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

SUGGESTED REVIEWERS:
Not Listed

REVIEWERS NOT TO INCLUDE:
Not Listed

The following information regarding collaborators and other affiliations (COA) must be separately provided for each individual identified as senior project personnel. The COA information must be provided through use of this COA template.

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.

If there are more than 10 individuals designated as senior project personnel on the proposal, or if there are print preview issues, each completed template must be saved as a .txt file [select the Text (Tab Delimited) option] rather than as an .xlsx or .xls file. This format will still enable preservation of searchable text and avoid delays in processing and review of the proposal.
Please note that some information requested in prior versions of the PAPPG is no longer requested. THIS IS PURPOSEFUL AND WE NO LONGER REQUIRE THIS INFORMATION TO BE REPORTED. Certain relationships will be reported in other sections (i.e., the names of postdoctoral scholar sponsors should not be reported, however if the individual collaborated on research with their postdoctoral scholar sponsor, then they would be reported as a collaborator). The information in the tables is not required to be sorted, alphabetically or otherwise.

There are five separate categories of information which correspond to the five tables in the COA template:

COA template Table 1:
List the individual's last name, first name, middle initial, and organizational affiliation (including considered affiliation) in the last 12 months.

COA template Table 2:
List names as last name, first name, middle initial, for whom a personal, family, or business relationship would otherwise preclude their service as a reviewer.

COA template Table 3:
List names as last name, first name, middle initial, and provide organizational affiliations, if known, for the following:
- **The individual's Ph.D. advisors; and**
- **All of the individual's Ph.D. thesis advisees.**

COA template Table 4:
List names as last name, first name, middle initial, and provide organizational affiliations, if known, for the following:
- **Co-authors on any book, article, report, abstract or paper with collaboration in the last 48 months (publication date may be later); and**
- **Collaborators on projects, such as funded grants, graduate research or others in the last 48 months.**

COA template Table 5:
List editorial board, editor-in chief and co-editors with whom the individual interacts. An editor-in-chief must list the entire editorial board.
- **Editorial Board: List name(s) of editor-in-chief and journal in the past 24 months; and**
- **Other co-Editors of journal or collections with whom the individual has directly interacted in the last 24 months.**

The template has been developed to be fillable, however, the content and format requirements must not be altered by the user. This template must be saved in .xlsx or .xls format, and directly uploaded into FastLane as a Collaborators and Other Affiliations Single Copy Document. Using the .xlsx or .xls format will enable preservation of searchable text that otherwise would be lost. It is therefore imperative that this document be uploaded in .xlsx or .xls only. Uploading a document in any format other than .xlsx or .xls may delay the timely processing and review of the proposal.

This information is used to manage reviewer selection. See Exhibit II-2 for additional information on potential reviewer conflicts.

1 Note that graduate advisors are no longer required to be reported.
2 Editorial Board does not include Editorial Advisory Board, International Advisory Board, Scientific Editorial Board, or any other subcategory of Editorial Board. It is limited to those individuals who perform editing duties or manage the editing process (i.e., editor in chief).

List names as Last Name, First Name, Middle Initial. Additionally, provide email, organization, and department
Fixed column widths keep this sheet one page wide; if you cut and paste text, set font size at 10pt or smaller, and
To insert *n* blank rows, select *n* row numbers to move down, right click, and choose Insert from the menu.
You may fill-down (crtl-D) to mark a sequence of collaborators, or copy affiliations. Excel has arrows that enable sorting.
For "Last Active Date" and "Last Active" columns dates are optional, but will help NSF staff easily determine which information remains relevant for reviewer selection.
"Last Active Date" and "Last Active" columns may be left blank for ongoing or current affiliations.

Table 1: List the individual's last name, first name, middle initial, and organizational affiliation (including considered affiliation) in the last 12 months.

1	Your Name:	Your Organizational Affiliation(s), last 12	Last Active Date
	Hickernell, Fred J.	Illinois Institute of Technology	present

Table 2: List names as last name, first name, middle initial, 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.

to disambiguate common names

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

Table 3: List names as last name, first name, middle initial, and provide organizational affiliations, if known, for the following.

G: The individual's Ph.D. advisors; and
T: All of the individual's Ph.D. thesis advisees.

to disambiguate common names

3	Advisor/Advisee Name:	Organizational Affiliation	Optional (email, Department)

G:	Howard, Louis N.	Massachussetts Institute of Technology	deceased
T:	Ding, Yuhan	Misercordia University	
T:	Hong, Regina	Germany	
T:	Huang, Fanglun	Anhui University	
T:	Jiang, Lan	Hyatt	
T:	Jiménez Rugama, Ll. A.	UBS	
T:	Li, Yiou	DePaul University	
T:	Liu, Kwong-IP	Hong Kong Baptist University	
T:	Niu, Ben	Ironbridge Capital Management	
T:	Rathnavel, Jagadeeswaran	Illinois Institute of Technology	
T:	Yue, Rongxian	Shanghai Normal University	
T:	Zhang, Yonglin		deceased
T:	Zeng, Xiaoyan	Shanghai University	
T:	Zhang, Kan	Illinois Institute of Technology	
T:	Zhang, Yizhi	Illinois Institute of Technology	
T:	Zhou, Xuan	J. P. Morgan	

Table 4: 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 the last 48 months (publication date may be later); and

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

to disambiguate common names

4	Name:	Organizational Affiliation	Optional (email, Department)	Last Active
A:	Berkaliev, Zaur	Illinois Institute of Technology	deceased	12/31/14
C:	Birge, John	University of Chicago		12/31/13
A:	Choi, Sou-Cheng Terrya	Illinois Institute of Technology		present
A:	Clancy, Nicholas	dunnhumby		12/31/14
C:	Constantine, Paul	University of Colorado, Boulder		present
A:	Devi, Shavila	Illinois Institute of Technology		12/31/14
A:	Ding, Yuhan	Misercordia University		present
A:	Élise Arnaud	Université Grenoble Alpes		12/31/17
C:	Fasshauer, Gregory E.	Colorado School of Mines		present
A:	Gilquin, Laurent	Inria Grenoble – Rhône-Alpes		12/31/17
A:	Hamilton, Caleb	NAG		12/31/14
A:	Hervé Monod	MaIAGE, INRA, Université Paris-Saclay		12/31/17
C:	Hyman, Mac	Tulane University		present
A:	Jiang, Lan	Hyatt		present
A:	Jiménez Rugama, Ll. A.	UBS		present
C:	Kang, Lulu	Illinois Institute of Technology		present
A:	Kartal, Ozgul	Illinois Institute of Technology		12/31/14
C:	Kritzer, Peter	Radon Institue for Comp. & App. Math.		present
C:	Kuo, Frances	University of New South Wales		present
C:	L'Ecuyer, Pierre	University of Montreal		present
A:	Li, Da	Illinois Institute of Technology		present
A:	Li, Xiaofan	Illinois Institute of Technology		12/31/14
C:	Li, Yiou	DePaul University		present
C:	Mak, Simon	Georgia Tech		present
A:	McCray, Patrick	Illinois Institute of Technology	retired	12/31/14

C:	Novak, Erich	Friedrich-Schiller-Universität Jena		present
C:	Owen, Art	Stanford University		present
A:	Prieur, Clémentine	Université Grenoble Alpes		12/31/17
C:	Rathnavel, Jagadeeswaran	Illinois Institute of Technology		present
C:	Roshan, V	Georgia Tech		present
C:	Tong, Xing	University of Illinois, Chicago		present
A:	Whitney, Stephanie	Illinois Institute of Technology		12/31/14
C:	Wozniakowski, Henryk	University of Warsaw		present
A:	Ye, Qi	South China Normal University		12/31/15
A:	Zawojewski, Judith S.	Illinois Institute of Technology	retired	12/31/14
A:	Zeng, Xiaoyan	Shanghai University		12/31/14
C:	Zhang, Kan	Illinois Institute of Technology		present
C:	Zhang, Yizhi	Illinois Institute of Technology		present
A:	Zhou, Xuan	J. P. Morgan		12/31/16

Table 5: List editorial board, editor-in chief and co-editors with whom the individual interacts. An editor-in-chief must list the entire editorial board.

B: Editorial Board: List name(s) of editor-in-chief and journal in the past 24 months; and

E: Other co-Editors of journal or collections with whom the individual has directly interacted in the last 24 months.

to disambiguate common names

5	Name:	Organizational Affiliation	Journal/Collection	Last Active
B:	Babuska, Ivo	Univesity of Texas, Austin	Intl. J. Numerical & Applied Math.	present
B:	Bochev, Pavel	Sandia National Laboratories	SIAM J. on Numerical Analysis	present
B:	Brenner, Susanne	Louisiana State University	Mathematics of Computation	1/31/17
B:	Cools, Ronald F. A.	K. U. Leuven	Mathematics of Computation	1/31/17
B:	Cui, Jun-zhi	Inst. Comp. Math., Chinese Acad. Sci.	Intl. J. Numerical & Applied Math.	present
B:	Dick, Josef	Univesity of New South Wales	Journal of Complexity	present
B:	Guo, Lei	Acad. of Math. \& System Sci., CAS	J. of Math. Research with Appl.	present
B:	Hinrichs, Aicke	Johann Kepler University Linz	Journal of Complexity	present
B:	Hsu, L. C.	Dalian University of Technology	J. of Math. Research with Appl.	present
B:	Kunoth, Angela	Universität zu Köln	SIAM J. on Numerical Analysis	present
B:	Lan, Yanping	University of Alberta	Intl. J. Numerical & Applied Math.	1/31/17
B:	Novak, Erich	Friedrich-Schiller-Universität Jena	Journal of Complexity	present
B:	Ritter, Klaus	Technische Universität Kaiserslautern	Journal of Complexity	present
B:	Shi, Zhongci	Inst. Comp. Math., Chinese Acad. Sci.	Intl. J. Numerical & Applied Math.	present
B:	Shparliniski, Igor E.	Macquarie University	Mathematics of Computation	1/31/17
B:	Shu, Chi-Wang	Brown University	Mathematics of Computation	1/31/17
B:	Sloan, Ian H.	University of New South Wales	Journal of Complexity	present
B:	Syzld, Daniel B.	Temple University	Mathematics of Computation	1/31/17
B:	Wang, Renhong	Dalian University of Technology	J. of Math. Research with Appl.	present
B:	Wasilkowski, Greg	Univesity of Kentucky	Journal of Complexity	present
B:	Wozniakowski, Henryk	University of Warsaw	Journal of Complexity	present

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Table 1: List the individual's last name, first name, middle initial, and organizational affiliation (including considered affiliation) in the last 12 months.

1	Your Name:	Your Organizational Affiliation(s), last 12	Last Active Date
	Choi, Sou Cheng	Illinois Institute of Technology (adjunct)	
	Choi, Sou Cheng	Allstate Insurance Company	

Table 2: List names as last name, first name, middle initial, 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.

to disambiguate common names

2	Name:	Organizational Affiliation	Optional (email, Department)	Last Active
R:	Lim, Lek Heng	Family	lekheng@galton.uchicago.edu, Statistics	

Table 3: List names as last name, first name, middle initial, and provide organizational affiliations, if known, for the following.

G: The individual's Ph.D. advisors; and
T: All of the individual's Ph.D. thesis advisees.

to disambiguate common names

3	Advisor/Advisee Name:	Organizational Affiliation	Optional (email, Department)
G:	Saunders, Michael	Stanford University	saunders@stanford.edu, Management Science and Engineering
G:	Golub, Gene (deceased)	Stanford University	Computer Science

Table 4: 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 the last 48 months (publication date may be later); and

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

to disambiguate common names

4	Name:	Organizational Affiliation	Optional (email, Department)	Last Active
A:	Saunders, Michael	Stanford University	saunders@stanford.edu, Management Science and Engineering	2/28/14
A:	Katz, Daniel S.	University of Illinois Urbana-Champaign	dskatz@illinois.edu, National Center for Supercomputing Applications (NCSA)	10/21/16
A:	Mulrow, Edward	NORC at the University of Chicago	Mulrow-Edward@norc.org, Statistics and Methodology	10/29/17
A:	Lin, Yongheng	Apple Inc.	yongheng.lin@gmail.com	10/29/17
A:	Ding, Yuhan	Misericordia University	Computer Science	
A:	Hickernell, Fred J.	Illinois Institute of Technology	hickernell@iit.edu, Applied Mathematics	
A:	Jiménez Rugama, Lluís Antoni	UBS AG	lluisantoni@gmail.com	
A:	Jiang, Lan	Hyatt Hotels Corporation	lanjiang61930@gmail.com	
A:	Li, Da			8/28/17
A:	Rathinavel, Jagadeeswaran	Illinois Institute of Technology	jrathin1@hawk.iit.edu, Applied Mathematics	
A:	Tong, Xin	University of Illinois at Chicago	xtong20@uic.edu, Mathematics, Statistics, and Computer Science	
A:	Zhang, Kan	Illinois Institute of Technology	kzhang23@hawk.iit.edu, , Applied Mathematics	
A:	Zhang, Yizhi	Illinois Institute of Technology	yzhang97@hawk.iit.edu, Applied Mathematics	8/28/17
A:	Zhou, Xuan	JPMorgan Chase and Co.	xuanjzhou@gmail.com	8/28/17
A:	Munson, Todd S.	Argonne National Laboratory	tmunson@mcs.anl.gov, Mathematics and Computer Science Division	3/31/14
A:	Niemeyer, Kyle	Oregon State University	Kyle.Niemeyer@oregonstate.edu, Mechanical Engineering	10/21/16
A:	Wilkins-Diehr, Nancy	San Diego Supercomputer Center	wilkinsn@sdsc.edu	2/22/16
A:	Venters, Colin C.	University of Huddersfield	C.Venters@hud.ac.uk, Software Systems Engineering	10/21/16

A:	Allen, Gabrielle	University of Illinois Urbana-Champaign	dallen@illinois.edu, Astronomy	10/21/16
A:	Löffler, Frank	Louisiana State University	knarf@cct.lsu.edu, Center for Computation & Technology	10/21/16
A:	Hetherington, James	University College London	j.hetherington@ucl.ac.uk, Research Software Development Group	10/21/16
A:	de Val-Borro, Miguel	Princeton University	Astrophysical Sciences	10/21/16
A:	Turk, Matthew J.	University of Illinois Urbana-Champaign	mjturk@illinois.edu, Astronomy	7/9/14
A:	Maheshwari, Ketan	Oak Ridge National Laboratory	ketan@mcs.anl.gov	7/9/14
A:	Elster, Anne C.	Norwegian University of Science and Technology	elster@idi.ntnu.no, Computer Science	7/9/14
A:	Howison, James	University of Texas at Austin	jhowison@ischool.utexas.edu, School of Information	2/22/16
A:	Hanwell, Marcus D.	Kitware Inc.	marcus.hanwell@kitware.com	7/9/14
A:	Lapp, Hilmar	Duke University	hlapp@duke.edu, Center for Genomic and Computational Biology	7/9/14
A:	Smith, Arfon M	Space Telescope Science Institute	Data Science Mission Office	9/19/16
A:	Cranston, Karen A.	Duke University	karen.cranston@gmail.com, Biology	2/22/16
A:	Gunter, Dan	Lawrence Berkeley National Laboratory	dkgunter@lbl.gov, Computational Research Division	10/21/16
A:	Idaszak, Ray	University of North Carolina at Chapel Hill	rayi@renci.org, Renaissance Computing Institute	10/21/16
A:	Brandt, Steven R.	Louisiana State University	sbrandt@cct.lsu.edu, Computer Science and Engineering	10/21/16
A:	Miller, Mark A.	San Diego Supercomputer Center	mmiller@sdsc.edu	10/21/16
A:	Gesing, Sandra	University of Notre Dame	sandra.gesing@nd.edu, Computer Science and Engineering	10/21/16
A:	Jones, Nick	The University of Auckland	n.jones@auckland.ac.nz, New Zealand eScience Infrastructure	10/21/16
A:	Weber, Nic	University of Washington	nmweber@uw.edu, Information School	10/21/16
A:	Marru, Suresh	Indiana University	smarru@iu.edu, Research Technologies	10/21/16
A:	Penzenstadler, Birgit	California State University Long Beach	birgit.penzenstadler@csulb.edu, Computer Science	10/21/16
A:	Davis, Ethan	University Corporation for Atmospheric Research	edavis@ucar.edu	10/21/16
A:	Hwang, Lorraine	University of California, Davis	lorraine@geodynamics.org, Earth and Planetary Sciences	10/21/16
A:	Todorov, Ilian T.	Science and Technology Facilities Council	ilian.todorov@stfc.ac.uk, Computational Chemistry Groups	10/21/16
A:	Patra, Abani	University at Buffalo	abani@buffalo.edu, Mechanical and Aerospace Engineering	10/21/16
A:	Hong, Neil Chue	University of Edinburgh	N.ChueHong@software.ac.uk, Software Sustainability Institute	2/22/16
A:	Seinstra, Frank	Netherlands eScience Centre	F.Seinstra@esciencecenter.nl, Computer Science	2/22/16
A:	Jones, Matthew	University of California Santa Barbara	jones@nceas.ucsb.edu, National Center for Ecological Analysis and Synthesis	2/22/16

A:	Clune, Thomas L	National Aeronautics and Space Administration	thomas.l.clune@nasa.gov, Goddard Space Flight Center	2/22/16
A:	Littauer, Richard	University of Saarland	richard.littauer@gmail.com, Computational Linguistics	2/22/16
A:	Swenson, Shel	Emory University	Mathematics and Computer Science	7/9/14
A:	Berriman, Bruce	California Institute of Technology	gbb@ipac.caltech.edu, Infrared Processing and Analysis Center	7/9/14
C:	Lim, Lek Heng	University of Chicago	lekheng@galton.uchicago.edu, Statistics	
C:	Huang, Jack	University of Chicago	jhuang11@uchicago.edu, Mathematics	
C:	Pao, Chrystal Ho	Trinity International University	chrystalhopao@gmail.com, Biology	
A:	Kochenderfer, Mykel J.	Stanford University	mykel@stanford.edu, Aeronautics and Astronautics	
A:	Wulfe, Blake	Stanford University	wulfebw@stanford.edu, Computer Science	
A:	Chintakindi, Sunil	Allstate Corporation	sunil.chintakindi@allstate.com, Automotive Innovation	
A:	Hartong-Redden, Rory	Allstate Corporation	rory.hartong-redden@allstate.com, Automotive Innovation	
A:	Kodali, Anuradha	Allstate Corporation	akoda@allstate.com, Automotive Innovation	
A:	Accomazzi, Alberto	Harvard University	Harvard–Smithsonian Center for Astrophysics	9/19/16
A:	Allen, Alice	Astrophysics Source Code Library		9/19/16
A:	Altman, Micah	Massachusetts Institute of Technology		9/19/16
A:	Billings, Jay Jay	Oak Ridge National Laboratory		9/19/16
A:	Boettiger, Carl	University of California, Berkeley		9/19/16
A:	Brown, Jed	University of Colorado Boulder		9/19/16
A:	Crick, Tom	Cardiff Metropolitan University		9/19/16
A:	Crosas, Mercè	Harvard University	Institute for Quantitative Social Science	9/19/16
A:	Edmunds, Scott	BGI Hong Kong	GigaScience	9/19/16
A:	Erdmann, Christopher	Harvard University	Harvard–Smithsonian Center for Astrophysics	9/19/16
A:	Fenner, Martin	DataCite		9/19/16
A:	Finkbeiner, Darel	The Office of Scientific and Technical Information		9/19/16
A:	Gent, Ian	University of St Andrews	School of Computer Science	9/19/16
A:	Goble, Carole	The University of Manchester	Software Sustainability Institute	9/19/16
A:	Groth, Paul	Elsevier Inc.	Elsevier Labs	9/19/16
A:	Haendel, Melissa	Oregon Health and Science University		9/19/16
A:	Hagstrom, Stephanie	University of California San Diego		9/19/16
A:	Hanisch, Robert	National Institute of Standards and Technology		9/19/16
A:	Henneken, Edwin	Harvard University	Harvard–Smithsonian Center for Astrophysics	9/19/16
A:	Herman, Ivan	World Wide Web Consortium (W3C)		9/19/16
A:	Ingraham, Thomas	F1000Research		9/19/16
A:	Jones, Catherine	Science and Technology Facilities Council		9/19/16

A:	Konovalov, Alexander	University of St Andrews		9/19/16
A:	Kratz, John	California Digital Library		9/19/16
A:	Lin, Jennifer	Public Library of Science		9/19/16
A:	Matthews, Brian	Science and Technology Facilities Council		9/19/16
A:	Mayes, Abigail Cabunoc	Mozilla Science Lab		9/19/16
A:	Mietchen, Daniel	National Institutes of Health		9/19/16
A:	Mills, Bill	TRIUMF		9/19/16
A:	Misshula, Evan	The City University of New York	Graduate Center	9/19/16
A:	Muench, August	American Astronomical Society		9/19/16
A:	Murphy, Fiona	Independent Researcher		9/19/16
A:	Nielsen, Lars Holm	CERN		9/19/16
A:	Ram, Karthik	University of California, Berkeley		9/19/16
A:	Rios, Fernando	Johns Hopkins University		9/19/16
A:	Sands, Ashley	University of California, Los Angeles		9/19/16
A:	Scott, Soren	Independent Researcher		9/19/16
A:	Thaney, Kaitlin	Mozilla Science Lab		9/19/16
A:	Van Hauwermeiren, Daan	Ghent University, Belgium		9/19/16
A:	Van Hoey, Stijn	Ghent University, Belgium		9/19/16
A:	Weaver, Belinda	The University of Queensland		9/19/16
C:	Fasshauer, Greg	Colorado School of Mines	Department of Applied Mathematics & Statistics	7/31/18

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to disambiguate common names

5	Name:	Organizational Affiliation	Journal/Collection	Last Active
B:	Chui, Charles K.	Stanford University; Hong Kong Baptist University	Mathematics of Computation and Data Science	4/24/17

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	Minh, David D. L.	Illinois Institute of Technology	

Table 2: List names as last name, first name, middle initial, 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.

to disambiguate common names

2	Name:	Organizational Affiliation	Optional (email, Department)	Last Active
R:	Minh, Do L.	Family	dminh@fullerton.edu	

Table 3: List names as last name, first name, middle initial, and provide organizational affiliations, if known, for the following.

G: The individual's Ph.D. advisors; and
T: All of the individual's Ph.D. thesis advisees.

to disambiguate common names

3	Advisor/Advisee Name:	Organizational Affiliation	Optional (email, Department)

G:	McCammon, J. Andrew	University of California, San Diego	Chemistry
T:	Xie, Bing (present student)	Illinois Institute of Technology	Chemistry

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to disambiguate common names

4	Name:	Organizational Affiliation	Optional (email, Department)	Last Active
A:	Akcakaya, Murat	University of Pittsburgh		
A:	Badger, John	DeltaG Technologies, San Diego, California		
A:	Bardhan, Jaydeep	Northeastern University, Boston, Massachusetts		
A:	Brooks, Dana H.	Northeastern University, Boston, Massachusetts		
A:	Chishti. Yasmin	Northeastern University, Boston, Massachusetts		
C:	Chong, Hyun-Soon	Illinois Institute of Technology		
A:	Erdogmus, Deniz	Northeastern University, Boston, Massachusetts		
A:	Fang, Xuan	Illinois Institute of Technology		
A:	Juarez, Oscar	Illinois Institute of Technology		
A:	Li, Chen	Illinois Institute of Technology		
A:	Liang, Pingdong	Illinois Institute of Technology		
A:	Makowski, Lee	Northeastern University, Boston, Massachusetts		
A:	Minh, Do	California State University, Fullerton		
A:	Nguyen, Andrew	California State University, Fullerton		
A:	Nguyen, Trung Hai	Illinois Institute of Technology		
A:	Onuk, Emre	University of California, Los Angeles		
A:	Raba, Daniel A.	Illinois Institute of Technology		
A:	Spiridon, Laurentiu	Institute of Biochemistry of the Romanian Academy		
A:	Tuz, Karina	Illinois Institute of Technology		
A:	Wang, Yu Jing	Illinois Institute of Technology		
A:	Xie, Bing	Illinois Institute of Technology		
A:	Zhou, Huan-Xiang	University of Illinois, Chicago		

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5	Name:	Organizational Affiliation	Journal/Collection	Last Active
B:				
E:				

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1	Your Name:	Your Organizational Affiliation(s), last 12 r	Last Active Date
	Sun, Xian-He	Illinois Institute of Technology	

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2	Name:	Organizational Affiliation	Optional (email, Department)	Last Active
R:	Zhang, Hong	Family		

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G: The individual's Ph.D. advisors; and

T: All of the individual's Ph.D. thesis advisees.

to disambiguate common names

3	Advisor/Advisee Name:	Organizational Affiliation	Optional (email, Department)
T:	Byna, Suren	Lawrence Berkeley National Lab	

T:	Cameron, Kirk W.	Virginia Tech	
T:	Chen, Yong	Texas Tech University	
T:	Du, Cong	EMC	
T:	Gurbani, Vijay K.	Alcatel-Lucent	
G:	Gustafson, John	Ceranovo Inc	
T:	Hui, Jin	Oracle	
G:	Ni, Lionel	University of Macau	
T:	Yang, Xi	Teradata	
T:	Yin, Yanlong	Bloomberg L.P.	

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to disambiguate common names

4	Name:	Organizational Affiliation	Optional (email, Department)	Last Active
A:	Chen, Chao	Texas Tech University		Aug. 2016
A:	Cheng, Yuanqi	Beihang University, China		Oct. 2016
A:	Dorier, Matthieu	Argonne National Lab		Oct. 2016
A:	Eslami, Hassan	University of Illinois at Urbana–Champaign		Dec. 2016
A:	Feng, Bo	Illinois Institute of Technology		Oct. 2015
A:	Feng, Chen	Institute of Computing Technology, China		Dec. 2015
A:	Fleck, Anthony	Illinois Institute of Technology		Nov. 2016
A:	Georgakopoulos, Dimitrios	Australian National University		June. 2015
C:	Gropp, William	University of Illinois at Urbana–Champaign		Aug. 2016
A:	Haider, Adnan	Illinois Institute of Technology		July. 2017
A:	He, Shuibing	WuHan University, China		Jan. 2018
A:	Huang, Chuanhe	Wuhan University		June. 2017
A:	Jenkins, Johnathan	Argonne National Lab		Nov. 2016
C:	Jin, Dong	Illinois Institute of Technology		July. 2017
A:	Jung, Eun-Sung	Jongik University, South Korea		Dec. 2016
A:	Kettimuthu, Raj	Argonne National Lab		Dec. 2016
A:	Kimpe, Dries	KCG Holdings, Inc.		June.2016
C:	Lan, Zhiling	Illinois Institute of Technology		Nov. 2016
A:	Lang, Michael	Los Alamos National Lab		Sept. 2015
A:	Latham, Rob	Argonne National Lab		Oct. 2016
A:	Li, Dandan	Beihang University, China		Oct. 2016
C:	Li, Dong	University of California Merced		Oct. 2016
A:	Li, Zheng	Western Illinois University		June. 2017
A:	Liang, Fan	Institute of Computing Technology, China		Sept. 2015
A:	Liu, Ning	IBM		July. 2017
A:	Liu, Yan	HuNan Univeristy, China		Nov. 2016
A:	Liu, Yuhang	Institute of Computing Technology, China		Oct. 2016
A:	Lu, Yin	Texas Tech University		Nov. 2015
A:	Papka, Michael	Argonne National Lab		Dec. 2016
C:	Raicu, Ioan	Illinois Institute of Technology		June. 2016
A:	Ranjan, Rajiv	Australian National University		June. 2015
C:	Ross, Robert	Los Alamos National Lab		June. 2016
A:	Sadooghi, Iman	Illinois Institute of Technology		Sept. 2015

C:	Thakur, Rajeev	Argonne National Lab		Nov. 2016
A:	Venkata, Manjunath Goren	Oak Ridge National Lab		Sept. 2015
A:	Wang, Bin	IBM		June. 2015
A:	Wang, Dawei	Juniper		May. 2014
A:	Wang, Guojun	Central South University, China		June. 2015
A:	Wang, Ke	Intel		Sept. 2015
A:	Wang, Lizhe	Chinese Academy of Science, China		June. 2015
A:	Wang, Senzhang	NUAA, China		Oct. 2016
A:	Wang, Xinning	Auburn University		June. 2015
A:	Wang, Yang	SIAT, Chinese Academy of Science, China		June. 2017
A:	Wang, Yang	Shanghai University		Jan. 2018
A:	Xu, Bao-yu	Shanghai University		Sep. 2016
A:	Xu, Chenzhong	Wayne State University		Jan. 2018
A:	Xu, Zhiwei	Institute of Computing Technology, China		Dec. 2015
A:	Yao, Shuzhen	Beihang University, China		Oct. 2016
A:	Yu, Weikuan	Florida State University		June. 2015
A:	Zhang, Wu	Shanghai University		Sep. 2016
A:	Zhao, Dongfang	University of Nevada, Reno		Oct. 2016
C:	Zhou, Shujia	Northrop Grumman Information Technology		Oct. 2016
A:	Zhou, Xiaobing	Illinois Institute of Technology		Sept. 2015
A:	Zhou, Xuehai	Texas Tech University		Sept. 2015
A:	Zomaya, Albert	University of Sydney		June. 2015

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	Manish Parashar	Rutgers University	IEEE TPDS	Feb. 2018

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	Wereszczynski, Jeffery M.	Illinois Institute of Technology	

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R:				

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to disambiguate common names

3	Advisor/Advisee Name:	Organizational Affiliation	Optional (email, Department)

G:	Andricioaei, Ioan	University of California, Irvine	Chemistry
T:	Carlson, Heather	Univeristy of Michigan, Ann Arbor	College of Pharmacy
T:	Perkins, Noel	University of Michigan, Ann Arbor	Mechanical Engineering
T:	Al-Hashimi, Hashim	Duke University	Chemistry

Table 4: List names as last name, first name, middle initial, and provide organizational affiliations, if known, for the following:

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4	Name:	Organizational Affiliation	Optional (email, Department)	Last Active
A:	Musselman, Catherine	University of Iowa		2/8/18
A:	Clubb, Robert T.	University of California, Los Angeles		2/8/18
A:	Strieter, Eric	Univeristy of Massachusetts, Amherst		6/1/17
A:	Jung, Michae E.	University of California, Los Angeles		9/1/17
A:	Miller, Llyoyd S.	Johns Hopkins University		9/1/17
A:	McCammon, J. A.	University of California, San Diego		9/1/17

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	Lederman, Norman G.	Illinois Institute of Technology	Present

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R:	None			

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to disambiguate common names

3	Advisor/Advisee Name:	Organizational Affiliation	Optional (email, Department)
G:	Druger, Marvin	Syracuse University	Department of Science Teaching

T:	Bell, Randy	Oregon State University	
T:	Gess-Newsome, Julie	Oregon State University	
T:	Abd-El-Khalick, Fouad	University of North Carolina	
T:	Akerson, Valarie	Indiana Uiversity	
T:	Morrison, Judy	Washington State University	
T:	Bartos, Stephen	Middle Tennessee State University	

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to disambiguate common names

4	Name:	Organizational Affiliation	Optional (email, Department)	Last Active
A:	Lederman, Judith	Illinois Institute of Technology		
A:	Bell, Randy	Oregon State University		
A:	Flick, Larry	Oregon State University		
A:	Kamporankis, Kostas	University of Geneva		
A:	McComas, William	University of Arkansas		

Table 5: List editorial board, editor-in chief and co-editors with whom the individual interacts. An editor-in-chief must list the entire editorial board.

B: Editorial Board: List name(s) of editor-in-chief and journal in the past 24 months; and

E: Other co-Editors of journal or collections with whom the individual has directly interacted in the last 24 months.

to disambiguate common names

5	Name:	Organizational Affiliation	Journal/Collection	Last Active
B:	van Driel, Jan	University of Melboune	International Journal of Science Ed.	Present
B:	Zeidler, Dana	University of South Florida	Journal of Research in Science Teaching	Present
B:	Settlage, John	University of Connecticut	Science Education	
B:	Wallace, John	University of Toronto	Canadian Journal of Science, Math, and Technology Ed.	
E:	Lederman, Judith	Illinois Institute of Technology	Journal of Science Teacher Education	

The following information regarding collaborators and other affiliations (COA) must be separately provided for each individual identified as senior project personnel. The COA information must be provided through use of this COA template.

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.

If there are more than 10 individuals designated as senior project personnel on the proposal, or if there are print preview issues, each completed template must be saved as a .txt file [select the Text (Tab Delimited) option] rather than as an .xlsx or .xls file. This format will still enable preservation of searchable text and avoid delays in processing and review of the proposal.
Please note that some information requested in prior versions of the PAPPG is no longer requested. THIS IS PURPOSEFUL AND WE NO LONGER REQUIRE THIS INFORMATION TO BE REPORTED. Certain relationships will be reported in other sections (i.e., the names of postdoctoral scholar sponsors should not be reported, however if the individual collaborated on research with their postdoctoral scholar sponsor, then they would be reported as a collaborator). The information in the tables is not required to be sorted, alphabetically or otherwise.

There are five separate categories of information which correspond to the five tables in the COA template:

COA template Table 1:
List the individual's last name, first name, middle initial, and organizational affiliation (including considered affiliation) in the last 12 months.

COA template Table 2:
List names as last name, first name, middle initial, for whom a personal, family, or business relationship would otherwise preclude their service as a reviewer.

COA template Table 3:
List names as last name, first name, middle initial, and provide organizational affiliations, if known, for the following:
- **The individual's Ph.D. advisors; and**
- **All of the individual's Ph.D. thesis advisees.**

COA template Table 4:
List names as last name, first name, middle initial, and provide organizational affiliations, if known, for the following:
- **Co-authors on any book, article, report, abstract or paper with collaboration in the last 48 months (publication date may be later); and**
- **Collaborators on projects, such as funded grants, graduate research or others in the last 48 months.**

COA template Table 5:
List editorial board, editor-in chief and co-editors with whom the individual interacts. An editor-in-chief must list the entire editorial board.
- **Editorial Board: List name(s) of editor-in-chief and journal in the past 24 months; and**
- **Other co-Editors of journal or collections with whom the individual has directly interacted in the last 24 months.**

The template has been developed to be fillable, however, the content and format requirements must not be altered by the user. This template must be saved in .xlsx or .xls format, and directly uploaded into FastLane as a Collaborators and Other Affiliations Single Copy Document. Using the .xlsx or .xls format will enable preservation of searchable text that otherwise would be lost. It is therefore imperative that this document be uploaded in .xlsx or .xls only. Uploading a document in any format other than .xlsx or .xls may delay the timely processing and review of the proposal.

This information is used to manage reviewer selection. See Exhibit II-2 for additional information on potential reviewer conflicts.

1 Note that graduate advisors are no longer required to be reported.
2 Editorial Board does not include Editorial Advisory Board, International Advisory Board, Scientific Editorial Board, or any other subcategory of Editorial Board. It is limited to those individuals who perform editing duties or manage the editing process (i.e., editor in chief).

List names as Last Name, First Name, Middle Initial. Additionally, provide email, organization, and department (optional)
Fixed column widths keep this sheet one page wide; if you cut and paste text, set font size at 10pt or smaller, and
To insert *n* blank rows, select *n* row numbers to move down, right click, and choose Insert from the menu.
You may fill-down (crtl-D) to mark a sequence of collaborators, or copy affiliations. Excel has arrows that enable sorting.
For "Last Active Date" and "Last Active" columns dates are optional, but will help NSF staff easily determine which information remains relevant for reviewer selection.
"Last Active Date" and "Last Active" columns may be left blank for ongoing or current affiliations.

Table 1: List the individual's last name, first name, middle initial, and organizational affiliation (including considered affiliation) in the last 12 months.

1	Your Name:	Your Organizational Affiliation(s), last 12 r	Last Active Date
	Ong, Kiah Wah	Illinois Institute of Technology	
		Indiana University, Bloomington	7/1/2017
		St Norbert College (interviewed)	2/5/2017
		Yale University (interviewed)	2/16/2017
		Siena College (interviewed)	2/27/2017

Table 2: List names as last name, first name, middle initial, 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.

to disambiguate common names

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

Table 3: List names as last name, first name, middle initial, and provide organizational affiliations, if known, for the following.

G: The individual's Ph.D. advisors; and
T: All of the individual's Ph.D. thesis advisees.

to disambiguate common names

3	Advisor/Advisee Name:	Organizational Affiliation	Optional (email, Department)
G:	Wang, Shouhong	Indiana University, Bloomington	showang@indiana.edu
T:			

Table 4: 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 the last 48 months (publication date may be later); and

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

to disambiguate common names

4	Name:	Organizational Affiliation	Optional (email, Department)	Last Active
A:	Hernandez, Marco	Indiana University	hernmarc@indiana.edu	
A:	Li, Limei	Sichuan Normal University, China	mathllm@163.com	1/1/17
A:	Cai, Ming	Florida State University	cai@met.fsu.edu	4/1/17
A:	Wang, Shouhong	Indiana University	showang@indiana.edu	

Table 5: List editorial board, editor-in chief and co-editors with whom the individual interacts. An editor-in-chief must list the entire editorial board.

B: Editorial Board: List name(s) of editor-in-chief and journal in the past 24 months; and

E: Other co-Editors of journal or collections with whom the individual has directly interacted in the last 24 months.

to disambiguate common names

5	Name:	Organizational Affiliation	Journal/Collection	Last Active
B:	Wang, Shouhong	Indiana University	Physica D	
E:	Wang, Shouhong	Indiana University	DCDS-B	

COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

PROGRAM ANNOUNCEMENT/SOLICITATION NO./DUE DATE
NSF 18-516 **02/14/18**

☐ Special Exception to Deadline Date Policy

FOR NSF USE ONLY

NSF PROPOSAL NUMBER

1829794

FOR CONSIDERATION BY NSF ORGANIZATION UNIT(S) (Indicate the most specific unit known, i.e. program, division, etc.)
OAC - CyberTraining - Training-based

DATE RECEIVED	NUMBER OF COPIES	DIVISION ASSIGNED	FUND CODE	DUNS# (Data Universal Numbering System)	FILE LOCATION
02/14/2018	**1**	**05090000 OAC**	**044Y**	**042084434**	**02/15/2018 2:11pm**

EMPLOYER IDENTIFICATION NUMBER (EIN) OR TAXPAYER IDENTIFICATION NUMBER (TIN)
362170136

SHOW PREVIOUS AWARD NO. IF THIS IS
☐ A RENEWAL
☐ AN ACCOMPLISHMENT-BASED RENEWAL

IS THIS PROPOSAL BEING SUBMITTED TO ANOTHER FEDERAL AGENCY? YES ☐ NO ☒ IF YES, LIST ACRONYM(S)

NAME OF ORGANIZATION TO WHICH AWARD SHOULD BE MADE
Illinois Institute of Technology

AWARDEE ORGANIZATION CODE (IF KNOWN)
0016915000

ADDRESS OF AWARDEE ORGANIZATION, INCLUDING 9 DIGIT ZIP CODE
Illinois Institute of Technology
10 West 35th Street
Chicago, IL. 606163717

NAME OF PRIMARY PLACE OF PERF
Illinois Institute of Technology

ADDRESS OF PRIMARY PLACE OF PERF, INCLUDING 9 DIGIT ZIP CODE
Illinois Institute of Technology
10 W. 35th St.
Chicago ,IL ,606163717 ,US.

IS AWARDEE ORGANIZATION (Check All That Apply) ☐ SMALL BUSINESS ☐ MINORITY BUSINESS ☐ FOR-PROFIT ORGANIZATION ☐ WOMAN-OWNED BUSINESS

☐ IF THIS IS A PRELIMINARY PROPOSAL THEN CHECK HERE

TITLE OF PROPOSED PROJECT **CyberTraining: CIC: Cross-Disciplinary Education for Next-Generation Computational Scientists**

REQUESTED AMOUNT	PROPOSED DURATION (1-60 MONTHS)	REQUESTED STARTING DATE	SHOW RELATED PRELIMINARY PROPOSAL NO. IF APPLICABLE
$ **499,783**	**36** months	**08/01/18**	

THIS PROPOSAL INCLUDES ANY OF THE ITEMS LISTED BELOW
☐ BEGINNING INVESTIGATOR
☐ DISCLOSURE OF LOBBYING ACTIVITIES
☐ PROPRIETARY & PRIVILEGED INFORMATION
☒ HISTORIC PLACES
☐ VERTEBRATE ANIMALS IACUC App. Date _____
PHS Animal Welfare Assurance Number _____
☒ TYPE OF PROPOSAL **Research**

☐ HUMAN SUBJECTS Human Subjects Assurance Number _____
Exemption Subsection _____ or IRB App. Date _____
☐ INTERNATIONAL ACTIVITIES: COUNTRY/COUNTRIES INVOLVED
_____
☒ COLLABORATIVE STATUS
Not a collaborative proposal

PI/PD DEPARTMENT
Applied Mathematics

PI/PD POSTAL ADDRESS
10 West 32nd Street

Chicago, IL 60616
United States

PI/PD FAX NUMBER
312-567-3135

NAMES (TYPED)	High Degree	Yr of Degree	Telephone Number	Email Address
PI/PD NAME **Fred J Hickernell**	**PhD**	**1981**	**312-567-8983**	**hickernell@iit.edu**
CO-PI/PD **Sou-Cheng Choi**	**PhD**	**2007**	**872-588-2118**	**schoi32@iit.edu**
CO-PI/PD **David D Minh**	**DPhil**	**2007**	**312-567-3411**	**dminh@iit.edu**
CO-PI/PD **Xian-He Sun**	**PhD**	**1990**	**312-567-5260**	**sun@iit.edu**
CO-PI/PD **Jeffery M Wereszczynski**	**PhD**	**2008**	**312-567-3322**	**jwereszc@iit.edu**

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 grant, 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 **Domenica G Pappas**	**Electronic Signature**	**Feb 14 2018 5:39PM**

TELEPHONE NUMBER	EMAIL ADDRESS	FAX NUMBER
312-567-3035	**pappas@iit.edu**	**312-567-6980**

PROJECT SUMMARY

Overview:

Computational scientists must learn how to take advantage of the rapidly evolving cyberinfrastructure (CI) eco-system to maximize scientific discovery. The education of computational scientists should begin in their pre-university studies, extend through their undergraduate and graduate studies, and continue throughout their careers. Key ideas to be learned include computing in diverse, advanced hardware environments; computing multi-lingually; utilizing and contributing to substantial software libraries; being an integral part of an interdisciplinary team; ensuring that computational results have scientific significance; and ensuring that computational results are trustworthy and reproducible.

This effort is led by the newly established Center for Interdisciplinary Scientific Computation (CISC) at Illinois Institute of Technology (Illinois Tech). CISC is partnering with Argonne National Laboratory, Fermilab, and the College of DuPage, leveraging our combined resources to educate future computational scientists with the required breadth of knowledge and skill to utilize advanced CI in responsible, efficient, and novel ways. This project is aimed primarily at educating CI contributors (CICs), but will also educate CI users (CIUs). To provide a thorough education of CICs and CIUs, our initiatives are aimed at four constituencies: high school students, community college students, Illinois Tech undergraduates, and Illinois Tech graduate students.

The PI consulted with Sushil Prasad in the course of developing this proposal. Keywords: computational science, cross-disciplinary, high school through doctoral, summer experiences.

Intellectual Merit:

A successful CIC must develop an interest in computing, master advanced computational skills, and acquire a cross-disciplinary perspective---all of which takes time. Thus, our initiatives are aimed at high school through doctoral students. We will implement a summer computational science course---requiring minimal computational background, but touching on parallel computing---aimed at high school students and college students. We will strengthen the content of our existing undergraduate and graduate computational science courses by adding the most up-to-date technologies and industry-proposed projects. We will add and expand courses targeted at large-scale computation, software design principles, and hands-on experience. Local community college students will be immersed in summer research experiences, working alongside our faculty and Illinois Tech students. CISC undergraduate and graduate fellows will join large-scale computation projects in nearby national labs or be embedded in Illinois Tech computational science research groups outside their own disciplines.

Broader Impacts:

Computational scientists trained by our new program will cross-pollinate their disciplines with the computational approaches that they learn from other fields of study. These computational scientists will be prepared and ready to contribute to large, interdisciplinary research efforts. The partnerships that we establish with national labs and industry will be mutually beneficial. Students will gain real-world experience working with our partners, while our partners will gain students better prepared to use advanced CI in research. The reach of this program will extend beyond Illinois Tech students to high school and community college students in greater Chicago, many of whom are underrepresented minorities. We will inspire and prepare them for careers as computational scientists. Our renovated computational science education will endure beyond the end of this project. The lessons that we learn and the resources that we develop will be shared with others via print and online publications as well as colloquium and conference talks.

TABLE OF CONTENTS

For font size and page formatting specifications, see PAPPG section II.B.2.

*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

Contents

1. Introduction

Computational scientists typically draw upon knowledge from several disciplines, including computer science, mathematical science, and natural science. Realizing the full potential of computational science for discovery requires interdisciplinary teams whose members can take full advantage of advanced hardware architectures and software environments, in addition to mathematical modeling and algorithm development. To conduct effective research, computational scientists should exhibit

- Depth within their chosen disciplines plus breadth across relevant disciplines, overcoming a silo mentality, and
- Experience with advanced cyberinfrastructure (CI), including some professional practices required for effective large-scale computation.

The newly established Center for Interdisciplinary Scientific Computation (CISC) http://cos.iit.edu/cisc at Illinois Institute of Technology (IIT or Illinois Tech) is proposing several new initiatives to educate computational scientists with qualities highlighted above. We will educate high school through doctoral students. Learning will be curricular and extra-curricular. We will partner with nearby national laboratories, companies engaged in advanced computing, and schools whose students have less access to research experience and high-end computing facilities.

The Challenges. Computing solutions to complex scientific problems require properly educated computational scientists. There are two kinds of challenges that must be addressed in providing this proper education.

Academic Silos. Computational science draws on multiple disciplines, including computer science, mathematical science, and natural science. Students must gain a deep understanding of their chosen discipline. Computational scientists should avoid becoming a jack of all trades and a master of none.

- Computer scientists must understand how emerging languages and architectures enable faster and more scalable computations, and they must be prepared to make the next advances.
- Computational mathematicians and statisticians must be able to describe and analyze truncation and round-off errors in numerical algorithms, as well as measurement and misspecification errors of statistical models. They must know how to construct the most efficient algorithms for different kinds of problems.
- Computational biologists, chemists, and physicists must grasp the important scientific ideas that need to be captured by computations. They must understand the benefits and limitations of using computer modeling in their respective disciplines and grasp the next opportunities for scientific advancement.

But this is not enough! Computational scientists should be a master of one trade and conversant with others. They must develop cross-disciplinary perspectives that will make them effective members of interdisciplinary teams tackling large, complex computational science problems.

Ignorance of Good Practice for Large-Scale Computation. Solving problems using advanced CI deviates in important ways from what students typically learn in their coursework. See [42, Sect. 2.4] for a more detailed discussion. Here are some highlights:

- Effective algorithms that take advantage of multi-core, distributed memory architectures may be substantially different than algorithms designed for a single CPU with only one core.
- The software required to solve large problems is often drawn from multiple sources, written in several languages, and developed over the course of years, by teams of experts, e.g., PETSc [2].
- Those who perform computational experiments and those who demonstrate the performance of their new algorithms must ensure that their results are reliable and can be reproduced by others [39].
- Software contributors must ensure that their software is robust, interacts well with other software, and can be extended by those who come afterwards. See [5] for a recent effort to promote these principles broadly.

We propose to overcome these challenges in educating the next generation of computational scientists.

Why CISC is Poised to Lead This. CISC was created in May 2017 to leverage Illinois Tech's existing strengths in computational science for greater impact. CISC has office space, a modest budget, and a 256-core cluster (see the section on Facilities, Equipment and Other Resources). We also have the good will of supporters among faculty and administrators. CISC has initiated a series of "matchmaking" seminars that introduce computational scientists to each others' research. The aim is to promote new interdisciplinary computational research groups that attract external funding. In support of this aim, CISC also sponsored a seed grant competition in Fall 2017. Fred J. Hickernell, PI and CISC's director, is one of several computational mathematicians at Illinois Tech and previously served for twelve years as chair of the applied mathematics department. Our computer science department has a historically strong group in high performance computing led by co-PI Xian-He Sun. In recent years, the biology, chemistry, and physics departments have hired computational scientists, including co-PIs David Minh (chemistry, CISC's associate director) and Jeff Wereszczynski (physics). Co-PI Sou-Cheng Choi is a lead researcher in machine learning at Allstate Insurance Company's Automotive and Life/Retirement innovation teams and also a research associate professor in applied mathematics at Illinois Tech.

In addition to the (co-)PIs, we have enlisted two senior personnel: Norman Lederman, who has a long and distinguished record in science education, and Kiah Wah Ong, an early-career colleague with strong teaching experience.

The (co-)PIs have experience developing curricula, mentoring high school students through PhD students, and partnering with College of DuPage, Argonne National Laboratory, and Fermilab. But our past record has been working primarily independently. The creation of CISC and the resources provided by Illinois Tech have provided us a platform with the potential to create a pipeline of computational scientists which starts at the high school level and extends to the doctoral level. The resources requested in this proposal will make that potential a reality by enabling the creation of a novel, strong, multi-faceted training program for cross-disciplinary computational scientists.

2. Results from Prior NSF Support

2.1. **Experience of Hickernell and Choi.** NSF-DMS-1522687, *Stable, Efficient, Adaptive Algorithms for Approximation and Integration*, $270,000, August 2015 – July 2018. Hickernell is PI and Choi is senior personnel.

2.1.1. *Intellectual Merit.* One of the primary outcomes of this project in relation to the present proposal is the development of the Guaranteed Automatic Integration Library (GAIL) [7]. This library comprises univariate and multivariate integration, as well as univariate function approximation and

optimization algorithms that automatically determine the sample size required to meet user-defined error tolerances. The library does not rely on interval arithmetic, as is done in INTLAB [35, 43, 44]; but like INTLAB, GAIL comes with theoretical guarantees that common adaptive algorithms lack. The recent GAIL developments include locally adaptive function approximation and optimization [6, 9], adaptive quasi-Monte Carlo cubature [18, 23], and the ability to set a hybrid error tolerance involving both absolute and relative error criteria [20]. Other articles, theses, software, and preprints supported in part by this grant include [1, 11, 22, 19, 17, 24, 28, 29, 31, 33, 34, 41, 48, 51, 52, 53].

2.1.2. *Broader Impacts.* Three students (two female) have completed their PhD degrees, and three students are in the midst of their PhD studies. One PhD graduate spent time as a student working at Fermilab helping physicists implement modern Monte Carlo methods. Another PhD student is picking up where the first one left off. Three students (two female) completed their MS theses. More than a dozen undergraduate students have been mentored (primarily during the summer), over the course of three summers. Some were supported by this grant, while most were supported by other funding sources. Hickernell has embedded the new adaptive (quasi-)Monte Carlo research in his graduate Monte Carlo course, and some students in that course have contributed to GAIL. Hickernell, Choi, and their students have written an encyclopedia article; given numerous conference and colloquium talks; organized a conference and arranged special conference sessions at multiple conferences. Hickernell has given an invited conference tutorial and is one of the program leaders for this year's SAMSI program on quasi-Monte Carlo sampling. Hickernell received the 2016 Joseph F. Traub Prize for Achievement in Information-Based Complexity.

2.2. **Experience of Sun.** NSF-CNS-1162540, *CSR: Medium: Collaborative Research: Decoupled Execution Paradigm for Data-Intensive High-End Computing,* $842,298 (IIT share $280,766), June 2012 – August 2016. Sun is the PI.

2.2.1. *Intellectual Merit.* This collaborative project developed a decoupled execution paradigm (DEP) to address input/output (I/O) bottleneck issues. This paradigm enables users to identify and handle data-intensive operations separately.

2.2.2. *Broader Impacts.* Technical hurdles have been identified for decoupled execution, spanning system architecture, programming model, and runtime system. Results are available as recent publications [12, 13, 16, 14, 15, 27, 45, 49, 50] and other I/O related publications. In addition, in the past five years, Dr. Sun has graduated 3 PhD and 11 masters students, and supervised 5 postdoctoral and 4 graduate researchers.

2.3. **Experience of Wereszczynski.** PI of NSF-MCB-1552743 "CAREER: The Effects of Post-translational Modifications and Histone Variants on Chromatin Fiber Dynamics" June 2016 – May 2021, $790,129.

2.3.1. *Intellectual Merit.* The aim of this CAREER award is to use and develop multiscale biophysical simulation techniques to study how DNA is compacted in the cell, and how these mechanisms are regulated to affect gene expression. The PI's group addresses these issues through the use of molecular dynamics (MD) simulations, along with collaborations at Argonne National Laboratory and the University of Iowa. Early results have been presented at the annual Biophysical Society Meeting in 2017 and 2018, and a manuscript detailing the mechanisms by which post-translational modifications to the "H3 tails" affect the structures and energetics of nucleosomes is under minor review at *eLife* [36].

2.3.2. *Broader Impacts.* To date, this proposal has funded four trainees: one postdoctoral scholar, one PhD student, and two undergraduates from the College of DuPage. Both undergraduates performed 10-week summer research projects, during which time they learned how to set up, perform, and analyze MD simulations of various biomolecular systems. Robert Hickok, who was in our lab

in the summer of 2016, is currently enrolled at the University of Illinois at Chicago, whereas Meet Patel, who worked with us in 2017, is enrolled at the Georgia Institute of Technology.

3. Intellectual Merit

3.1. **Skills to Be Learned.** Our primary emphasis is educating CI contributors (CICs), and our secondary emphasis is educating CI users (CIUs). Our goal is to train students from high school through PhD level in skills of various difficulty, some building upon others. These include the skills in the table below. The sections describing our initiatives where these skills will be learned are listed in the far right column.

Learning Outcomes	**CIU**	**CIC**	**Learned**
Use			
1. Write and run numerical programs on a single CPU	HS	HS	3.3, 3.4.1, 3.5
2. Run numerical programs that utilize multiple cores and/or a GPU on a single machine	UG	HS	3.3, 3.4.1, 3.4.3, 3.4.4, 3.5
3. Run jobs that require more than one node with tight connectivity	G	UG	3.4.2, 3.4.4, 3.4.5, 3.6
4. Run jobs on a top-500 supercomputer	G	UG	3.4.2, 3.4.4, 3.5, 3.6
5. Use tools for analysis and visualization of large-scale simulations	G	G	3.4.2, 3.4.5, 3.6
6. Solve scientific problems that require multiple libraries and languages	G	UG	3.4.3, 3.4.5, 3.6
7. Execute reproducible scientific computations	UG	UG	3.4.2, 3.4.3
Develop & Optimize			
8. Write numerical programs that take advantage of multiple cores and/or a GPU on a single machine	UG	HS	3.3, 3.4.2, 3.4.3, 3.4.4
9. Make additions to a well-documented numerical software library consisting of documented, tested, robust routines		G	3.4.3, 3.6
10. Contribute to a numerical software library that takes advantage of high performance computing architectures		G	3.4.5, 3.6
11. Analyze the computational efficiency of individual algorithms and identify performance bottlenecks		UG	3.4.1, 3.4.2
12. Analyze the computational efficiency of large-scale simulations and identify performance bottlenecks		G	3.4.5, 3.6
Apply			
13. Evaluate whether simulation output accurately reflects the natural phenomenon it is designed to emulate	UG	UG	3.4.1, 3.4.2, 3.6
14. Appreciate how a computational result informs decision-making in the application domain and its effect on what kind of computational result is needed	G	G	3.4.1, 3.4.2, 3.6
15. Know how different modeling assumptions in the application domain are tied to the choice of different computational methods and computing environments	G	G	3.4.2, 3.5, 3.6
16. Collaborate with computational scientists outside their own majors	UG	UG	3.4.1, 3.6

Many of the learning outcomes above parallel to those provided in Table 1 of [42]. However, that table focuses on the outcome for a PhD in computational science. Our table above provides intermediate outcomes for those in high school, bachelor's, and master's study. A future CIC should ideally develop all of the skills labeled HS in high school, all of the skills labeled UG during undergraduate studies, and all of the skills labeled G during graduate studies. The analogous interpretation applies to CIUs. Our proposed innovations, outlined in the remainder of this section, provide opportunities to future CICs and CIUs to develop these skills.

The degree of mastery of any particular skill may depend on whether the computational scientist is majoring in computer science, mathematical science, or natural science. Moreover, our students may only be with us for part of their high school through PhD studies. We are ready to help those whose preparation is lacking catch up to where they need to be. When students leave our program, they should be fully prepared for the next steps in their growth as computational scientists.

3.2. **Proposed Innovations.** Our innovations will better prepare CICs and CIUs via several modes of learning for different kinds of students. They can be summarized as follows:

Section	Innovation	Target	
3.3	Summer computational science course	CIU	CIC
3.4.1	Enriched existing computational science offerings	CIU	CIC
3.4.2	Graduate theses incorporating advanced CI	CIU	CIC
3.4.3	Professional practices for computational science course		CIC
3.4.4	Undergraduate parallel and distributed computing course		CIC
3.4.5	Large-scale scientific computation course		CIC
3.5	Research experiences for community college students	CIU	CIC
3.6	CISC undergraduate and graduate summer fellowships		CIC

Several of these innovations involve permanent expansions of our curriculum. The others are extra-curricular activities designed to complement what is learned in the classroom. We have a track record in most of these areas, but we want to go far beyond our past experience to establish something new and substantial.

3.3. **Summer computational science course.** Since 2013, Illinois Tech's College of Science has run a (non-residential) three-week computational science summer course for Chicago area high school students. The goal has been to introduce them to solving mathematical and scientific problems using Mathematica. The Undergraduate Admissions Office publicizes and recruits students for the course, which has had an average enrollment of 9–10 students in the past. Starting in the summer of 2018, this summer course has an academic home in CISC, while continuing to partner with the Undergraduate Admissions Office, and in particular, Ms. April Welch. Dr. Kiah Wah Ong is the instructor.

We will broaden this course to include computing on the CISC cluster to introduce these high school students to multi-core computing (Skills 1, 2, and 8). Mathematica has the capability to perform computations in parallel, and we will also investigate the use of other languages, such as Python. This summer course will encourage the students to pursue degrees involving high performance computation and better prepare them for potential careers as computational scientists. We also hope to attract the students to Illinois Tech's computational science offerings.

Because our students are expected to have diverse backgrounds in computing, we will begin the course by assessing their existing skills and then break them into groups so that those who need to learn more fundamental skills may do so, while those with more advanced knowledge can be given more challenging assignments. Illinois Tech students will serve as teaching assistants (TAs) for the course, which will provide them with the opportunity to reinforce their own learning by teaching the computational science that they have learned.

The timing of this course will overlap with the summer research experiences for community college students (Sect. 3.5) and the research experiences of the CISC fellows (Sect. 3.6). We will inspire the students in this summer course by introducing them to the work of those who are a few steps ahead of them in their development as computational scientists.

Our goal is to host 15 high school students in the summer of 2019 and increase the number each year to 30 high school students steady state in the summer of 2021. The summer course has been and will continue to be funded by tuition fees. In order to broaden access, we plan to offer tuition scholarships to those with financial need. We will also track their career trajectories through annual surveys.

To attain these goals, we will create hard- and soft-copy fliers describing our revamped computational science course. Ms. Welch's colleagues in the Undergraduate Admissions Office will help us promote the course as they visit Chicagoland high schools. Hickernell and Ong will make themselves available to brief admissions counselors about the course and tell visiting high school students about it.

We also plan to open this summer computational science course to undergraduate students, primarily from Illinois Tech. Our goal is to attract 5–10 such students per year. Many of our students have scholarships or financial aid, which covers the summer term as well. We expect students who may not have a strong computing background—but have an curiosity in knowing more—will be attracted to this course. This will provide them a stepping stone to our more advanced computational science offerings.

3.4. **Strengthened undergraduate and graduate level computational science coursework.** Illinois Tech already has a substantial computational science curriculum. However, it has several deficiencies, which we aim to address.

CISC will post fliers around campus and publish pages on the CISC website describing our existing computational science offerings as well as our new and expanded offerings described below. Each semester we will broadcast information about the courses being offered to Illinois Tech students and their advisors to recruit more and better students into these classes.

3.4.1. *Enriched existing computational science offerings.* Illinois Tech offers quite a number of computational science courses. Computer science offers high performance computing at the undergraduate and graduate levels. Applied mathematics BS through PhD students are required to take at least one computational mathematics course and may also choose from a rich variety of computational mathematics electives. There are two undergraduate computational physics courses, a computational chemistry course, and a computational biology course.

These courses teach Skills 1, 11, and 13. However, students tend to take only the courses in their own major. Thus an applied mathematics student may not really have the chance to develop Skill 13. The (co-)PIs, who teach some of these courses, will liaise with other course instructors and the host departments to encourage non-majors to take these courses (Skill 16). We will explore how we might lower the pre-requisite barriers to help students break into new silos. We also will explore introducing some parallel computing (Skill 2) into these courses.

Minh has been playing a key role in developing the Bachelor of Science in Computational Chemistry and Biochemistry at Illinois Tech. To our knowledge, it is the first program of its kind in the country. In addition to a standard Bachelor of Science curriculum certified by the American Chemical Society, the recently introduced degree program requires courses from computer science and three specialized courses: computational quantum chemistry, computational biochemistry and drug design, and cheminformatics. The former has been offered on an annual basis and the latter two will be developed by Minh. Minh will develop the courses in a way that does not require advanced knowledge of physical chemistry and is therefore maximally inclusive to different majors.

The Monte Carlo methods graduate course taught by Hickernell every fall requires every student to complete a course project. Each year since 2015, HAVI, a global logistics company, has offered

a simulation project for this class that arises from their practical research. Two to three groups of five students each have dealt with the complexities of understanding data, formulating appropriate mathematical models to answer the question posed by HAVI, settling on a suitable simulation platform, performing and refining their simulations, and reporting their results to HAVI. These projects have gone well beyond the simple problems used to teach fundamental Monte Carlo concepts and have given students an added a dimension of industrial research to their education. The approaches and the insights provided by the students have impressed the HAVI researchers.

We propose to forge additional partnerships between local industry and our computational courses, which will help our students acquire Skill 14. This may take the form of course projects, guest lectures, and/or internship opportunities. As was the case with HAVI, we will harness our alumni connections. We will also make cold calls on companies performing extensive computation in the course of their work.

3.4.2. *Graduate theses incorporating advanced CI.* With the support of the other initiatives described above and below, we will be able to direct our graduate students towards more meaningful MS and PhD thesis topics that rely upon large-scale computation. This will help them learn Skills 3, 4, 5, 7, 8, 11, 13, 14, and 15.

3.4.3. *Professional practices for computational science course.* A few years ago, Choi and Hickernell piloted a one-credit course, MATH 573 Reliable Mathematical Software, primarily for their own research group. The course covered truncation and round-off errors, stopping criteria for adaptive software, creating software collaboratively via Git and GitHub, documentation, input parsing and validation, and reproducible computation. The rationale for the course was feedback from those outside academia that our computational mathematics students, while very knowledgeable about numerical algorithms, lacked some of the skills required to implement these algorithms in an industrial or government research setting. Students completed a project consisting of creating a small software library or extending an existing library. Several of the students in this course participated in developing GAIL [7]. This experience helped one student land an academic job teaching computer science, three students land computationally oriented positions in industry, and a fifth student gain admission to a PhD program.

We will grow this course to a standard three-credit undergraduate/graduate elective course. In addition to a fuller treatment of the above topics, which address Skills 7–9, we will add material on working in a multi-lingual environment (Skill 6) and small-scale parallel computation (Skills 2 and 8). The prerequisite will be any undergraduate course that covers numerical computation, therefore making this course accessible to a wider audience.

3.4.4. *Undergraduate parallel and distributed computing course.* Sun will be responsible for enhancing CS451 Introduction to Parallel and Distributed Computing. This new class is designed for CS students to learn the basic concepts and skills of parallel and distributed computing systems (Skills 2–4, 8). Sun will lead the effort to extend and enhance this class to attract and benefit students from other disciplines of science and engineering. There are definitely aspects of computer systems that are important for all computational scientists to know, but it is not clear how much non-computer science students can absorb if they are placed in the same class as computer science students. This is a non-trivial task, given that computer science students will typically have a much stronger foundation than other students, and one wants to benefit all students in the class. Sun, Hickernell, and Choi will share their experiences in teaching this class and the above-mentioned one. The aim will be to adjust the content and pre-requisites of these classes—keeping in mind the diversity of the intended audiences—and deciding whether the educational objectives are best served by having one, two, or even three classes. The three faculty may also engage in guest lecturing in each other's courses.

3.4.5. *Large-scale scientific computation course.* Since 2006 the computer science department has offered a graduate course, Advanced Scientific Computation, which covers Skills 3, 5, 6, 10, and 12. Dr. Hong Zhang from Argonne National Laboratory has taught this course to students majoring in computer science, mathematics, physics, and engineering. Students were exposed to cutting-edge analytic and algorithmic research projects and gained hands-on large-scale numerical programming experience. This course has been a launching point for many students into careers in computational science. Several of the course projects were integrated into the Portable Extensible Toolbox for Scientific Computing (PETSc) [2], benefiting the scientific community in large. At least eight students received summer internships at Argonne after taking her course, and three of her students eventually became post-doctoral researchers at Argonne.

In the past, this course has run only every other year. We plan to increase the frequency of this course to annually, serving a dozen or more students, by advertising its existence and benefits.

Students desiring to be CISC fellows (see Sect. 3.6) will be more competitive if they take one or more of the courses mentioned above in Sect. 3.4.3–3.4.5. We will use this as marketing point to recruit students into these courses.

3.5. **Research experiences for community college students.** To encourage the pursuit of bachelor's and advanced degrees by community college students, Wereszczynski has partnered in the past with the College of DuPage (CoD) to recruit students from their associate degree programs to engage in a ten-week summer internship program in his research group. CoD, with more than 28,000 students, is the second largest provider of undergraduate education in the State of Illinois. Many students who wish to pursue a career requiring an undergraduate or graduate degree start their college studies at CoD because for financial reasons.

We propose to broaden this program to include several CISC associated research groups at Illinois Tech. Each year we will work with Prof. Tom Carter of the physics department to advertise and recruit students to this program, with a particular focus on underrepresented minorities. These students will be matched with CISC labs based on their research interests and career goals. Our goal is to inspire and prepare these students for careers as computational scientists.

In the first phase of their internships, Minh will teach the cohort of CoD students in a week-long intensive computing "crash course" that will include topics such as an introduction to Linux, programming in Python, and the use of high performance computing resources. We will request an educational allocation on NSF XSEDE for students to run short benchmark molecular dynamics simulations on different computing architectures, including single CPUs, multiple cores on a single node, parallel jobs across multiple nodes, graphical processing units, and Intel Xeon Phis. Simulations of proteins in water including dihydrofolate reductase (23558 atoms) and cellulose (408609 atoms) will be run with NAMD [40]. Based on the results, students will compare the speed and scalability of the algorithms on different architectures and for different system sizes.

For the remaining nine weeks, CoD students will work directly in IIT labs on various computational projects, such as high performance Monte Carlo methods in Choi and Hickernell's group, binding free energy calculations in the Minh's group, parallel programming and performance optimization in Sun's group, and simulations of biomolecular complexes in Wereszczynski's group. To foster discussions among the CoD students, weekly lunches will be organized. In addition, at the end of the summer a research symposium will be organized in which students will present a short presentation on their work. Following the summer period, we will track the career trajectories of these students with annual follow up surveys, and we will maintain mentoring relationship with these students as are appropriate.

We will aim for four CoD students in 2019, six in 2020, and six in 2021. Students will be provided $5000 stipends. After the project ends, we hope to secure funding to continue from other sources, such as Research Experience for Undergraduate (REU) funding and REU add-on supplemental funding.

3.6. **CISC undergraduate and graduate summer fellowships.** To provide more opportunities for the practice of the advanced CI skills that we are teaching our Illinois Tech undergraduate and graduate students, we plan to offer summer fellowships. These will be awarded on a competitive basis and be provided to students who partake in one of the following experiences

- Embedding themselves in a computational science research group outside their major, or
- Joining a large-scale computational science research project at Argonne, Fermilab, or in a local company.

The former opportunity moves our students outside their silos. The broadening experience will make them more valuable members of interdisciplinary teams performing large-scale computations. It will help them learn and practice Skills 13–16. For example, a natural science student embedded in a mathematical science research group might experiment with how well the group's new algorithms solve a practical science problem. A computer science student embedded in a natural science research group might lead the adaption of a scientific application from a single core to a high-performance computing architecture.

CISC began a series of lunchtime matchmaking seminars in the fall of 2017 to introduce computational scientists and engineers at Illinois Tech to each others' research. CISC also hosted a seed grant competition and awarded one grant to an interdisciplinary team. These continuing activities will generate more opportunities for CISC fellows and more quality fellowship applications. Moreover, the CISC fellowships, along with the matchmaking seminars and the seed grants, will help CISC achieve its goal to promote more competitive proposals for external funding of interdisciplinary computational science research.

The ongoing large-scale computational projects at Argonne and Fermilab will provide students the opportunity to learn and practice Skills 4, 5, 6, 14, and 15. Argonne has several software development projects including PETSc [2] and xSDK [4]. Fermilab has a heterogeneous computing environment for high energy physics (HEPCloud) [10] under continuous development. Two of our external advisory board members, Lois Curfman McInnes (Argonne) and Burt Holzman (Fermilab) will aid us in placing CISC Fellows in these two national labs.

The (co-)PIs have had collaborations and contacts with Chicago-area companies involved in supporting or performing large-scale calculations as part of their research, such as HAVI (see Sect. 3.4.1) and NAG. We will further develop these contacts and identify sources of possible projects for CISC fellows.

At the end of the summer the CISC fellows will present their work in posters, possibly coinciding with the presentations by the COD students. During their presentations the CISC Fellows will interact with the summer computational science course students (Sect. 3.3).

Each year, starting in 2019, we will offer CISC fellowships to two or more undergraduates ($5000 stipend each) and five or more graduate students ($7000 stipend each). Announcement of the fellowships will be made to science students near the beginning of the calendar year. The students applying will provide a synopsis of their proposed projects, their curriculum vitae, and letters of recommendation from their advisor and the project supervisor. The (co-)PIs will decide who will receive the fellowships. Brochures describing the CISC fellowships will be provided to the departments to use in recruiting new students with interest in computational science.

By the time that this grant is completed, we expect that our overall training program for computational scientists will have prepared a significant number of our students to compete for funded internship opportunities in the national laboratories. Moreover, we anticipate that embedding students in research groups outside their silos will spark interdisciplinary collaborations among research groups. This in turn will lead to external funding of interdisciplinary computational projects that will draw together and financially support computational science students from diverse majors.

4. Broader Impacts

4.1. **Educating Next-Generation Computational Scientists.** Standard science curricula have not kept pace with the potential of advanced CI for computational science. Computer science courses teach the architectures and languages for large-scale computation, but they do not teach their students how to team up with domain experts to solve important scientific problems. Computational mathematics, biology, chemistry, and physics courses do teach computing, but not educate their students enough in advanced computing technologies and computation thinkings to lead the use and contribution to advanced CI.

Our proposed computational science education program will set students on a path so that by the time they finish their PhD studies, they can be cross-disciplinary computational scientists making vital contributions to interdisciplinary research teams discovering new science. Their work will lead to breakthroughs in our understanding nature, from the sub-atomic to the astrophysical scale. Their work will lead to breakthroughs in health, medicine, manufacturing and finance, which will improve the quality of our lives and the national economy.

The students leaving our programs will carry their academic and practical knowledge of advanced CI to their new research groups in universities, government labs, and companies that they will join. They will share what they have learned with those who need to use more powerful computing capability, but do not yet know how. The knowledge that we impart will be multiplied.

4.2. **Impacting Research in Computer Science, Mathematical Science, and Natural Science.** The interdisciplinary computational research promoted by our program will generate interesting research problems for the contributing disciplines:

- Complex quantitative models of natural science phenomena will challenge computational mathematicians and computer scientists to develop new algorithms that can utilize more advanced software and hardware.
- The advances in CI will alter how computational mathematicians and computer scientists design algorithms and measure algorithmic efficiency. Efficiency measures for algorithms running on single processors do not apply to advanced CI, and new efficiency measures are needed. Given the variety of architectures and languages, operation count or clock time are not adequate good choices.
- Large-scale scientific computation enabled by advanced CI will answer existing questions in natural science and prompt new research questions in these sciences.

The computational scientists educated by our program will be prepared to tackle these new research problems because they will be proficient contributors and users of advanced CI, i.e., CICs and CIUs. They will know there own disciplines deeply enough to have the new ideas required to solve these new problems. Because they are cross-disciplinary, they will understand how their expertise meshes with the ideas from other disciplines to solve the problem at hand.

Consider an example involving quasi-Monte Carlo (qMC) methods (Hickernell's research), which are used to evaluate multi-dimensional integrals. From their 1960s until the early 1990s the progress in qMC was mainly theoretical. Then in the mid-1990s, Paskov and Traub [38] showed that qMC could price a collateralized mortgage obligation much more efficiently than independent and identically distributed Monte Carlo (IIDMC). This was surprising, since existing theory supporting showed that qMC was better than IIDMC up to dimension only five or so, whereas Paskov and Traub's problem had dimension 360. This computational result challenged mathematicians and theoretical computer scientists to re-visit the long-held theory, and the result was dozens of articles and a more complete understanding of the situations in which qMC is superior to MC, even for infinite dimensional integration. New computation raised new research questions, which were then answered.

As another example, a couple of years ago, Jiménez Rugama, the former PhD student of Hickernell, was invited to join a research group of physicists at Fermilab to explore whether their Monte Carlo (MC) computations could be sped up. The default IIDMC algorithm being used was several decades old. Jiménez Rugama was able to introduce the Fermilab group to the much more efficient qMC methods. In the course of implementing these methods, Jiménez Rugama observed an anomaly in the calculations, which was traced to a bug in the long-standing physics code that generated the particle collision events.

4.3. **Modeling How Silos Can be Broken.** We recognize that computer science, mathematical science, and the several natural sciences are well-defined disciplines. Someone living in one of these silos cannot take full advantage of advanced CI for scientific computation. The solution is not to build a new computational science silo. The solution is to develop cross-disciplinary computational scientists that are deep in one discipline but break out of their own silo to be conversant in others.

This project will show other educational institutional how to break down the major discipline silos to foster high quality computational science. The activities that we will implement will be models for others. We will make our syllabi, training materials, and procedures available on repositories for others to follow and model. (See the Data Management plan for more specifics.) We will publicize our successes and the lessons learned from failures in conference talks. We will advise those interested to adopt our best practices.

4.4. **Codifying Good Computational Science Practice.** The practice of good computational science is built upon diverse ideas that are not necessarily contained in one text or reference book. Some texts on computational science, such as [47], focus on numerical methods, while others, such as [46], focus on scientific applications. Neither of these types of texts give significant attention to parallel computing or software engineering for high performance computational science software libraries. Texts on high performance computing for computational scientists, such as [30], are incomplete in their coverage of numerical methods or important applications.

As we initiate, develop, and expand the new courses described in Sects. 3.4.3–3.4.5 and as we work with the CISC fellows, we will gather digestible resources describing good computational science practice. These resources will be referenced on the CISC webpage and published in journal articles.

4.5. **Broadening Access to Computational Science Opportunities.** Illinois Tech's summer programs are aimed at serving the Chicago area high school students, especially those who are underrepresented minorities. The goal is to provide intellectually stimulating experiences for them that will better prepare them for undergraduate and graduate study. In particular, our summer course in computational science (see Sect. 3.3) will broaden access to a career in computational science. By teaching our students how compute answers to scientific problems *and* giving them two college credits as well, we will be giving our students a head start that they would not have otherwise.

Community colleges enroll approximately 45% of the nation's undergraduate students, a disproportionate number of which are underrepresented minorities [26, 37]. Nearly 90% of these students have a goal of transferring to four-year institutions to complete their bachelor's degree, however the actual transfer rate is estimated to be only 25–40% [21, 32]. Studies have shown that involving students, especially those from underrepresented groups, in research activities decreases their attrition rate and increases the probability they will pursue further education [3, 25]. Our research experience for CoD students (Sect. 3.5) will ignite their interest in computational science, giving them motivation to complete their undergraduate degrees and pursue advanced degrees.

4.6. **Sharing What We Have Learned.** In the course of carrying out our proposed work, we will be learning from

- The background work we do in preparing our new and enhanced courses,

- The ongoing formal assessment that we will undertake (see Sect. 6),
- The continual advice from our external advisors (see Sect. 5),
- Informal student feedback, and
- Our experience.

We will distill the insights gained and share them in articles, talks, and posts on our website. We will seek out venues where our experience can gain a broader audience, such as conferences, websites, and online forums aimed at (potential) computational science educators. We will also make available the course materials, software packages, and code templates that we have developed so that they are available to others.

5. Partnerships and External Advisory Board

To maximize the impact of our project, we are partnering with Ms. April Welch, Associate Vice-President of Strategic Initiatives at Illinois Tech. Ms. Welch and her colleagues in Illinois Tech's Office of Enrollment will assist us in recruiting students for the Summer Computational Science Course (see Sect. 3.3).

Ms. Welch and her colleagues have established multiple programs for recruiting and supporting high school students with disadvantaged socio-economic backgrounds and preparing them to succeed at a rigorous university like Illinois Tech. The Undergraduate Admissions Office has a network of staff members and alumni actively recruiting African-American and Hispanic students for admission to Illinois Tech and the summer programs that her office supports.

We are also partnering with three other organizations through key contacts:

- Dr. Tom Carter, Professor of Physics at College of DuPage (CoD), the largest community college in Illinois, located in the western suburbs of Chicago,
- Dr. Lois Curfman McInnes, Senior Computational Scientist in the Mathematics and Computer Science Division at Argonne National Laboratory, where she was former PETSc co-lead and is presently xSDK co-lead, and
- Dr. Burt Holzman, Assistant Director of the Scientific Computing Division at Fermi National Accelerator Laboratory (Fermilab), where he oversees the HEPCloud program and coordinates cross-cutting initiatives and solutions across the facility.

Dr. Carter will partner with us to identify CoD students most suited to take advantage of our summer research experience for under-served undergraduates (see Sect. 3.5). He will help communicate to the students our expectations for the summer and feedback to us any difficulties that the students are having. He will also let us know these students' next steps after finishing their CoD studies.

Dr. Curfman McInnes will help us identify large-scale computation projects and advisors at Argonne that are suitable for CISC Fellows (see Sect. 3.6). Particular attention will be given to PETSc and xSDK related projects. She will advise in the selection of the CISC Fellows to be placed at Argonne.

Dr. Holzman will help us identify large-scale computation projects and advisors at Fermilab that are suitable for CISC Fellows (see Sect. 3.6). Particular attention will be given to HEPcloud projects involving heterogeneous systems. He will advise in the selection of the CISC Fellows to be placed at Fermilab.

Our External Advisory Board will be comprised of Dr. Carter, Dr. Curfman McInnes, and Dr. Holzman. This board will meet with the (co-)PIs and Senior Personnel twice a year (by teleconference if necessary), to review the progress of our project and advise us on how our efforts can be even more effective. Apart from these formal meetings, we will welcome their advice at any time and solicit their advice as needed.

6. Assessment

The proposed project is both ambitious and complex. There are four levels of participants (i.e., high school students, community college students, undergraduate students, and graduate students) as well as participants that are classified as cyberinfrastructure (CI) users (CIUs) and contributors (CICs). There are 16 different learning outcomes, all of which are performance tasks as opposed to understandings that are assessed with paper and pencil exams. In addition, the proposed project will also track the post project trajectory of the various participant levels (e.g., future course enrollments, employment situations, etc.). In order to insure the trustworthiness of data collected, all assessments will have established content validity as well as inter-rater agreement (i.e., reliability).

6.1. **Content Validity of Assessments.** The specific learning outcomes (see Sect. 3.1) are all performance tasks. Some are independent of each other and some are interrelated. Consequently, a single assessment instrument would not be appropriate. Rather, assessment tasks will need to be developed for each performance task and validity will need to be established for each task. A group of five individuals, derived from the project staff, will develop a task purported to assess each of the learning objectives. After development, Advisory Board members (and additional experts in the field if needed) will independently assess whether each item assesses what it purports to measure. An agreement level of 80% will be desired. Five individuals, as is convention, will be needed for this assessment. If an agreement level of 80% is not reached, the task will be revised and subjected to another independent evaluation. This process will be repeated until an agreement level of 80% is reached for each performance task.

6.2. **Inter-Rater Agreement (Reliability) of Assessments.** It is one thing to establish whether an assessment task is aligned with the learning outcome for which it is designed, but it is another to document that the assessment of student/participant performance is consistent. Given that all of the learning outcomes are performance tasks, the consistency of assessment will need to be established by documenting that those individuals evaluating the task performance do so in a consistent manner. A scoring rubric will need to be developed for each performance task. This will involve the specification of what each respondent will need to include in their performance of the specified task. In short, the rubric defines what should be included for a particular "grade" on the task. Sample student responses (e.g., 3–5) will be evaluated by a group of scorers (preferably five) to document whether there is agreement in how a student's performance is evaluated. By convention, the target level of agreement should be at least 80% for each performance task. This will establish that students' performance on the learning tasks are being scored in a consistent manner. Once inter-rater agreement is established it is not necessary for every student task to be scored by multiple evaluators. Ordinarily, inter-rater agreement is established at the beginning of an investigation. However, in this case, every effort will be made to check this consistency midway through the scoring of student tasks and at the end of the evaluation process.

It is important to note that high school students, community college students, undergraduate students, and graduate students are not expected to achieve each of the learning outcomes at the same level. Consequently, the sample student responses scored for reliability will be performed separately for each student level.

6.3. **Research Questions and Data Analysis.** The sample for the proposed project consists of four different levels of students. The accomplishments of these four groups of students will be analyzed independently. That is, their performance levels for each of the 16 learning outcomes will be determined independently. Clearly, students at these different levels cannot be expected to perform at the same level on each of the learning outcomes. Additionally, it would be inappropriate to assume that contributors (CICs) and users (CIUs) would be expected to perform at the same level.

Although it would not be likely that the students would have the ability to perform the learning outcomes in advance of the program, using a pretest/posttest design will potentially provide important information relative to the range of students involved in the project. changes will not be determined. Since categorical data (students with varying abilities to complete the performance tasks) simple percentages of performance will be documented to establish success of the proposed project. Specially, Chi-Square tests will be performed comparing the pretest scores with posttest scores with a significance level of 0.05 considered to be statistically significant.

Project participants will be located in different contexts (e.g., research labs, IIT, and community colleges, high schools), hence it will be of interest to see if there are differences in performance relative to such contexts. Consequently, Chi-Square comparisons ($p < 0.05$) will be used to compare differences in learning outcome performances on each of the learning outcomes at each of the different educational levels. Such comparisons may have implications for future interventions for students at various academic levels.

Finally, it will be of particular interest to follow the professional trajectories of participants in this proposed program following their participation. For example, do high school students enter university programs related to CI following their participation or do they become directly employed in the field through various occupations? In a similar manner it will be of interest to follow the trajectories of community college, undergraduate, and graduate students. What, if any, was the impact of participation in the program? Data on post program trajectories will be compiled with simple frequencies related to university and/or career paths. Given that the proposed program is a three year program, participants will be followed for a period of up to two years after participation.

One of the most intriguing driving motivations for the proposed project is the breaking down of disciplinary silos with respect to the program focus on an area that is clearly interdisciplinary. Participants in this project will come from a variety of subject matter areas, as well as different educational levels. It is unclear if there is any relationship among disciplinary areas, educational levels, and potential professional trajectories within CI. One final focus of data analysis, although clearly exploratory, will be a correlation matrix that includes educational level, disciplinary background, program success (with respect to outcomes), and career trajectory. Depending on the results of such an analysis, further more targeted analyses may be pursued.

6.4. **Tracking the Career Outcomes of Our Students.** In addition to assessing the skills learned by our students, we plan to track their career paths. We will survey our students to identify their next program of studies or their job, whichever the case may be. This will allow us to determine how many pursue careers as computational scientists. We will also ask them what skills they are finding important in their next degree program or job.

7. Timeline

The chart below highlights when certain project tasks are expected to be performed.

Time	Sect.	Task
2018		
November		Proposed work begins
	5	Meet with CISC External Advisory Board—confirm priorities and first steps
	3.3	Prepare advertising for the summer computational science course
	3.5	Prepare advertising for the research experience for CoD students
	3.6	Advertise the CISC summer fellowships
	3.4.1	Post information on existing computational science courses on the CISC website

2019		
January	3.3	Begin promoting summer computational science course
	3.4.3	Pilot new professional practices for computational science course
	3.4.4	Offer undergraduate parallel/distributed computing course
	3.5	Begin promoting research experience for CoD students
	3.6	Identify potential projects/research groups to receive CISC fellows
February	3.6	Accept applications for CISC summer fellowships
	3.4.1	Begin seeking more industrial partners to propose course progress
March	3.6	Announce CISC summer fellowship awardees
	3.5	Announce COD students accepted for the summer research experience
May	3.5	Begin research experience for CoD students; start with the "crash" course
	3.6	Begin summer CISC fellowships
July	3.3	Begin summer computational science course
August	3.4.5	Offer advanced scientific computing course
September	5	Meet with CISC External Advisory Board
	3.3	Evaluate summer computational science course
	3.5	Evaluate research experience for CoD students
	3.6	Evaluate summer CISC fellowships
October	4.6	Ensure that materials developed during the first year are published on the web
December	3.3	Begin promoting summer computational science course
	3.5	Begin promoting research experience for CoD students
	3.6	Identify potential projects/research groups to receive CISC fellows
2020 January – 2021 October		Same schedule for major course offerings and summer activities as in 2019, but with promotion for the summer activities starting the December beforehand
	4.6	Analyze assessment data and prepare publications documenting what has been learned
	4.6	Attend conferences to share what has been learned

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Frederick John Hickernell

Professional Preparation

Institution	Location	Major	Degree	Year
Pomona College	Claremont, CA	mathematics & physics	BA	1977
Massachusetts Institute of Technology	Cambridge, MA	mathematics	PhD	1981

Appointments

2017–present	Director, Center for Interdisciplinary Scientific Computation, Illinois Institute of Technology
2005–present	Professor, Illinois Institute of Technology
2005–2017	Chair of Applied Mathematics, Illinois Institute of Technology
1995–2005	Associate Professor & Professor of Mathematics, Hong Kong Baptist University
1989–2002	Head of Mathematics, Hong Kong Baptist College/University
1985–1995	Lecturer & Senior Lecturer of Mathematics, Hong Kong Baptist College

Products (for citation counts see scholar.google.com (Fred J. Hickernell))

Five Products Closely Related to the Proposal

[1] S.-C. T. Choi, Y. Ding, F. J. Hickernell, L. Jiang, Ll. A. Jiménez Rugama, D. Li, J. Rathinavel, X. Tong, K. Zhang, Y. Zhang, and X. Zhou, *GAIL: Guaranteed Automatic Integration Library (versions 1.0–2.2)*, MATLAB software, gailgithub.github.io/GAIL_Dev/, 2013–2017.

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Synergistic Activities

[1] My research has included dozens of high school, BSc, MS, MPhil and PhD students as well as post-doctoral scholars. My mentoring has included summer research experiences for students funded by NSF support as well as other sources of financial support. Not only have students gained experience in discovery of new mathematics, they have been required to organize and communicate their discoveries in research group meetings, conference presentations, and publications. Students and post-docs that I have mentored have gone on to further study, academic positions, and various positions in commerce industry.

For over twelve years I was department chair at Illinois Tech before stepping down in 2017. During that time I hired and encouraged eight new tenure track assistant professors: three were women, six earned tenure and promotion to associate professor, and six successfully competed for external funding. Two of the women hires, who have received tenure and been promoted to associate professor and have received external funding, were in statistics, an area where our department previously lacked strength. In May, 2017, I was appointed director of a newly created Center for Interdisciplinary Scientific Computation (CISC), and charged with raising the profile of our scientific computation research and education at Illinois Tech. CISC is connecting faculty from science, engineering, business, and human sciences.

[2] Associate Editor, *International Journal of Numerical Analysis and Modeling* (2003–present), *Journal of Complexity* (1999–present), *Journal of Mathematical Research with Applications* (2010–present), *Mathematics of Computation*, 2008–2017, *SIAM Journal on Numerical Analysis*, 2005–present.

[3] Organizer, Program Committee Member, and/or Steering Committee Member for a number of international conferences, including the *Third through Eleventh International Conferences on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing*, biennially 1998–present. Program Leader for the Statistical and Applied Mathematical Sciences Institute (SAMSI) 2017–18 Program on Quasi-Monte Carlo and High-Dimensional Sampling Methods for Applied Mathematics (QMC).

[4] Worked with developers to promote the inclusion of software for generating low discrepancy sequences in the MATLAB Statistics Toolbox, since R2008a, and in routine G05YNF of the NAG library, since 2009.

[5] Fellow of the Institute of Mathematical Statistics (elected 2007). Recipient of the 2016 Joseph F. Traub Prize for Achievement in Information-Based Complexity.

Sou-Cheng (Terrya) Choi

Professional Preparation

Institution	Location	Major	Degree	Year
National University of Singapore	Singapore	Computational Science, Mathematics	B.S. (Hons)	1997
National University of Singapore	Singapore	Statistics and Applied Probability	M.S.	1997
Stanford University	Stanford, CA	Computational and Mathematical Engineering	Ph.D.	2007

Appointments

2017–present Research Associate Professor, Illinois Institute of Technology, Chicago, IL
2018–present Lead Researcher in Machine Learning and Data Mining Applications, Allstate Corporation, Chicago, IL
2016–2017 Principal Data Scientist (Consultant), Allstate Corporation, Chicago, IL
2014–2017 Research Assistant Professor, Illinois Institute of Technology, Chicago, IL
2010–2013 Research Scientist, Computation Institute, University of Chicago, Chicago, IL with joint appointment in the Argonne National Laboratory, Argonne, IL
2007–2013 University Affiliate, Department of Management Science and Engineering, Stanford University, Stanford, CA
2007–2010 Senior Member of Technical Staff, Server Technology/Business Intelligence, Oracle USA, Inc., Redwood Shores, CA
1998–2000 Financial Software Engineer, Kamakura Corporation, Singapore
1997–1998 Systems Analyst, Warburg Dillon Read, Union Bank of Switzerland, Singapore

Products.

FIVE PRODUCTS MOST CLOSELY RELATED

1. Smith, A. M., Katz, D. S., Niemeyer, K. E, and FORCE11 Software Citation Working Group (2016). Software Citation Principles, PeerJ Computer Science, Volume 2, e86.
2. Katz, D., Choi, S.-C. T., Lapp, H., Maheshwari, K., Loffler, F., Turk, M., Hanwell, M., Wilkins-Diehr, N., Hetherington, J., Howison, J., Swenson, S., Allen, G., Elster, A., Berriman, B., and Venters, C. (2014). Summary of the First Workshop on Sustainable Software for Science: Practice and Experiences (WSSSPE1). Journal of Open Research Software, Volume 2, Number 1, e6.
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FIVE FURTHER PRODUCTS

1. Choi, S.-C. T., Lin, Y., and Mulrow, E. (2017). Comparison of Public-Domain Software and Services for Probabilistic Record Linkage and Address Standardization. In Towards Integrative Machine Learning and Knowledge Extraction: BIRS Workshop, Banff, AB, Canada, July 24-26, 2015, Springer International Publishing, Cham, 51–66.
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5. Donoho, D. L., Flesia, A., Huo, X., Levi, O, Choi, Choi, S.-C. T., and Shi, D. (2003). BEAMLAB (Version 200) [Software]. Available from http://www-stat.stanford.edu/~beamlab/

Synergistic Activities

1. Since 2013, I have served as a mentor to 12 graduate (8 doctoral and 4 master's) students who are Applied Mathematics majors at the Illinois Institute of Technology (IIT). I have guided them on various aspects of reliable reproducible research in computational mathematics and statistics. I also served as thesis committee members for two of the students. The research and mentoring efforts have resulted in publications of multiple papers and presentations in conferences and journals, as well as an ongoing software package called GAIL. Four of our PhD graduates are now working in either academia or industries. At least one MS student went on to pursue PhD degree in mathematical sciences. We continue to collaborate with our current students as well as alumni working in both industries and academia.
2. I taught four research seminar courses at IIT and the University of Chicago (UC) between 2013 and 2016. Each course has between one to eight students at undergraduate or master's levels from applied mathematics or computer science. We explored, for instance, modern machine learning methods for problems and big data sets stemming from computational social sciences. In Summer 2017, a group of my students examined Chicago crime rates and city safety at geographical blocks, each of which has an area of approximately 0.24 square miles. We won a second prize in a poster competition organized by the IIT College of Science.
3. I have been collaborating with an undergraduate student from the Department of Mathematics, University of Chicago on a research project related to probabilistic record linkage of big datasets and address standardization since Summer 2017. I seeded the student with some research ideas from a paper my coauthors and I had published. The student was able to enhance the code base quickly. Starting this Fall, we have extended the code with new methodology based on neural networks showing highly accurate classification results of address components. We have involved a mathematically well-prepared high school student since Dec 2017 to test and refine the computational results for submission to a major conference in 2018.
4. I have given over 78 scientific talks locally and internationally in the past ten years. Three of them are plenary talks at international conferences. At least twenty of them are invited talks at various intuitions or conferences. I have also co-organized multiple international conferences (e.g., WSSSPE1 to WSSSPE4, which are annual conferences on sustainable scientific software from 2013 to 2016) and (co-)hosted at least eight mini-symposiums in major conferences organized by, for example, the Society of Industrial and Applied Mathematics (SIAM), the American Mathematical Society (AMS), and the International Linear Algebra Society (ILAS) over the years in order to encourage exchange of ideas among researchers in computational sciences and research software.
5. I offer scientific consulting services to public members or private corporations on problems related to my research expertise in computational sciences and algorithms. For instance, in the past few years, I received inquiries from members of Stanford University and Peking University, China on questions related to my mathematical software MINRES-QLP Pack. I helped debug the researcher's programs and discussed potentially more efficient approaches to solve their problems. These researchers have applied my algorithms to enhance nonlinear algorithms such as deep learning or for solving complex problems arising in studies of nanophysics. Another example involves my consulting services offered to Allstate Corporation between Jun 2016 to Dec 2017 that used multi-core machines to perform parallel computations of risk modeling as well as instantaneous traffic and incident analysis for over 20 million road segments in America. I also collaborate with Stanford University on a challenging project related to rea-time collision risk prediction over immediate time horizons using multi-core GPU machines; the work has resulted in a paper accepted by the 17th International Conference on Autonomous Agents and Multiagent Systems (AAMAS 2018). A third example is a recent ongoing collaboration with Professor Chrystal Ho Pao, a biologist from a local university, to develop an interdisciplinary approach for teaching a biology and statistics research course at undergraduate level; we plan to publish a paper in an education journal.

Biographical Sketch for David Minh

(a) Professional Preparation

- University of California, Berkeley, CA. Chemistry. B.A. 2003
- University of California, San Diego, CA. Chemistry. Ph.D. 2007
- National Institutes of Health, Bethesda MD. Statistical Mechanics. Postdoc. 2007-2009
- Argonne National Laboratory, Argonne IL. Biophysics. Postdoc. 2009-2011
- Duke University. Computational Chemistry. Postdoc. 2011-2013

(b) Appointments

- Illinois Institute of Technology. Assistant Professor of Chemistry. 2013-present

(c) Products

(i) Five Products Most Closely Related:

- Nguyen TH, Zhou HX, Minh DDL. Using the Fast Fourier Transform in Binding Free Energy Calculations. Journal of Computational Chemistry. in press. `http://dx.doi.org/10.1002/jcc.25139`
- Spiridon, L, Minh DDL. Hamiltonian Monte Carlo with Constrained Molecular Dynamics as Gibbs Sampling. J Chem Theory Comput, 13(10), 4649-4659 (2017).
- Xie B, Nguyen TH, Minh DDL. Absolute Binding Free Energies between T4 Lysozyme and 141 Small Molecules: Calculations Based on Multiple Rigid Receptor Configurations. J Chem Theory Comput, 13(6), 2930-2944 (2017).
- Nguyen TH, Minh DDL. Intermediate Thermodynamic States Contribute Equally to Free Energy Convergence: A Demonstration with Replica Exchange. J Chem Theory Comput, 12(5): 2154-2161 (2016).
- Minh DDL, Minh DL, Nguyen L. Layer Sampling. Commun Stat Simulat Comput, 45:1, 73-100 (2016).

(ii) Five Further Products:

- Onuk E, Badger J, Wang YJ, Bardhan J, Chishti Y, Akcakaya M, Brooks DH, Erdogmus D, Minh DDL, and Makowski L. Effects of Catalytic Action and Ligand Binding on Conformational Ensembles of Adenylate Kinase. Biochemistry, 56(34), 4559-4567 (2017).
- Minh DDL. Implicit Ligand Theory: Rigorous binding free energies and thermodynamic expectations from molecular docking. J Chem Phys, 137: 104106 (2012).
- Nilmeier JP, Crooks GE, Minh DDL, Chodera JD. Nonequilibrium candidate Monte Carlo is an efficient tool for equilibrium simulation, Proc Natl Acad Sci USA, 108(45): E1009-1018 (2011).
- Minh DDL. Optimized replica gas estimation of absolute integrals and partition functions. Phys Rev E, 82(3): 031132 (2010).
- Minh DDL, Adib AB. Optimized free energies from bidirectional single-molecule force spectroscopy. Phys Rev Lett, 100(18): 180602 (2008).

(d) Synergistic Activities

- I have been extensively involved in mentoring undergraduates and high school students.

  IIT undergraduates have been involved in my research group since I started my faculty position. Two students, John Clark and Rachael Youngworth, have completed honors theses with my group. Clark worked on algorithms for clustering receptor snapshots in binding free energy calculations based on implicit ligand theory. Youngworth worked on molecular dynamics simulations of succinate dehydrogenase. Clark now works on laboratory information management systems at Accenture and Youngworth is pursing a Ph.D. at the University of Chicago. I currently have two undergraduate students in my group, William Menzer and Natalie Jumonville, who both plan to pursue Ph.D. degrees.

  My group has hosted summer internships for 23 undergraduates, mostly from the Brazil Scientific Mobility Program. The students have worked on a variety of projects in small teams mentored by a long-term group member. Some projects have involved implementing new features into a software package developed by my group, AlGDock. These include a Markov chain Monte Carlo method, a grid interpolation algorithm, and restraints to confine a ligand to a particular pose. Other projects have been more applied, such as constructing homology models and running free energy calculations to explore structural ramifications of binding different ligands.

  My group has also hosted 6 high school students. Like the undergraduates, they have worked in teams mentored by a long-term group member. They have worked on projects related to molecular docking, translating computer code from MATLAB to python, and predicting residence time based on BPMFs.

- In October 2015, I was the local arrangements chair for the Midwest Enzyme chemistry conference, which was held at IIT. I worked with the program chair to help ensure smooth progress for the free one-day conference for approximately 200 individuals.

- In the summer of 2015, I helped develop and organize a workshop for high school chemistry teachers entitled "Choose Your Own Adventure: Solving Real-World Problems with Spectroscopy." After a lecture about spectroscopic techniques and a tour of instruments, the teachers devised and implemented laboratory-based solutions to a set of realistic scenarios. The teachers responded enthusiastically, asking many questions and performing careful sample preparation and measurement. One teacher effused that if we held the workshop again, he would return to work on scenarios that he missed the first time!

- Much of my research can be described as development and refinement of research tools, computation methodologies, and algorithms for problem-solving. Throughout my scientific career, I have made source code publicly available on the internet.

- I have reviewed 33 articles for 15 different journals: ACS Omega (1), Biophysical Journal (2), Biopolymers (2), Journal of Chemical Physics (10), Journal of Chemical Information and Modeling (2), Journal of Chemical Theory and Computation (5), Journal of Computer-Aided Molecular Design (1), Journal of Molecular Biology (1), Journal of Physical Chemistry (3), Journal of Statistical Physics (1), Journal of Structural Biology (1), Langmuir (1), Physics Letters A (1), Physical Biology (1), and PloS One (1). The number in parentheses is the number of articles reviewed for each journal.

Xian-He Sun (US citizen)

Department of Computer Science (CS)	+1 312 567 5260
Illinois Institute of Technology (IIT)	+1 312-567 5067 fax
10 W. 31st Street	sun@iit.edu
Chicago, IL 60616	www.cs.iit.edu/~sun/

Professional Preparation

Beijing Normal Univ., Beijing, China	Mathematics	BS, 1982
Michigan State University, East Lansing, MI	Mathematics	MS, 1985
Michigan State University, East Lansing, MI	Computer Science	PhD, 1990
DoE Ames National Laboratory, Ames, IA	Post-Doctoral Researcher	1990-1991

Appointments

1999-present	Distinguished Professor (since 2014), Chair (9/2009-8/2014), Professor (since 2002), Associate Professor, Dept. of Computer Science, Illinois Institute of Technology, Guest Faculty, Argonne National Laboratory
2006-2010	Visiting Scientist, Fermi National Accelerator Laboratory
1994-1999	Assistant & Associate Professor, Department of Computer Science, Louisiana State University
1992-1993	Staff Scientist, ICASE, NASA Langley Research Center
1991-1992	Visiting Assistant Professor, Dept. of Mathematical Science, Clemson University

Five Closely Related Products

[1] N. Liu, A. Haider, D. Jin and X.-H. Sun, "Modeling and Simulation of Extreme-Scale Fat-Tree Networks for HPC Systems and Data Centers," ACM Transactions on Modeling and Computer Simulation (TOMACS), vol. 27, no. 2, pp. 13:1--13:23, July. 2017.

[2] S. He, Y. Wang, X.-H. Sun, and C. Xu, "Using MinMax-Memory Claims to Improve In-Memory Workflow Computations in the Cloud," IEEE Transactions on Parallel and Distributed Systems (TPDS), vol. 28, no. 4, pp. 1202-1214, April 2017.

[3] Y. Liu and X.-H. Sun, "Evaluating the Combined Effect of Memory Capacity and Concurrency for Many-core Chip Design," ACM Transactions on Modeling and Performance Evaluation of Computing Systems (TOMPECS), vol. 2, no. 2, pp. 9:1-9:25, Apr. 2017.

[4] D. Wang and X.-H. Sun, "APC: A Novel Memory Metric and Measurement Methodology for Modern Memory System", in IEEE Transactions on Computers, vol. 63, no. 7, pp. 1626-1639, July 2014

[5] X.-H. Sun and D. Wang, "Concurrent Average Memory Access Time," IEEE Computer, Vol.47, no.5, pp.74-80, May 2014.

Five Other Related Significant Products

[1] Y. Liu and X.-H. Sun, "CaL: Extending Data Locality to Consider Concurrency for Performance Optimization," IEEE Transactions on Big Data. (Accepted)

[2] A. Kougkas, H. Eslami, R. Thakur, W. Group and X.-H. Sun, "Rethinking Key Value Store for Parallel I/O Optimization," in International Journal of High Performance Applications, vol. 31, no. 4, pp. 335-356, 2017
[3] Shuibing He, Yang Wang, and Xian-He Sun, "Boosting Parallel File System Performance via Heterogeneity-Aware Selective Data Layout," in IEEE Transactions on Parallel and Distributed Systems (TPDS), vol. 27, no. 9, pp. 2492-2505, Sept. 2016.
[4] D. Zhao, N. Liu, D. Kimpe, R. Ross, X.-H. Sun, and I. Raicu, "Towards Exploring Data-Intensive Scientific Applications at Extreme Scales through Systems and Simulations," in IEEE Transactions on Parallel and Distributed Systems (TPDS), vol. 27, no. 6, pp. 1824-1837, June 2016.
[5] B. Xu, W. Zhang, X.-H. Sun, and Y. Wang, "A memory-driven scheduling scheme and optimization for concurrent execution in GPU," Journal of Cluster Computing, vol. 19, pp2241-2250, 2016.

Synergistic Activities

Awards and Honors

- The Office of Naval Research (ONR) & The American Society for Engineering Education (ASEE*), Certificate of Recognition* award, 1999, The IEEE Computer Society Golden Core Award, IEEE Computer Society, 2017, Meritorious Service Certificate, IEEE Computer Society, 2016, ACM SIG Governing Board ACM Service Award, 2014. Best Paper Award, IEEE ISPA 2016, ACM SIGSIM PADS 2015, IEEE ISPA2011, ICPP01, 2001. Best Poster Award, SC03, 2003, Best Paper Finalist, SC08, 2008, Sigma Xi senior research award, 2009. IEEE CS Distinguished Visitor, 2001-2003.

Conference Organizing

- Chairman and Member of Program and Steering Committee: for more than twenty international conferences and workshops, including serving as the general chairman of ACM/IEEE IPDPS 2016, ACM/IEEE CCGrid 2014.

Publication Editorships

- Associate Editor-in-Chief (AEIC): IEEE Trans. on Parallel and Distributed Systems (TPDS), Editorial Board: TPDS (2010-2014), *Journal of Parallel and Distributed Computing* (2006-2012), *Journal of Web Services Research* (since 2006), *Journal of Performance Evaluation and Modeling for Computer Systems* (since 1997), *International Journal of High Performance Computing and Networking* (since 2003), *International Journal of Grid and Utility Computing* (since 2003)

Grant Review

- NSF Panelist: ANIR, ACIR, CCF, ITR, SBIR/STTR, CNS; Department of Energy; NASA; Natural Sciences and Engineering Research Council of Canada; Louisiana Board of Regents; University Grants Committee of Hong Kong, Hong Kong Research Grants Council, AAAS

Member-ship

- Member: IEEE (**Fellow** since 2012), ACM (**Senior Member** since 2009), IEEE-CS, New York Academy of Sciences, PHI KAPPA PHI, Sigma Xi

Jeff Wereszczynski, Ph.D. (http://www.iit.edu/∼jwereszc)

Biographical Sketch

Professional Preparation

Rensselaer Polytechnic Institute, Troy NY	Physics	B.S.	2004
University of Michigan, Ann Arbor, Ann Arbor MI	Biophysics	Ph.D.	2008
University of California, San Diego, San Diego CA	Chemistry	Postdoc	2008-2013

Appointments

2013-Present Assistant Professor, Department of Physics, Illinois Institute of Technology

Publications

Five Publications Most Closely Related to the Proposed Project:

1. S. Bowerman, A. S. J. B. Rana, A. Rice, G. H. Pham, E. R. Strieter, and J. Wereszczynski. Determining Atomistic SAXS Models of Tri-Ubiquitin Chains from Bayesian Analysis of Accelerated Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, 13(6):2418–2429, Jun 2017
2. A. Rice and J. Wereszczynski. Probing the disparate effects of arginine and lysine residues on antimicrobial peptide/bilayer association. *Biochimica et Biophysica Acta – Biomembranes*, 1859(10):1941–1950, 10 2017
3. S. Bowerman and J. Wereszczynski. Effects of macroH2A and H2A.Z on nucleosome structure and dynamics as elucidated by molecular dynamics simulations. *Biophysical Journal*, 110(2):327–337, 2016
4. A. W. Jacobitz, E. B. Naziga, S. W. Yi, S. A. McConnell, R. Peterson, M. E. Jung, R. T. Clubb, and J. Wereszczynski. The "Lid" in the Streptococcus pneumoniae SrtC1 Sortase Adopts a Rigid Structure that Regulates Substrate Access to the Active Site. *Journal of Physical Chemistry B*, 120(33):8302–8312, Aug 2016
5. E. B. Naziga and J. Wereszczynski. Molecular mechanisms of the binding and specificity of streptococcus pneumoniae sortase c enzymes for pilin subunits. In Press

Five Other Significant Publications:

1. S. Bowerman and J. Wereszczynski. Detecting allosteric networks using molecular dynamics simulation. *Methods in Enzymology*, 578:429–447, 2016
2. J. Wereszczynski and J. A. McCammon. Nucleotide-dependent mechanism of Get3 as elucidated from free energy calculations. *Proceedings of the National Academy of Sciences, USA*, 109(20):7759–7764, 2012
3. K. Kappel, J. Wereszczynski, R. T. Clubb, and J. A. McCammon. The binding mechanism, multiple binding modes, and allosteric regulation of Staphylococcus aureus Sortase A probed by molecular dynamics simulations. *Protein Science*, 21(12):1858–1871, Dec 2012
4. J. Wereszczynski and J. A. McCammon. Using Selectively Applied Accelerated Molecular Dynamics to Enhance Free Energy Calculations. *Journal of Chemical Theory and Computation*, 6:3285–3292, Nov 2010

5. J. Wereszczynski and J. A. McCammon. Statistical mechanics and molecular dynamics in evaluating thermodynamic properties of biomolecular recognition. *Quarterly Reviews of Biophysics*, 45(1):1–25, Feb 2012

Synergistic Activities

1. XSEDE "Campus Champion." Responsibile for interfacing with IIT community to promote usage and become familiar with XSEDE resources.
2. Member of the XSEDE Resource Allocation Committee. This committee meets quarterly to review supercomputer allocation requests for the NSF sponsored Extreme Science and Engineering Discovery Environment (XSEDE) project.
3. Mentor for six community college students from the College of DuPage over the summers of 2015-2017. These students each performed ten week summer internships in computational biophysics, which involved learning how to setup, perform, and analyze simulations. Students have gone on to
4. Recipient of NSF CAREER Award (2016). Recipient of NIH Career Transition Award (K22, 2013). Recipient of NIH Ruth L. Kirschstein Postdoctoral Fellowship (F32, 2010). Recipient of Rackham Reagents Fellowship (2004).

NORMAN G. LEDERMAN
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Illinois Institute of Technology
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PROFESSIONAL PREPARATION

Institution	Location	Major	Degree	Year
Bradley University	Peoria, IL	Biology	B.S.	1971
New York University	New York, NY	Biology	M.S.	1973
Bradley University	Peoria, IL	Secondary Education	M.S.	1977
Syracuse University	Syracuse, NY	Science Education	Ph.D.	1983

APPOINTMENTS

2001 – Present	Professor and Chair, Department of Mathematics and Science Education, Illinois Institute of Technology, Chicago, IL
1997 – 2001	Professor of Science and Mathematics Education and Director of the Academy for Excellence in Science and Mathematics Education, Oregon State University, Corvallis, OR
1991 – 1997	Associate Professor, with Tenure, of Science and Mathematics Education, Oregon State University, Corvallis, OR
1985 – 1991	Assistant Professor of Science and Mathematics Education, Oregon State University, Corvallis, OR
1984 – 1985	Assistant Professor of Teacher Education, State University of New York at Albany, Albany, NY
1979 – 1981	Biology Teacher, North Syracuse (NY) High School
1974 – 1979	Biology Teacher, Eureka (IL) High School
1979 – 1982	College Biology Instructor, Onondaga Community College, Syracuse, NY
1976 – 1979	College Biology Instructor, Illinois Central College, East Peoria, IL

PUBLICATIONS RELATED TO THE PROPOSED PROJECT

1. Lederman, N. G. (1992). Students' and teachers' conceptions of the nature of science: A review of the research. *Journal of Research in Science Teaching, 29*(4), 331-359.

2. Lederman, N.G., Sweeney, J.K., & Bell, R.L. (2004) *Constructing science in elementary classrooms.* New York: Allyn and Bacon.

3. Lederman, N.G., Abd-El-Khalick, F., Bell, R.L., & Schwartz, R.S. (2002). Views of nature of science questionnaire: Toward valid and meaningful assessment of learners' conceptions of nature of science. *Journal of Research in Science Teaching*, *39*(6), 497-521.

4. Flick, L., & Lederman, N.G. (2004). *Scientific inquiry and nature of science: Implications for Teaching, learning, and teacher education*. The Netherlands: Kluwer Academic Publishers.

5. Lederman, N.G. (2007). Nature of science: past, present, and future. In S.K. Abell & N.G. Lederman (Editors), *Handbook of research on science education* (pp. 831-880). Mahwah, NJ: Lawrence Erlbaum Associates.

OTHER SIGNIFICANT PUBLICATIONS

1. Lederman, N. G. (1999). Teachers' understanding of the nature of science and classroom practice: Factors that facilitate or impede the relationship. *Journal of Research in Science Teaching*, *36*(8), 916-929.

2. Lederman, N.G, Lederman, J.S. (2012). Nature of scientific knowledge and scientific inquiry: Building capacity through professional development. In B.J. Fraser, K. G. Tobin, & C. J. McRobbie (Eds.), *Second international handbook of science education*. (pp. 335-360). New York, NY: Springer.

3. Lederman, N.G., Antink, A., & Bartos, S. (2013). Nature of science, scientific inquiry, and socio-scientific issues arising from genetics: A pathway to developing a scientifically literate citizenry. *Science and Education*, *22*(4)**,** (pp. 285-302). New York, NY: Springer.

SYNERGISTIC ACTIVITIES

- Co-Principal Investigator (with Rob Bonichsen and Barbara Crawford), Project Mammoth Park, National Science Foundation (98-19633), $809,282, 1999-2002.

- Principal Investigator, Inquiry, Context, and Nature of Science: Project ICAN, National Science Foundation (99-11734), $2,070,432, 2000-2004.

- Has served as Director of Teacher Education for the National Science Teachers Association (NSTA), Director of the Northwest Region of the Association for the Education of Teachers in Science (AETS), and President and Board of Directors of NSTA, AETS, National Association for Research in Science Teaching (NARST), and the School Science and Mathematics Research Association. Past president of AETS and the Oregon Educational Research Association.

- Co-Editor (with M. Niess), School Science and Mathematics, 1996-2001 and Editorial Board Member (Current and Previous): American Educational Research Journal, Journal of Science Teacher Education, Journal of Elementary Science Education, Journal of Research in Science Teaching, Science and Education, Science Education.

Kiah Wah Ong

Professional Preparation

Institution	Location	Major	Degree	Year
University of Malaya	Kuala Lumpur, Malaysia	mathematics	BSc	2004
Universiti Tunku Abdul Rahman	Kuala Lumpur, Malaysia	mathematics	MMath	2010
Indiana University	Bloomington, IN	mathematics	PhD	2017

Appointments

2017–present	Lecturer, Department of Applied Mathematics, Illinois Institute of Technology
2011–2017	Associate Instructor, Department of Mathematics, Indiana University
2010–2011	Lecturer, Universiti Tunku Abdul Rahman
2006–2008	Assistant Lecturer, Universiti Tunku Abdul Rahman
2004–2006	Mathematics Teacher, Chong Hwa Independent High School

Publications

[1] K.W.Ong, *Dynamic transitions of generalized Kuramoto-Sivashinsky equation*, Discrete Contin. Dyn. Syst. Ser. B, **21** (2016), no. 4, 1225-1236, DOI 10.3934/dcdsb.2016.21.1225.

[2] L.Li and K.W.Ong, *Dynamic transitions of generalized Burgers equation*, J. Math. Fluid Mech, **18** (2016), no. 1, 89-102, DOI 10.1007/s00021-015-0240-7.

[3] K.W.Ong, S.L.Tan and Y.E.Tu, *Integral operators and univalent functions*, Tamkang J. Math **43** (2012), no. 2, 215-221, DOI: http://dx.doi.org/10.5556/j.tkjm.43.2012.630.

[4] L.Li, M.Hernandez, K.W.Ong, *Stochastic attractor bifurcation for the two-dimensional Swift-Hohenberg equation*, Math Methods Appl Sci, to appear.

[5] M.Cai, M.Hernandez, K.W.Ong and S.Wang, *Baroclinic Instability and Transitions in a Two-Layer Quasigeostrophic Channel Model*, submitted, arXiv:1705.07989.

Synergistic Activities

[1] Planning Committee Member, Preparing Future Faculty Conference, Indiana University, 2015-2016.

[2] Volunteer for Indiana University Science Fest 2015 Outreach Event.

[3] Faculty advisor for Actuary Today, Universiti Tunku Abdul Rahman, Malaysia, 2010-2011. The 2011 Actuary today is an inaugural two days event design to illustrate the role of actuaries in insurance, and to provide information on current actuarial employment outlook in Malaysia.

SUMMARY PROPOSAL BUDGET

YEAR 1

FOR NSF USE ONLY		
PROPOSAL NO.	DURATION (months) Proposed	Granted
AWARD NO.		

ORGANIZATION
Illinois Institute of Technology

PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR
Fred Hickernell

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-months CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Fred J Hickernell - PI**	0.00	0.00	0.50	**8,905**	
2. **Norman G Lederman - Senior Personnel**	0.00	0.00	0.60	**10,000**	
3. **David D Minh - Co-PI**	0.00	0.00	0.50	**4,966**	
4. **Jeffery M Wereszczynski - Co-PI**	0.00	0.00	0.50	**5,268**	
5.					
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00	**0**	
7. (**4**) TOTAL SENIOR PERSONNEL (1 - 6)	0.00	0.00	2.10	**29,139**	
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	0.00	**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)				**29,139**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**2,301**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**31,440**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS)				**6,000**	
2. INTERNATIONAL				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **65,000**					
2. TRAVEL **7,000**					
3. SUBSISTENCE **400**					
4. OTHER **0**					
TOTAL NUMBER OF PARTICIPANTS (**11**) TOTAL PARTICIPANT COSTS				**72,400**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**2,000**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**2,000**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**111,840**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **MTDC (Rate: 53.0000, Base: 39440)**					
TOTAL INDIRECT COSTS (F&A)				**20,903**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**132,743**	
K. SMALL BUSINESS FEE				**0**	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				**132,743**	

M. COST SHARING PROPOSED LEVEL $ **0** AGREED LEVEL IF DIFFERENT $

PI/PD NAME
Fred Hickernell

ORG. REP. NAME*
Domenica Pappas

FOR NSF USE ONLY		
INDIRECT COST RATE VERIFICATION		
Date Checked	Date Of Rate Sheet	Initials - ORG

 ***ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET**

SUMMARY PROPOSAL BUDGET

YEAR 2

FOR NSF USE ONLY		
PROPOSAL NO.	DURATION (months) Proposed	Granted
AWARD NO.		

ORGANIZATION
Illinois Institute of Technology

PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR
Fred Hickernell

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-months CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Fred J Hickernell - PI**	0.00	0.00	0.50	**9,261**	
2. **Norman G Lederman - Senior Personnel**	0.00	0.00	0.57	**10,000**	
3. **David D Minh - Co-PI**	0.00	0.00	0.50	**5,165**	
4. **Xian-He Sun - Co-PI**	0.00	0.00	0.50	**11,084**	
5. **Jeffery M Wereszczynski - Co-PI**	0.00	0.00	0.50	**5,478**	
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00	**0**	
7. (**5**) TOTAL SENIOR PERSONNEL (1 - 6)	0.00	0.00	2.57	**40,988**	
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	0.00	**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)				**40,988**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**3,239**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**44,227**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS)				**6,240**	
2. INTERNATIONAL				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **90,480**					
2. TRAVEL **7,000**					
3. SUBSISTENCE **416**					
4. OTHER **0**					
TOTAL NUMBER OF PARTICIPANTS (**15**) TOTAL PARTICIPANT COSTS				**97,896**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**2,080**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**2,080**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**150,443**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **MTDC (Rate: 53.0000, Base: 52547)**					
TOTAL INDIRECT COSTS (F&A)				**27,850**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**178,293**	
K. SMALL BUSINESS FEE				**0**	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				**178,293**	

M. COST SHARING PROPOSED LEVEL $ **0** AGREED LEVEL IF DIFFERENT $

PI/PD NAME
Fred Hickernell

ORG. REP. NAME*
Domenica Pappas

FOR NSF USE ONLY		
INDIRECT COST RATE VERIFICATION		
Date Checked	Date Of Rate Sheet	Initials - ORG

 ***ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET**

SUMMARY PROPOSAL BUDGET

YEAR 3

FOR NSF USE ONLY		
PROPOSAL NO.	DURATION (months) Proposed	Granted
AWARD NO.		

ORGANIZATION
Illinois Institute of Technology

PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR
Fred Hickernell

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-months CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Fred J Hickernell - PI**	0.00	0.00	0.50	**9,632**	
2. **Norman G Lederman - Senior Personnel**	0.00	0.00	0.55	**10,000**	
3. **David D Minh - Co-PI**	0.00	0.00	0.50	**5,372**	
4. **Xian-He Sun - Co-PI**	0.00	0.00	0.50	**11,527**	
5. **Jeffery M Wereszczynski - Co-PI**	0.00	0.00	0.50	**5,698**	
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00	**0**	
7. (**5**) TOTAL SENIOR PERSONNEL (1 - 6)	0.00	0.00	2.55	**42,229**	
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	0.00	**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)				**42,229**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**3,336**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**45,565**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS)				**6,490**	
2. INTERNATIONAL				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **101,670**					
2. TRAVEL **7,000**					
3. SUBSISTENCE **433**					
4. OTHER **0**					
TOTAL NUMBER OF PARTICIPANTS (**16**) TOTAL PARTICIPANT COSTS				**109,103**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**0**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**0**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**161,158**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **MTDC (Rate: 53.0000, Base: 52055)**					
TOTAL INDIRECT COSTS (F&A)				**27,589**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**188,747**	
K. SMALL BUSINESS FEE				**0**	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				**188,747**	

M. COST SHARING PROPOSED LEVEL $ **0** AGREED LEVEL IF DIFFERENT $

PI/PD NAME
Fred Hickernell

ORG. REP. NAME*
Domenica Pappas

FOR NSF USE ONLY		
INDIRECT COST RATE VERIFICATION		
Date Checked	Date Of Rate Sheet	Initials - ORG

 ***ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET**

SUMMARY PROPOSAL BUDGET

Cumulative

FOR NSF USE ONLY		
PROPOSAL NO.	DURATION (months) Proposed	Granted
AWARD NO.		

ORGANIZATION: **Illinois Institute of Technology**

PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR: **Fred Hickernell**

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-months CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Fred J Hickernell - PI**	0.00	0.00	1.50	**27,798**	
2. **Norman G Lederman - Senior Personnel**	0.00	0.00	1.72	**30,000**	
3. **David D Minh - Co-PI**	0.00	0.00	1.50	**15,503**	
4. **Xian-He Sun - Co-PI**	0.00	0.00	1.00	**22,611**	
5. **Jeffery M Wereszczynski - Co-PI**	0.00	0.00	1.50	**16,444**	
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00	**0**	
7. (**5**) TOTAL SENIOR PERSONNEL (1 - 6)	0.00	0.00	7.22	**112,356**	
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	0.00	**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)				**112,356**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**8,876**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**121,232**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS)				**18,730**	
2. INTERNATIONAL				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **257,150**					
2. TRAVEL **21,000**					
3. SUBSISTENCE **1,249**					
4. OTHER **0**					
TOTAL NUMBER OF PARTICIPANTS (**42**) TOTAL PARTICIPANT COSTS				**279,399**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**4,080**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**4,080**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**423,441**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS (F&A)				**76,342**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**499,783**	
K. SMALL BUSINESS FEE				**0**	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				**499,783**	

M. COST SHARING PROPOSED LEVEL $ **0** AGREED LEVEL IF DIFFERENT $

PI/PD NAME: **Fred Hickernell**

ORG. REP. NAME*: **Domenica Pappas**

FOR NSF USE ONLY		
INDIRECT COST RATE VERIFICATION		
Date Checked	Date Of Rate Sheet	Initials - ORG

C ***ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET**

BUDGET JUSTIFICATION

Senior Personnel[1]
Hickernell, Lederman, Minh, Sun, and Wereszczynski are each budgeted for roughly half a month of summer salary per year. They will each lead certain initiatives as detailed in the Management and Coordination Plan.

Fringe Benefits
IIT's federally negotiated fringe benefit rates are: faculty academic salary, 23.8%; faculty summer salary, 7.9%; staff salary, 24.5%; and student stipends, 0.0%.

Travel
The PI will travel to the NSF PIs meeting each year. Co-PIs and Senior Personnel will travel to report the results arising from this project at conferences.

Participant Support
Summer CoD students will be paid stipends of $5000 each. We expect to recruit four students in 2019, six students in 2010, and six students in 2021. CISC Summer Undergraduate Fellows will also be paid stipends of $5000 each. We expect to recruit two students in 2019, three students in 2010, and three students in 2021. CISC Summer Graduate Fellows will be paid stipends of $7000 each. We expect to recruit five students in 2019, six students in 2010, and seven students in 2021.

Several hundred dollars is budgeted each year for weekly lunchtime discussions for the summer CoD students.

Summer CoD students and the CISC Fellows program who achieve significant results may apply for travel grants to (partially) support their attendance at conferences to present their work. Each year $7000 will be available to support participant travel.

Other Direct Costs
Materials and Supplies
Materials will be developed and printed to recruit participants for the summer computational science course, the summer research experience for CoD students, and the CISC fellowships. Certain minor software purchases may be needed for these activities.

Indirect Costs
IIT's current federally negotiated indirect cost rate (agreement date 03/02/2017) is 53% of modified total direct costs (MTDC). MTDC include all salaries and wages, fringe benefits, materials, supplies, services, travel and up to the first $25,000 of each subaward. MTDC excludes equipment, capital expenditures, student tuition, rental costs of off-site facilities, as well as the portion of each subaward in excess of $25,000.

	Y1	Y2	Y3	Total
Direct Costs	$111,840	$150,443	$161,158	$423,441
Indirect Costs	$20,903	$27,850	$27,589	$76,342
Total Costs	$132,743	$178,293	$188,747	$499,783
Modified Base	*$39,440*	*$52,547*	*$52,055*	*$144,042*

[1] For purposes of NSF PAPPG section II.C.2.g(i)(a), the term "year" at Illinois Institute of Technology refers to IIT's fiscal year (June 1 – May 31)

Current and Pending Support

(See PAPPG Section II.C.2.h for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Fred Hickernell	Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: CyberTraining: CIC: Cross-Disciplinary Education for Next-Generation Computational Scientists (this proposal)

Source of Support: NSF

Total Award Amount: $ 499,783 Total Award Period Covered: 08/01/18 - 07/31/21

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.50

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Theoretically Justified Adaptive Numerical Algorithms for Integration and Approximation

Source of Support: NSF

Total Award Amount: $ 429,160 Total Award Period Covered: 07/01/18 - 06/30/21

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 2.00

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Stable, Efficient, Adaptive Algorithms for Approximation and Integration

Source of Support: NSF

Total Award Amount: $ 270,000 Total Award Period Covered: 08/01/15 - 07/31/18

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.50

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:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See PAPPG Section II.C.2.h for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Sou-Cheng Choi	Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: CyberTraining: CIC: Cross-Disciplinary Education for Next-Generation Computational Scientists (this proposal)

Source of Support: NSF

Total Award Amount: $ 499,783 Total Award Period Covered: 08/01/18 - 07/31/21

Location of Project: Illinois Institute of Technology

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: Theoretically Justified Adaptive Numerical Algorithms for Integration and Approximation

Source of Support: NSF

Total Award Amount: $ 429,160 Total Award Period Covered: 07/01/18 - 06/30/21

Location of Project: Illinois Institute of Technology

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: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See PAPPG Section II.C.2.h for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: David Minh	Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: CyberTraining: CIC: Cross-Disciplinary Education for Next-Generation Computational Scientists (this proposal)

Source of Support: NSF

Total Award Amount: $ 499,783 Total Award Period Covered: 08/01/18 - 07/31/21

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.50

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Entropy for End-Point and FFT-Based Binding Free Energy Calculations

Source of Support: NIH

Total Award Amount: $ 1,475,706 Total Award Period Covered: 07/01/18 - 06/30/22

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 1.00

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Novel biochemical strategies of ion transport and electron transfer in the essential bacterial respiratory complex Na+-NQR

Source of Support: NIH

Total Award Amount: $ 1,388,166 Total Award Period Covered: 07/01/18 - 06/30/23

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 1.00

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Gibbs Sampling of Multimeric Proteins

Source of Support: NSF

Total Award Amount: $ 408,645 Total Award Period Covered: 06/01/18 - 05/31/21

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 1.00

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Novel Small Molecule Inhibitors for Targeted Cancer Therapy: In Vitro and In Silico Identification of Molecular Targets

Source of Support: NIH

Total Award Amount: $ 138,688 Total Award Period Covered: 04/01/18 - 03/31/20

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Summ: 0.30

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See PAPPG Section II.C.2.h for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: David Minh

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Sound-stage Virtual Screening Based on Implicit Ligand Theory

Source of Support: NIH

Total Award Amount: $ 337,373 Total Award Period Covered: 09/25/15 - 08/31/18

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.77

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:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See PAPPG Section II.C.2.h for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Xian-He Sun	Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: CyberTraining: CIC: Cross-Disciplinary Education for Next-Generation Computational Scientists (this proposal)

Source of Support: NSF

Total Award Amount: $ 499,783 Total Award Period Covered: 08/01/18 - 07/31/21

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.50

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: SPX: Collaborative Research: Pace Data Transfer: Layered Architecture Matching for Memory System Optimization

Source of Support: NSF

Total Award Amount: $ 499,999 Total Award Period Covered: 06/15/18 - 06/14/21

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 1.00

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: CSR: Small: IRIS: A unified data access framework for the merging of compute-centric and data-centric storage

Source of Support: NSF

Total Award Amount: $ 499,999 Total Award Period Covered: 05/01/18 - 04/30/21

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 1.00

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Eager: Collaborative Research: DiRecMR: Reconciling the Dichotomy of MapReduce for Efficient Speculation and Resilience

Source of Support: NSF

Total Award Amount: $ 80,038 Total Award Period Covered: 08/01/17 - 07/31/18

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 1.00

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: CRI: II-NEW: MYSTIC: prograMmable sYstems reSearch Testbed to explore a stack-wIde adaptive system fabriC

Source of Support: NSF

Total Award Amount: $ 1,000,000 Total Award Period Covered: 07/15/17 - 06/30/20

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Summ: 0.50

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See PAPPG Section II.C.2.h for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Xian-He Sun	Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: CRI: II-NEW: A Big Data Professing Infrastructure for Smart Energy Systems

Source of Support: NSF

Total Award Amount: $ 400,000 Total Award Period Covered: 08/01/17 - 07/31/20

Location of Project: Illinois Institute of Technology

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: Utilizing Memory Parallelism for High Performance Data Processing

Source of Support: NSF

Total Award Amount: $ 191,000 Total Award Period Covered: 08/01/15 - 07/31/18

Location of Project: Illinois Institute of Technology

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: CSR: Small: Empower Data-Intensive Computing: The Integrated Data Management Approach

Source of Support: NSF

Total Award Amount: $ 416,000 Total Award Period Covered: 09/01/15 - 08/31/18

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 1.00

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: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See PAPPG Section II.C.2.h for guidance on information to include on this form.)

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: Jeffery Wereszczynski

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: CyberTraining: CIC: Cross-Disciplinary Education for Next-Generation Computational Scientists (this proposal)

Source of Support: NSF

Total Award Amount: $ 499,783 Total Award Period Covered: 08/01/18 - 07/31/21

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.50

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Science Excellency through Residency (SER)

Source of Support: National Louis University; Department of Education

Total Award Amount: $ 99,231 Total Award Period Covered: 10/01/17 - 09/30/18

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 1.00 Sumr: 0.00

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Collaborative Research: Molecular Mechanism of Heme Extraction by IsdH

Source of Support: NSF

Total Award Amount: $ 250,000 Total Award Period Covered: 08/01/17 - 07/31/20

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.50

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Probing the Structure/Function/ Dynamics Relationship in Biomolecuar Complexes With Multiscale Computational Techniques

Source of Support: NIH

Total Award Amount: $ 1,615,843 Total Award Period Covered: 09/01/16 - 08/31/21

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 1.00 Sumr: 0.50

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: CAREER: The Effects of Post-Translational Modifications and Histone Variants on Chromatin Fiber Dynamics

Source of Support: NSF

Total Award Amount: $ 789,893 Total Award Period Covered: 06/01/16 - 05/31/21

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Summ: 1.00

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*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See PAPPG Section II.C.2.h for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Jeffery Wereszczynski

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Molecular Simulations of the Structure/Function Relationship Histone Variants

Source of Support: NIH

Total Award Amount: $ 324,753 Total Award Period Covered: 04/01/15 - 03/31/18

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 1.00

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: The Biophysics Collaborative Access Team

Source of Support: NIH

Total Award Amount: $ 6,353,675 Total Award Period Covered: 04/01/16 - 12/31/20

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 1.00

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: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See PAPPG Section II.C.2.h for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Norman Lederman	Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: CyberTraining: CIC: Cross-Disciplinary Education for Next-Generation Computational Scientists (this proposal)

Source of Support: NSF

Total Award Amount: $ 499,783 Total Award Period Covered: 08/01/18 - 07/31/21

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.57

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: REU Site: Summer Engineering Research Experiences in Diabetes for Undergraduates

Source of Support: NSF

Total Award Amount: $ 322,510 Total Award Period Covered: 04/01/15 - 03/31/18

Location of Project: Illinois Institute of Technology

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.25

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:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See PAPPG Section II.C.2.h for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Kiah Ong

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: CyberTraining: CIC: Cross-Disciplinary Education for Next-Generation Computational Scientists (this proposal)

Source of Support: NSF

Total Award Amount: $ 499,783 Total Award Period Covered: 08/01/18 - 07/31/21

Location of Project: Illinois Institute of Technology

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:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

 USE ADDITIONAL SHEETS AS NECESSARY

Facilities, Equipment and Other Resources

Sou-Cheng Terrya Choi (co-PI), Research Associate Professor of Applied Mathematics, will join the regular management team meetings, in addition to working remotely. She is employed full-time outside academia but will contribute to the project on a volunteer basis. No salary is requested for her, but her travel related to the project will be supported.

Kiah-Wah Ong (Senior Personnel), Lecturer in Applied Mathematics, will contribute to the project as a regular faculty member, whose summer teaching is supported by tuition income.

April Welch (Internal Collaborator), Associate Vice-President of Strategic Initiatives, is supporting this project through the resources of the Admissions Office. No salary is requested for her.

All Illinois Tech faculty, PhD students, and visitors have offices provided at Illinois Tech. Summer CoD students and CISC Fellows will be provided shared work areas. In addition to offices and conference rooms provided by the home departments of the (co-)PIs and senior personnel, the Center for Interdisciplinary Scientific Computation (CISC) also has office and meeting space available for this project.

CISC has a 256-core cluster named von Neumann funded by the College of Science. An increase in the number of cores within 2018 is likely. Von Neumann is available available to all Illinois Tech research faculty and is centrally managed by Illinois Tech Office of Technology (OTS) Services.

Sun directs the Scalable Computing Software (SCS) Laboratory at IIT. The computing facilities at the SCS Laboratory include a 64-node Sun Microsystems ComputeFarm, a 17-node Dell cluster, a 14-node IBM Linux-based cluster, a 12-node Cray XD1 supercomputer, a 72-processor SiCortex cluster, and other advanced computing and communication facilities. The Sun ComputeFarm is connected fully with Gigabit Ethernet and partially with InfiniBand.

Sun and his group also have access to the Chameleon Cloud platform. Chameleon is consisted with two clusters located in Texas Advanced Computing Center (TACC) at Texas and University of Chicago. Chameleon has 291 compute nodes fully connected with 10Gbps Ethernet network, and 41 of them are also double connected via Fourteen Data Rate (FDR) InfiniBand (56Gbps).

Wereszczynski's lab has exclusive access to a cluster that has 12 compute nodes, each of which is comprised of 16 CPU cores running at 2.6 GHz, 64 GB of RAM, and four NVIDIA GTX 1080 GPU cards. The cluster has an infiniband interconnect, a head node, and 100 TB of storage. This lab also has access to desktops with NVIDIA GTX 980, 1080, and 1080 Ti GPUs.

Illinois Tech is connected to the Open Science Grid through its own GridIIT. Wereszczynski is the campus champion for XSEDE. He can assist research groups who wish to take advantage of that facility apply for time.

Illinois Tech is partnering with our advisory board, which is comprised of scientists at College of DuPage, Argonne National Laboratory, and Fermilab (see Sect. 5). Argonne and Fermilab have large-scale computational facilities that our students will be able to access when involved in projects with these two laboratories.

Illinois Tech has site licenses for Mathematica, MATLAB, SAS, and JMP. Other open source software is also installed in our research and teaching laboratories.

Illinois Tech's university library provides access to journals, research monographs, and databases, either on-site, online, or via inter-library loan.

Illinois Tech was listed on the National Federal Register of Historic Places in 2005. The proposed research activities will not make any physical changes to Illinois Tech's campus and buildings.

Data Management Plan

This plan will make certain that the data produced during the period of this project is appropriately managed to ensure its usability, access, and preservation. The data produced by the proposed project will consist of CI theory, new software, good practices for CI training, course materials, and program guidelines.

Publications and Lectures. The goal of this project is training CICs and CIUs to contribute to research, and we expect original research to arise in the training process. The participants, including (co-)PIs, senior personnel, external advisors, and students, will disseminate the results of their theoretical discoveries, their computational investigations, and their new insights into CI education as early as appropriate in the form of peer-reviewed journal articles, conference abstracts, and lectures at various conferences and institutions. Authorship will accurately reflect the contributions of those involved. Students will be particularly encouraged to publish their work. When allowed by publishers, pre-prints of publications will be posted on arXiv.

Software. Software packages of libraries resulting from this project will be stored on public repositories, such as GitHub, and made available for adoption and improvement by others. This is the practice already with our Guaranteed Integration Library (GAIL) [7] and many major software libraries developed by others. Software may also be published through ACM-TOMS and similar journals. Our software developments will be publicized through colloquium and conference talks and e-newsletters such as the NA-Digest.

Course Materials. Lecture notes and example code developed for our key courses, including the summer computational science course, the crash course for CoD students, the new professional practices course, the undergraduate parallel and distributed computing course, and the large-scale computation course, will be made available on public repositories such as GitHub or Google Drive.

Web Publication. The CISC website will serve as an index to the data generated by this project. This will include pointers to publications arising from this project, software arising out of this project, and course materials, as mentioned above.

We find that sample or template code, e.g., demonstrating how to run a job on a cluster, how to run a job utilizing multiple cores, or how to run a job based on a specialized package, are useful teaching devices. We will store these samples on public repositories and provide pointers to them on the CISC website.

Information about to our initiatives, including goals, policies, and benchmarks will also be available on the CISC website.

The best practices that we discover disseminated on public computational science forums, such as the newly established Better Scientific Software [5].

We will fully comply with all applicable guidelines and policies on model and data sharing as mandated or recommended by NSF. This Data Management Plan addresses NSF's policy on the dissemination and sharing of research results within a reasonable time. In accordance with this policy, this plan does not include preliminary analyses (including raw data), drafts of scientific papers, plans for future research, peer reviews, or communications with colleagues.

College of DuPage

Ann E. Rondeau, President

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Glen Ellyn, Illinois 60137-6599

(630) 942-2200 *phone*
(630) 942-2869 *fax*

rondeau@cod.edu
cod.edu

February 8, 2018

To Whom It May Concern:

If the proposal submitted by Prof. Fred J. Hickernell and co-PIs entitled "Cyber Training: CIC: Cross-Disciplinary Education for Next-Generation Computational Scientists" is selected for funding by NSF; College of DuPage and specifically Dr. Tom Carter will collaborate as detailed in the Project Description section of the proposal.

Sincerely,

Ann E. Rondeau

Dr. Ann E. Rondeau
President
College of DuPage
Vice Admiral, U.S. Navy (Ret.)

February 8, 2018

Burt Holzman
Asst. Division Head

Scientific Computing
P.O. Box 500, MS 234
Kirk Road and Pine Street
Batavia, Illinois 60510-5011
USA
Office: 630.840.5753
burt@fnal.gov

Attn: Fred Hickernell
Director, Center for Interdisciplinary Scientific Computation (CISC)
Illinois Institute of Technology

To whom it may concern:

If the proposal submitted by Prof. Fred J. Hickernell and co-PIs entitled "CyberTraining: CIC: Cross-Disciplinary Education for Next-Generation Computational Scientists" is selected for funding by NSF, it is my intent to collaborate as detailed in the Project Description section of the proposal.

Sincerely,

Dr. Burt Holzman
Assistant Division Head
Scientific Computing Division
Fermi National Accelerator Laboratory

Lois Curfman McInnes
Senior Computational Scientist

Mathematics and Computer Science Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439

630-252-5170
curfman@mcs.anl.gov

February 12, 2018

Re: **Letter of Collaboration**

To whom it may concern:

If the proposal submitted by Professor Fred J. Hickernell and co-PIs entitled "CyberTraining: CIC: Cross-Disciplinary Education for Next-Generation Computational Scientists" is selected for funding by NSF, it is my intent to collaborate as detailed in the Project Description section of the proposal.

Sincerely,

Lois Curfman McInnes
Senior Computational Scientist
Mathematics and Computer Science Division
Argonne National Laboratory

April Welch
Associate Vice President for Strategic Initiatives
Director, Exelon Summer Institute
Director, Freelance Coder Camp
Illinois Institute of Technology, Enrollment
10 West 35rd Street, 9F7-1
Chicago, Illinois 60616

312-567-3196
welcha@iit.edu

ILLINOIS INSTITUTE OF TECHNOLOGY

February 12, 2018

To whom it may concern:

If the proposal submitted by Prof. Fred J. Hickernell and co-PIs entitled "CyberTraining: CIC: Cross-Disciplinary Education for Next-Generation Computational Scientists" is selected for funding by NSF, it is my intent to collaborate as detailed in the Project Description section of the proposal.

Sincerely,

April Welch
Associate Vice President for Strategic Initiatives

Management and Coordination Plan

The (co-)PIs, all of whom are from Illinois Tech, will serve together as the Management Team for this project:

- Fred J. Hickernell (PI), Professor of Applied Mathematics and Director of the Center for Interdisciplinary Scientific Computation (CISC),
- Sou-Cheng Choi (co-PI), Research Associate Professor of Applied Mathematics and Lead Researcher at Allstate,
- David Minh, Assistant Professor of Chemistry and Associate Director of CISC,
- Xian-He Sun, Distinguished Professor of Computer Science, and
- Jeff Wereszczynski, Assistant Professor of Physics.

The Management Team will meet bi-monthly to share progress of the project initiatives, discuss challenges that arise, and strategize on how to make our initiatives more effective.

The Management Team will be assisted by the following Illinois Tech colleagues:

- Norman Lederman (Senior Personnel), Distinguished Professor of Science Education,
- Kiaw Wah Ong (Senior Personnel), Lecturer in Mathematics, and
- April Welch (Internal Collaborator), Associate Vice-President of Strategic Initiatives.

They will meet with the whole Management Team or with individual (co-)PIs as needed.

As mentioned in Sect. 5 of the Project Description, an External Advisory Board will be formed, consisting of the following members:

- Dr. Tom Carter, Professor of Physics at College of DuPage (CoD),
- Dr. Lois Curfman McInnes, Senior Computational Scientist in the Mathematics and Computer Science Division at Argonne National Laboratory, and
- Dr. Burt Holzman, Assistant Director of the Scientific Computing Division at Fermi National Accelerator Laboratory (Fermilab).

The table below shows the persons responsible for each major task. The first person listed for each task takes the lead. The budget column lists the financial support from the proposed grant for each item, including materials and supplies (Mat), summer salaries (Sal), stipends (Sti), substinence (Sub), and travel (Tra). HSal denotes salary for Hickernell, and LSal, MSal, SSal, and WSal have analogous meanings. Budget entries "Tuition" are covered by the tuition received from enrolled students.

Task (with reference to the Project Description)		**Persons**	**Budget**
3.3	Summer computational science course		
	— Course design and content creation	Ong, Hickernell	HSal
	— Advertisement to prospective students	Welch, Ong	Mat
	— Instruction and supervision of TAs	Ong	Tuition
	— Evaluation	Lederman, Ong	LSal
3.4	Advertisement of our computational course offerings	Hickernell	Mat
3.4.1	Enriched existing computational science offerings		
	— Applied mathematics	Hickernell	HSal
	— Chemistry	Minh	MSal
	— Computer science	Sun	SSal
	— Physics	Wereszczynski	WSal
3.4.3	Professional practices for computational science course		
	— Course design and content creation	Hickernell, Choi	HSal
	— Instruction	Hickernell, Choi	Tuition

	— Evaluation	Lederman, Hickernell	LSal, HSal
3.4.4	Undergraduate parallel and distributed computing course		
	— Content revision	Sun	SSal
	— Instruction	CS faculty	Tuition
	— Evaluation	Lederman, Sun	LSal, SSal
3.4.5	Large-scale scientific computation course		
	— Content revision	Sun	SSal
	— Instruction	CS faculty	Tuition
	— Evaluation	Lederman, Sun	LSal, SSal
3.5	Research experiences for community college students		Sti
	— Recruiting students from CoD	Wereszczynski, Carter	WSal
	— Crash course design and instruction	Minh, Wereszczynski	MSal, WSal
	— Weekly lunchtime discussions	Wereszczynski	Sub
	— Evaluation	Lederman, Minh, Wereszczynski	LSal, MSal, WSal
3.6	CISC undergraduate and graduate summer fellowships		Sti
	— Identifying project opportunities in national labs and companies	Hickernell, Choi, Minh, Sun, Wereszczynski, Curfman McInnes, Holzman	HSal, MSal, SSal, WSal
	— Advertisement of opportunities	Hickernell, Minh	HSal, MSal
	— Selection of CISC Fellows	Hickernell, Choi, Minh, Sun, Wereszczynski	HSal, MSal, SSal, WSal
	— Concluding poster session for CISC Fellows and CoD students	Minh, Hickernell	MSal, HSal
	— Evaluation	Lederman, Hickernell	LSal, HSal
4.6	Attend PI meeting at the NSF	Hickernell	Tra
4.6	Publish findings in journals and online	Hickernell, Choi, Minh, Sun, Wereszczynski, Lederman, Ong	HSal, MSal, SSal, WSal, LSal
4.6	Share findings at conferences	Hickernell, Choi, Minh, Sun, Wereszczynski, Lederman, Ong	Tra, HSal, MSal, SSal, WSal, LSal
5	Organizing meetings of the Management Team and the External Advisory Board	Hickernell	HSal