REU Site: Bio-Grid Initiatives for Interdisciplinary Research and Education[☆]

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[☆]Extended from an earlier version that appeared in Proceedings of the Workshop on Education for High-Performance Computing (EduHPC), Nov. 15-20, 2015, Austin, TX.

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Abstract

Recently more and more universities have been incorporating HPC (High Performance Computing) in their computing curriculum [1]. The Bio-Grid REU (Research Experience for Undergraduates) Site offers undergraduate students interested or experienced in HPC a summer research opportunity to participate in projects that apply HPC in various life-science disciplines. The projects are associated with the *Bio-Grid Initiatives* conducted at the University of Connecticut. Training seminars are designed to equip students with background knowledge such as basic parallel programming, large-scale data analytics, and middleware support, *etc.*, as well as some ongoing projects using these computing methods. Students participate in several collaborative projects supported by a campus-wide computational and data grid. The REU project introduces such interdisciplinary research work to students in the early stage of their academic career to spark their interest. The project aims at preparing future software engineers to formalize and solve emerging life-science problems, as well as life-science researchers with a strong background in high-performance computing. The Bio-Grid REU Site was supported by the National Science Foundation from 08-10 and 12-14, with a website located at <http://biogrid.engr.uconn.edu/REU>

Keywords: HPC, Computational Biology, Grid and Cloud Computing

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1. Instruction

Research work in life sciences increasingly relies on globally distributed information and knowledge repositories. The quality and performance of future computing and storage infrastructure in support of such research depends heavily on the ability to exploit these repositories, to integrate these resources with local information processing environments in a flexible and intuitive way, and to support information extraction and analysis in a timely and on-demand manner.

With an ever-increasing throughput, the next-generation sequencing technologies have led to generate a large amount of DNA data, to the extent that in its first six months, next-generation sequencing outpaced what already have been generated in the past 21 years by old technologies [2]. This wealth of genomic information dramatically accelerates progress toward a comprehensive understanding of the genetic mechanisms involved in diverse biochemical processes pertinent to bioremediation, medicine, biotechnology and agriculture. Efficiency and accuracy of genetic sequence analysis are achieved by the use of diverse CPU-intensive bioinformatics tools and algorithms (*e.g.*, analysis of global similarities [3], domain and motif analysis [4], analysis of the relevant structural [5] and functional data). Running these tools on the rapidly growing data is a time-consuming process and needs high-throughput computations to get results in a timely fashion.

Modern HPC technology and infrastructures represent an emerging and expanding instrumentation, computing, information and storage platform that often allows geographically distributed resources, which are under distinct control, to be linked together in a transparent fashion [6, 7]. The power lays not only in the aggregate computing ability, data storage, and network bandwidth that can readily be brought to bear on a particular problem, but also on its ease of use. After research efforts in nearly two decades, computing infrastructures such as the grids and clouds have matured and been widely applied to computation-intensive applications, optimized storage of large-scale distributed data, and the intelligent use of these data [8, 9, 10].

UConn Bio-Grid Initiatives. The UConn *Bio-Grid Initiatives* aim at advancing the application of modern information technology and infrastructure to various life-science disciplines. The research activities center on the development and deployment of modern Grid and Cloud technologies toward an infrastructure for automated life-science information integration, extraction and analysis [11, 12, 13]. The computing infrastructure is based on a campus-wide computational and data Grid, an effort initiated in 2004. This infrastructure is supporting several collaborative, interdisciplinary research projects, led by our project staff from Schools of Engineering and Medicine. Also an ongoing effort is the development of general-purpose middleware support for the transfer of sensitive data. Educational programs associated with the Bio-Grid Initiatives include the development of new and re-development of current courses to incorporate inventions coming out of the research, a new cross-disciplinary *bio-computing* minor, as well as new degree tracks emphasizing the application of High-Performance Computing to different life-science disciplines. An annual scientific meeting, the *International Bio-Grid Workshop* has been held in conjunction with the research and educational activities since 2003 and has been serving as a major scientific venue for our research community.

Project Goals. This Bio-Grid REU Site is a 10-week summer site supporting ten undergrad students annually. Student participants are expected to have a sufficient background in computing or biological science and be interested in HPC. A series of training seminars, conducted by the project staff, is designed to equip students with preliminary background knowledge. The seminars introduce to students concepts about modern grid and cloud computing infrastructure and related information technology. Ongoing life-science research projects deploying the campus grid are presented to the students. The seminar series also include talks on research projects that are at the planning stage of being grid-enabled.

The Bio-Grid Initiatives are enriched in research, outreach and educational activities. Associated faculty members are enthusiastic about the REU Site to continue offering the opportunity for nation-wide undergraduate students to in-

volve in the various interdisciplinary activities. In addition to the faculty members, graduate students currently on the collaborative projects also participate in mentoring.

The REU goals with associated objectives, including learning outcomes for
65 students are as follows.

GOAL 1: Promote an interest in the interdisciplinary research work associated with the Bio-Grid initiatives by targeting NSF-targeted student participants - underrepresented minorities, students with disabilities, women, and veterans
70 from primarily NSF-targeted institutions in the early stages of their academic careers. Anticipated results/objectives follow.

1.1 Identify, recruit and receive at least 25% applications from NSF targeted students.

1.2 REU program will be made up of at least 30% NSF-targeted
75 students.

1.3 70% of REU students will be from targeted institutions (non-PhD-granting institutions).

1.4 100% of REU students will have completed sophomore or junior year of college.

80 1.5 Program will be made up of 50% life science students and 50% CSE students with an interest or course experience in HPC.

GOAL 2: Promote the acquisition of skills allowing computer scientists and biologists to function in an interdisciplinary working/research environment. Anticipated results/objectives follow.

85 2.1 Software engineering students will be introduced to methods to formalize and solve problems emerging from life-science disciplines.

2.2 Life-science students will be introduced to information processing techniques.

2.3 Students will value the importance of interdisciplinary knowledge.
90

2.4 Students will be able to apply the scientific method in hypothesis-driven research.

2.5 Students will be able to engage in self-directed research.

2.6 Students will be able to communicate research results in verbal
95 and written form.

2.7 Students will practice taking responsibility as members of a research team.

2.8 Students will value the importance of teamwork in scientific research.

100 **GOAL 3:** Attract NSF-targeted students to become researchers and professionals in their specialized discipline (computer science/biological sciences) but with the ability for interdisciplinary work. Anticipated results/objectives follow.

3.1 Students will be able to make informed decisions about a career in science/engineering after discovering if such a life appeals to them.

105 3.2 Students who so desire will make the successful transition to appropriate grad programs.

2. Program Structure and Associated Activities

The REU Site actively incorporates feedback from students and mentors while structuring the program. Social activities such as cook-outs, pizza parties
110 and baseball games are jointly planned with other REU programs hosted at UConn and are scheduled at the organizational meeting before program starts. In general, the program time lines are as follows:

Day 1: Orientation, Campus Tour, Program Overview, Lunch with Faculty,
115 Ice Cream Social

Week 1: Technical Seminars (mornings); Responsible Conduct of Research Seminars (afternoons)

Week 2: Lab Tours, Center (BiBCI: Bioinformatics and Biocomputing Institute) Tours

- 120 Week 3: Invited HPC Talks from BECAT (Booth Engineering Center for Advanced Technologies)
- Week 4: Seminar on Proposal Writing, targeting NSF Graduate Research Fellowships
- Week 5: Remote Bio-Grid Workshop (may be in conjunction with the student
- 125 Mini-Symposium)
- Week 6: Student Proposal Presentations
- Week 7: Seminar on Grad School Application
- Week 8: Seminar on Technical Writing and Presentations
- Week 9: Diversity Forum: Challenges and Choices in Higher Education (Panel
- 130 Discussions)
- Week 10: Bio-Grid Symposium (Final Project Presentations)

A major component of the program is for students to actively involve in one research project. After the training seminars in the first week, students discuss

135 with the project staff about their interests and a research supervisor is assigned to each student. Under the supervision of the project staff, students have their lab space and closely interact with their supervisor and graduate students currently on the project. Project supervisors design a component of the assigned project for students to work on. Mismatches between student and mentor are

140 resolved early in the program, allowing these students to successfully complete the project. REU students also have the opportunity to remotely attend the annual International Bio-Grid Workshop. Faculty members associated with the Bio-Grid Initiatives are all welcome to propose student projects.

Example Project: Basic Grid/Cloud Infrastructure. The development of the

145 Bio-Grid portal focuses on establishing an extensible and robust Application Programming Interface (API), based on standard procedures many life-science applications require when executing in a grid environment [14, 15, 16, 17, 18, 19, 20, 21]. This involves various compute platforms, using several different native queue managers (*e.g.*, OpenPBS, Condor, fork), a variety of operating systems

150 (e.g., RedHat Linux, IRIX, Windows), and various Wide Area Network (WAN)
connections (e.g., GigE, Fast Ethernet, T1) on campus.

The Bio-Grid is based on the Globus Toolkit middleware version 2.2.4 and the web portal is served by Apache HTTP Server version 2.0. (All of the web portal pages are dynamically created using the PHP hypertext preprocessor
155 scripting language, JavaScript, and real-time MySQL database access.) Each web portal page also allows the strict use of security and authentication procedures, defining a fine grained custom interface for each grid user. Several grid user Access Control Levels (ACLs) are defined for un-authenticated, general, system administrator, and grid administrator web portal page access. The base
160 Globus Toolkit middleware Meta computing Directory Service (MDS) information is stored in the Bio-Grid database and can be queried and displayed directly. The job monitoring system are designed to be an extremely lightweight and non-intrusive tool for monitoring applications and resources on the Bio-Grid.

Example Project: HPC Middleware Development. For a grid or cloud to serve
165 as the infrastructure for on-demand integration of sensitive clinical practice and health-care information, additional data management and replication mechanisms should be provided, as the current middleware mainly deals with flat files but not to the metadata level. This project concentrates on creating a *Bio Data Management unit* (BDM unit) that interfaces with the middleware and provides
170 additional metadata management capabilities. For example, medical images are stored in DICOM servers [22, 23, 24] in the hospital. Each image may consist of one or several DICOM files representing portions of the imaged body. The first role of the BDM unit is therefore to serve as an interface between the grid Storage Element and the DICOM server by assigning a logical file name to each
175 image. For each new DICOM image generated by an image producer, a logical file name is created and registered into the replication system. There is not necessarily a physical file instance behind this logical file number but rather a virtual file consisting of a set of DICOM files, that can be reconstructed on the fly by the BDM unit if a request for this logic file number comes in. For

180 efficiency reasons, assembled files are cached in a scratch space before leaving.

Example Project: Distributed Image Retrieval. This project integrates the BDM and the middleware installed on the Bio-Grid. Take the following test case for example. A cardiologist is looking for medical images similar to a case of his/her patients to confirm the diagnosis. He/She uses a high-level application
185 interface to select the Magnetic Resonance Image (MRI) sequence corresponding to his/her patient and request for similar images. A set of ranked MRI sequences are returned to the physician and he/she can visualize these new cases and read the corresponding diagnosis. This application can be decomposed into a sequence of steps below.

190 First, the physician enters a query (*e.g.* find the MRI of Mr. X acquired yesterday in this hospital) through the BDM user interface. The BDM unit sends a query for retrieving metadata to the Grid metadata interface. The user authorizations to access the data are checked by the external metadata service and the patient file logical identifier and its associated parameters (imaging
195 modality, region of interest, dynamic sequence, MR acquisition parameters, *etc.*) are returned to the user interface. A request to find all images similar to that of the patient for which a medical diagnosis is known is made. The BDM is then used to route the request to all sites (*e.g.* hospitals) with metadata services. The logical identifiers of all images matching the patient's parameters are returned.
200 A computation to determine level of similarity is conducted. The job submission service of the grid middleware is then used to distribute computations over available working nodes. For each job, the grid replica manager triggers a replication of the input files.

Example Project: Protein Function Studies. The complete sequencing of nu-
205 merous genomes now brings up the next major challenge in biology to understand how these genes function. Presently, scientists have only unraveled the functions of a small percentage of the proteins in these genes. Often protein functions ascribe to some recurring sub-structural *motifs* (or *minimotifs*, as they often contain less than 15 amino acids), which usually present specific positional

210 characteristics in the protein sequences [25, 26, 27, 28, 29, 30]. Devising efficient
 models, computationally or stochastically, to identify potentially *functional mo-*
tifs is the first essential step toward realizing protein functions. This project
 has yielded a web-based program (MnM, *Minimotif Miner*, [31, 32]) to search
 the proteome database for the presence of minimotifs, computationally, in pro-
 215 tein queries. The MnM downloads our minimotif database and several other
 NCBI databases (RefSeq, LocusLink, HomoloGene, Taxonomy, Pfam, and db-
 SNP databases) as the input and analyze for potentially functional minimotifs.
 The MnM program searches proteins for the presence of minimotifs in our min-
 imotif database. A proteome enrichment factor for each minimotif is calculated
 220 by dividing the observed number of a minimotif in a proteome divided by the
 predicted number which is based on its probability and the amino acid fre-
 quencies in each proteome. We used the MnM to analyze several proteomes.
 Statistics show that several minimotifs are enriched in the human proteome
 [31, 33].

225 *Example Project: Genomic Knowledge Inference.* It is crucial that the massive
 genomic data produced are well represented so that useful biological informa-
 tion may be efficiently extracted/inferred. A useful tool for effective knowledge
 representation is the *semantic network* system [34]. A semantic network is a
 conceptual model for knowledge representation, in which the knowledge entities
 230 are represented by nodes , while the edges are the relations between entities
 [35, 36, 37, 38]. A semantic network is an effective tool, serving as the backbone
 knowledge representation system for genomic, clinical and medical data. Usu-
 ally these knowledge bases are stored at locations geographically distributed.
 This highlights the importance of an efficient distributed semantic network sys-
 235 tem enabling distributed knowledge integration and inferences. The semantic
 network is a key component of the *Unified Medical Language System* (UMLS)
 project initiated in 1986 by the U.S. National Library of Medicine (NLM). The
 goal of the UMLS is to facilitate associative retrieval and integration of biomed-
 ical information so researchers and health professionals can use such information

240 from different (readable) sources [39, 40]. Our research team has developed a distributed semantic network system, based on a task-based and message-driven model to exploit both task and data parallelism while processing queries.

Bio-Grid Workshop Participation. We initiated in 2003 the Annual *Bio-Grid* Workshop (International Workshop on Biomedical Computations on the Grid).
245 The aims of the Bio-Grid workshop are to promote and reinforce awareness of the possibilities and advantages linked to the development, deployment and evaluation of Grid technologies in broadly biology-related research and practice. Here the context of “biology” covers the whole range of information from molecular level (genetic and proteomic information) through cells and tissues,
250 to the individual (clinical practice) and the population level (social healthcare). Since its initiation in 2003, BioGrid events have usually been held world wide in June or July in such cities as Tokyo, Chicago, Cardiff (UK), Singapore, Rio de Janeiro, and Berlin (Germany), all featuring invited speeches, a technical program and plenary sessions. In 2009 we were able to work with the European
255 Health-Grid Association to design a Berlin-Storrs joint session of the Bio-Grid program and had our summer REU students remotely attend this session.

3. The Research Environment

The project investigators all have extensive experience in undergraduate teaching, research supervision, and curriculum development. The REU staff
260 and faculty affiliated with Bio-Grid Initiatives have long collaborated on interdisciplinary research projects and have been involving undergraduate students in the research work.

The CSE faculty represents a wide diversity of research disciplines and are recipients of major research grants from federal agencies such as the NSF, NIH,
265 DARPA, ONR, DoEd, *etc.* The twenty-eight faculty members came from eleven different countries, representing another dimension of diversity. The department has a long tradition of being at the forefront of computing education, offering

broad based educational programs in computer Science and Engineering with bachelor, master and doctoral degrees.

270 The university has a *104-node HPC Cluster* and a *64-node SGI Altix 3700* available for summer students. The 104-node (1,408-core) HPC cluster contains both CPU and GPU resources, enabling a massive amount of computing power. There are 3 classes of nodes available in the cluster: (1) *60 Intel Westmere compute nodes*, each node with 12 Intel Xeon X5650 Westmere cores (total of
275 720 cores) and 48 GB of RAM. (2) *40 Intel Sandy Bridge compute nodes*, each node with 16 Intel Xeon E5-2650 Sandy Bridge cores (total of 640 cores) and 64 GB of RAM; and (3) *4 NVIDIA GPU nodes*, each node with 8 NVIDIA Tesla M2050 GPUs, 12 Intel Xeon X5650 Westmere cores and 48 GB of RAM. The nodes are configured to use LSF job scheduler, and uses low-latency
280 Infiniband network interconnect. 200 TB of high-performance GPFS storage is made available to the cluster. The SGI Altix system consists of (1) an SGI Altix 350 system with 8 Intel Itanium 2 Processors (1.5GHz with 6MB cache), each with 8 GB Memory, and an 80 GB SATA Hard Drive as the front-end server; and (2) an SGI Altix 3700 Bx2 system with 64 Intel Itanium 2 Processors
285 (1.5GHz with 4MB cache), each with 64 GB memory and 146 GB 10K RPM SCSI Hard Drive, with additional four 300 GB 10K RPM Ultra320 SCSI Hard Drives. These twin systems are networked to the School's existing SGI Onyx-4 Visualization System to provide a complete compute-to-visualization package for project staff and summer students.

290 **4. Student Recruitment and Selection**

In addition to a dedicated REU website linked from the NSF, we encourage student applicants from across the nation by extensively sending out brochures and invitations. Students from institutes where less research opportunities are available are especially encouraged to apply. We have previously collaborated
295 with investigators from minority institutions on NSF funded research and educational projects. UConn has a rich history of working closely with minority

institutions. We work closely with the university to publicize the REU site among those traditionally minority institutions¹ and among student members of the *National Society of Black Engineers*, the *Society for Hispanic Professional Engineers*, and the *Society of Women Engineers* in the nation through emails,
300 phone contacts, posters and brochures. We work closely with the *National Center for Women & Information Technology* (NCWIT) to actively promote and advocate the ten-week summer REU program to women. Through the academic alliance, NCWIT assists in reaching out across the nation for the purposes of
305 recruitment of women to participate in the Bio-Grid summer REU program. The NCWIT academic alliance includes such NSF targets as minority-serving colleges and institutions lacking research opportunities.

We also contact collaborators and administrative staff at minority institutions to distribute the REU Site posters. Every effort is made to encourage
310 undergraduate student participation from these institutions. Due consideration is given to minority applicants. At the state level, we host workshops at the Connecticut State University System (Central, Southern, Eastern and Western) and the CT Community College System to advertise the REU program, especially minority institutions in CT such as the *Capital Community College*
315 (Hartford) and the *Housatonic Community College* (Bridgeport), *etc.* We work closely with the University to encourage underrepresented students registered at the University of Connecticut to participate in the planned activities. Local students may participate in selected activities at their interests in a flexible manner. They are counted in the quota of 10 students to be accommodated by
320 this REU site. Local students may also participate by registering an independent study session for credits with the faculty supervisor whose project they feel interested in.

We work with the *Office of Veterans Affairs and Military Programs* at UConn to actively recruit veteran students via the *National Association of Veterans' Programs Administrators* (NAVPA). NAVPA's member institutions include such
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¹United States Department of Education Accredited Postsecondary Minority Institutions.

NSF targets as minority-serving community colleges and other institutions lacking research opportunities. The primary role of the office at the university is to provide direct support for student veterans as well as to create a university-wide support network for veterans throughout the university. Additionally, the
330 Division of Student Affairs at UConn owns a house that serves as a drop in center for student veterans. This house has been available to REU student veterans. The office also assists in accessing student veterans across the nation for recruitment.

We work with the *Center for Students with Disabilities* (CSD) at UConn to
335 actively recruit disabled students from UConn and other institutions to participate in the summer REU. UConn's CSD has seen the rapid growth in the number of students with disabilities accessing higher education. In 1993, the University served approximately two hundred students with disabilities. In 2008-2009, the CSD worked with more than one thousand. The CSD program has been
340 recognized as a "model program" by the *Association on Higher Education and Disability* (AHEAD). The CSD has an extensive peer mentor network where entering students with disabilities are paired with current students to assist with their transition to the university community. The service is extended to summer REU students with disabilities. The CSD is also committed to offering
345 specialized training required for mentors to accommodate REU students.

The application requires (1) personal information including prior research, project and any course experiences in HPC; (2) a brief research statement about personal and professional goals and how the REU experience would further these goals; (3) the selection and prioritization of three potential research topics; and
350 (4) provide two letters of reference, at least one of which should be from the applicant's institution.

Our recruitment goals are to attract a group of highly motivated students, roughly half majoring in computer science and half majoring in a biology-related field, with appropriate academic records and a targeted percentage from non-
355 PhD granting institutions. However, due to the partnerships we have established with former participants' schools and other institutions, we have been using our

contacts at each to help select promising students whose academic background may miss the bar yet show high potential in non-GPA ways. Participating faculty of the REU project performs preliminary evaluations of applications, based
360 on academic performance, research statement, and letters of reference. Final decisions are based on the student's (a) academic background and perceived interest and enthusiasm for the interdisciplinary research, (b) home institution (non-PhD or limited research given preference), (c) ethnic and gender diversity, if available (applicant's gender, race and ethnic background are requested on
365 an optional basis), and (d) disability and veteran status. A modified rolling admission procedure is employed until all slots are filled. Mentors and students are matched based on mutual preferences.

5. Program Evaluation and Reporting

Evaluation of the student experience commences with an initial survey in
370 which REU students articulate their goals for the program. Formative evaluation, *i.e.*, continued evaluation with the possibility of program modification as indicated, is conducted during the first two-three weeks and at the mid-point in addition to summative evaluation (end-of-program surveys for both students and mentors, and follow-up communication with students). The project applies
375 both qualitative and quantitative evaluation methods to assess the goals, as well as the outcome-based objectives for each goal. Assessment is aimed at measuring objectives/outcomes associated with students' acquisition of research skills, especially in the appropriate cross-discipline, gaining an understanding of life in the research lab, and eventual enrollment in appropriate graduate programs.
380 To assess success of the project in recruiting diverse REU students, we track all applications, including demographic data that is supplied by the applicant. We determine what level of recruitment (personal letter, phone call, recruitment visit, *etc.*) provides the best return - both in attracting applicants and in attracting participants - for our recruitment effort. Both qualitative (individual
385 and group interview) and quantitative (survey) approaches are used to assess

student experiences and outcomes, and focus on the specific objectives.

Upon arrival, REU students are given a questionnaire on their goals and expectations. Each lab is visited at least once/week during the first month of the program to informally monitor progress as part of ongoing formative evaluation.

390 Interview questions and observations are aimed at determining how well the REU student "fits" in the lab, including the level of interaction with other lab personnel and the student's perceptions regarding how s/he is progressing on a project. We plan a formal mid-program evaluation, possibly in the context of a group breakfast or lunch meeting. Mentors (REU faculty) are also surveyed (a)
395 within the first few weeks; (b) at midpoint and (c) at the end of the program to determine their perceptions of each student's progress. Students' ability to communicate results are assessed both by mentor's observations and by the final presentation which culminate the summer REU experience. At the end of the summer, REU students are given comprehensive survey questionnaires
400 designed to elicit feedback on all aspects of the program, from housing and social activities to a detailed evaluation of their research experience and their intellectual experiences in the form of seminars and ancillary activities. This mixed method designed for assessment can, especially after the program is in place for a few years, provide data to assess the efficacy of our REU site at
405 promoting increased representation of underrepresented minorities, veterans and persons with disabilities in research.

Maintaining Contact. Post-program contact with the students has been facilitated by the mentor-student relationships developed over the summer program, in addition to utilizing traditional phone numbers and email addresses. We
410 encouraged students to take home their posters from the end-of-summer conference, and contacted a faculty member at each student's home institution to let them know about the poster and encourage them to have the REU student give a talk. Students were contacted by email periodically during the following semesters and polled as to their plans and career choices. We also solicited the
415 first year REU students as ambassadors and asked them to encourage future

applicants from their home colleges.

6. Project Outcomes

Our Goal (1) was to "*promote an interest in the interdisciplinary research work associated with the Bio-Grid initiatives by targeting NSF-targeted student participants - underrepresented minorities, students with disabilities, women, and veterans from primarily NSF-targeted institutions in the early stages of their academic careers*", with an objective of anticipating half participants with an interest or background in HPC and another half with a biology-related background. Tables 1 and 2 summarize our results about participants, offers made and applicants. "Target Schools" refers to Non-PhD granting institutions. Our Goal (1) was met. The objective of recruiting half CS students and half Bio-related students was being approached, with an improvement from 8:2 (CS:Bio) in 2008 to 6:4 (CS:Bio) in 2010. The ratio slightly dropped in 2012 to 4:2 (CS:Bio) and in 2013 to 7:2 (CS:Bio). We believe this drop has to do with the rather small cohort funded in 2012 and 2013 (15 total). Note that the classification of students into CS or BIO was simply to assist in making offers and organizing student teams. The classification was more based on experience, not on student's major. A CS student is one who is experienced in computing, especially HPC. A BIO student is one who had prior exposure to biology courses or wet-lab experience. For example, a Mechanical Engineering major with significant HPC experience is put in the CS group. A Computer Science major with a Bioinformatics concentration and relevant wet-lab experience is regarded as a BIO student.

Our Goal (3) was to "*attract NSF-targeted students to become researchers and professionals in their specialized discipline (computer science/biological sciences) but with the ability for interdisciplinary work*". In this regard, the percentage of female participants has risen from 10% (1/10) in 08 to 60% in 2010, with a drop to 33% (2/6) in 2012 and 22% in 2013 (2/9). While there is certainly room for improvement in this outcome, we did observe that more than

Table 1: Bio-Grid REU Site Statistics 2008-2010: Participants/Offer Made/Applicants

Year	Total	# Fe- male	# Under- repre- sented Minori- ties	# from Target Schools	# of CS- related Major	# of Bio- related Major
2008	10/14/38	1/4/9	1/4/7	4/7/18	8/12/31	2/2/7
2009	10/17/54	3/6/19	1/4/8	2/6/20	7/10/40	3/4/14
2010	10/15/68	6/8/22	2/6/12	5/9/37	6/10/41	4/5/27
Total	30/46/160	10/18/50	4/14/27	11/22/75	21/32/112	9/11/48

30% (36/117) of the 2013 applicants were women. Percentage of participants from non-PhD granting institutions rises from 40% (4/10) in 2008 to 67% (6/9) in 2013. In addition, we have been continuing our efforts in recruiting students that are under-represented minorities (Black, Hispanic, Native American, Native Hawaiian). In 2013, 6 offers were made to underrepresented minorities, while 4 such offers were made in each of 08 and 09, and 3 in 12. Although not all offers to under-represented minorities were taken, we did observe a significant increase of minority applicants, especially from institutes we've targeted. The lower yield rate from female and minority applicants is likely due to the fact that the federally sponsored REU programs specifically encourage diversity and broadening participation, and qualified female and minority applicants are likely to receive more offers to choose from. Finally, we made two offers in 2013 to two applicants who indicated disability. A student who was diagnosed with Crohn's Disease joined us for the summer of 2013. We worked with the housing department and the Center for Students with Disabilities at UConn to accommodate the student's medical needs.

Bio-Grid students were recruited from universities as follows.

- Bowdoin College

Table 2: Bio-Grid REU Site Statistics 2012-2013: Participants/Offers Made/Applicants

Year	Total	# Fe- male	# Under- repre- sented Minori- ties	# from Target Schools	# of CSE Major	# of Bio (or non- CSE) Major
2012	6/8/88	2/4/18	1/3/9	2/4/33	4/5/60	2/3/28
2013	9/16/117	2/6/36	1/6/18	6/9/42	7/9/72	2/7/45
Total	15/24/205	4/10/54	2/9/27	8/13/75	11/14/132	4/10/73

- Carnegie Mellon University
- City University of New York - Hunter
- 465 - Colorado Mesa University
- Duke University
- East Coast Polytechnic Institute
- Fairfield University
- Hobart College
- 470 - Lewis-Clark State College
- Loyola Marymount University
- Manchester Community College
- Manhattanville College
- Rhode Island College
- 475 - Siena College
- Swarthmore College
- Tufts University
- University of California San Diego
- University of Connecticut
- 480 - University of Delaware
- University of Hartford

- University of Maine, Orono
- University of Massachusetts Amherst
- University of Pennsylvania
- 485 - University of Puget Sound
- University of Tennessee at Chattanooga
- University of Texas Dallas
- Western New England College

Our Goal (2) was to "*promote the acquisition of skills allowing computer*
 490 *scientists and biologists to function in an interdisciplinary working/research environment*". Students conducted research under the supervision of mentors, interacting with graduate students and postdocs, participating in research meetings and experienced life as a researcher. Whenever possible, a Bio student and a CS student were teamed up to experience interdisciplinary teamwork. Students
 495 all reported that the REU gave them the understanding they needed to assess whether a research career is for them. Ongoing formative evaluation, consisting of meetings with students at the end of the first week as well as mid-experience, allowed for timely corrections of any problems. All mentors reported that students were good team members. All students reported viewing research
 500 as largely a team effort, and gave specific examples of being able to ask questions of different grad students, or of learning different techniques from different groups. All mentors reported students made progress toward independence in research, with a majority reporting students were able to work with complete independence by the end of the program, indicating the immediate objectives
 505 of Goal (2) were met.

Although the extent to which Goals (2) and (3) are successfully accomplished can only be determined with the passage of time, the structured interviews during the course of the summer program and through follow-up interviews immediately after the completion of the program has a strong indication of the
 510 successful accomplishment of these goals. It's also noted that most students indicated there was no direct cause-effect relationship between the Bio-Grid

summer program and their career choice, although all students acknowledged the interdisciplinary research experience and agreed it has provided valuable input in their post-program research and course activities.

515 Technical seminars in the first week of program invited mentors to give a research presentation (Figures 1, 2 and 3). This provided sufficient project and mentor information to students before the project assignment at the end of the first week. Departmental seminars on the *graduate school application process*, *research proposal writing* targeting the NSF graduate fellowship application, 520 *technical report writing* and *effective scientific presentation* have also been very well received. *Weekly group meetings* with the project staff helped resolve any potential problems in a timely manner. *Joint REU seminars* were integral to our program. Among them are an *Ethics workshop* presentation addressing ethics in research, a *stem cell ethics seminar*, and a discussion regarding ethics. 525 Starting 2010, the ethics workshop evolved into an RCR (*Responsible Conduct of Research*) seminar series (Figure 4), spanning the entire first week of program. The *Diversity in the Sciences Workshop* evolved from a presentation to a panel discussion, utilizing faculty and staff from across the campus (Figures 5 and 6). The mid-term *Bio-Grid mini-Symposium* required all Bio-Grid students to 530 prepare a 15-min or so oral presentation, accompanied by a one-page research summary. The mini-symposium was designed to get students familiar with the "proposal defense" stage when in graduate school. It also equipped students with knowledge about grant proposal writing. The final Bio-Grid Symposium program was the culminating event. Each project was allotted 30-min for an 535 oral presentation. A technical report was due before students left the program. Collegiality was fostered by many social events - most of them involving all summer research participants (ice cream social, barbecue, baseball game) and others just the Bio-Grid REU program (initial orientation). Summer research students were housed together in a separate section of the summer dormitory, 540 and interacted with Community Assistants (grad students working in Housing) who were connected to the summer research program.

Outcomes of continued post-program mentoring for REU participants. We regularly contact Bio-Grid alumni and offer assistance in recommendation letters and in preparation for graduate fellowship applications for those applying to graduate school. As of April 2016, Bio-Grid alumni have won the NSF Graduate Research Fellowship in 2016 (Stephanie Kowlton, Bio-Grid 2012) and 2012 (Brittany Nkounkou, Bio-Grid 10), an Alfred P. Sloan Foundation Graduate Scholarship in 2012 (Brittany Nkounkou, Bio-Grid 10), an honorable mention of the NSF Graduate Research Fellowship in 2012 (Michael Zuba, Bio-Grid 09), and a GAANN Fellowship by US Dept. of Education in 2010 (Michael Zuba, Bio-Grid 10).

Among the 15 REU students recruited from 12-13, 8 are now in graduate school (6 PhD, 2 MS). 4 students are in the process applying to graduate school. By the summer of 2016 around 80% of REU students recruited from 12-13 will be pursuing a graduate degree. Among the 29 students recruited from 08-10, 13 students are attending or have finished graduate school (7 PhD, 1 MD/PhD, 1 MD, 4 MS). 6 students currently in industry are applying to graduate school and expect to start an MS/PhD program within a year. One student is applying to medical school. In summary, by next summer around 70% of REU students recruited from 08-10 will have completed (or be pursuing) a graduate degree.

Many of the Bio-Grid alumni have indicated their experience in HPC have helped them throughout their graduate study.

Bio-Grid alumni entered such graduate schools or medical schools as

- Boston University
- Columbia University
- Cornell University
- Rensselaer Polytechnic Institute
- Stanford University
- University of California, Santa Barbara
- University of Connecticut (grad school and medical school)
- University of Maryland, College Park

- University of North Carolina Chapel Hill
- University of Pennsylvania
- University of Pittsburgh (Medicine)
- University of Texas (Medicine)

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Additional student outcomes include peer-reviewed scientific publications in both HPC and bioinformatics co-authored with summer REU students in major journals and conferences [41, 42, 43, 44, 45, 46, 47, 48, 49].

Outcome of Faculty From REU Student Mentoring. The outcome of the REU program also involves the benefits faculty and the CSE department would gain from the investment of time and resources in mentoring REU students. Experience gained from our REU Site program concerning assessment and recruitment was used extensively in a few current and pending grants by colleagues. Throughout the funding periods, twelve faculty members and fifteen graduate students have mentored summer students.

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7. Lessons Learned: Incorporating HPC in an Interdisciplinary REU

This section discusses the experience gained and lessons learned from the perspectives of an REU Site designed to incorporate High-Performance Computing in interdisciplinary research and education.

Recruiting Students with Sufficient Exposure to HPC. Concepts of HPC arises from every aspect of parallelism in computing, which is relevant to most of the courses offered in a typical undergraduate Computer Science or Computer Engineering curriculum. Ideally participants on the computing side should have finished such courses as Operating Systems, Computer Architecture and Algorithm Analysis; have some experience in parallel programming; and are interested in life-science related research work.

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Recruiting Students in Biology-Related Majors. Students on the BIO side may be in such majors as Molecular Biology, Evolutionary Biology, Neuroscience,

Biomedical Engineering, *etc.*; preferably have finished one year of courses in
600 their concentrations; and are interested in informatics research.

Educating Students the Essence of Interdisciplinary Research. Undergrad stu-
dents do not often get the chance to work with others from different disci-
plines. To truly spark their interest in interdisciplinary research early in their
academic career, the REU program should be designed to educate students
605 that interdisciplinary research is not just people of different specialized disci-
plines collaborating with each other. Instead, interdisciplinary work signifies
true convergence. Namely, people learn from the very best of others' technolo-
gies, bring the essence to their own discipline and create something that goes
beyond boundaries in terms of moving forward through new technologies and
610 new solutions.

Stimulating Enthusiasm of Faculty and Participants. Whenever possible, re-
cruit qualified applicants who indicate interest in pursuing graduate study in a
particular lab or with a particular faculty member. After presentations of avail-
able projects, allow students to interact more closely with Lab PIs before project
615 assignment. Mismatches between student and mentor should be observed and
resolved early in the program, allowing students to successfully complete the
project.

Encouraging Participants to Pursue Research Resources. A Bio-Grid partici-
pant in 2009 attended the *International Bioinformatics Conference* in Spain
620 in 2010 to present her research results. We did not have enough travel fund
to sponsor the student's trip but decided to encourage the student to pursue
funding from her home institution (UCSD) for the trip. The student eventually
secured travel fund from the Provost's office to make the trip.

Using the Right Student Mentors. Our experience indicated that an effective
625 way to mentor minority REU students and to encourage them to pursue an aca-
demic career is to have them work with minority doctoral students. A Bio-Grid
participant in 2010, who did not have a plan to do a PhD when admitted to

Bio-Grid, later published a paper in 2011, won two graduate research fellowships as a college senior in 2012 and as of now has been a CS PhD student
630 (Cornell) and has been serving as President of Black Graduate and Professional Student Association. One of the student’s mentors was our Cloud Computing GAANN (Graduate Assistance in Areas of National Need) doctoral fellow, an underrepresented minority student as well.

8. Acknowledgement

635 *Funding.* The Bio-Grid REU Site acknowledged funding by the National Science Foundation in grants CCF-0755373 (2008-2010) and OCI-1156837 (2012-2014).

Faculty mentors. Faculty mentors and consultants include Jun-Hong Cui (CSE), Swaminathan Hariharan (Educational Psychology), Richard Jones (Physics), Aggelos Kiayias (CSE, formerly), Kristen Kimbal (Physiology and Neurobiol-
640 ogy), Ion Mandoiu (CSE), Thomas J. Peters (CSE), Sanguthevar Rajasekaran (CSE), Heather Read (Psychology and Biomedical Engineering), Bing Wang (CSE) and Xiaoyan Wang (Family Medicine).

Collaborating UConn REU Sites. The Bio-Grid REU Site also acknowledged the joint events co-hosted by collaborating REU Sites at UConn by the Depart-
645 ments of Chemical Engineering, Chemistry, Electrical Engineering, as well as Physiology and Neurobiology.

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Figure 1: Technical Seminar: Model Organism Databases

Figure 2: Technical Seminar: GPU Programming

Figure 3: Technical Seminar: Storage Clouds

Figure 4: Responsible Conduct of Research Seminar

Figure 5: Diversity in the Sciences Workshop: Panel Discussions

Figure 6: Diversity in the Sciences Workshop: Group Discussions

Model Organism Databases / Organism Specific Databases

- DBs that describe the genome and other information about an organism
- Every sequenced organism with an active organizational community requires a MOD
 - Integrate genome data with information about the life history and genetic network of the organism
 - Integrate literature-based information with computational predictions
- Curated by experts for that organism
 - No one group can curate all the world's genomes
 - Distribute workload across a community of experts to create a community resource

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Keywords:

High-Performance Computing, Algorithm Design and Analysis, Computational Biology, Cyber-Infrastructure, Life Science Informatics, Experimental Algorithmics

Summary:

Chun-Hsi Huang is an Associate Professor with the Department of Computer Science and Engineering at the University of Connecticut. Dr. Huang's research interests are primarily in the areas of High Performance Computing, Computational Biology and Algorithm Design & Analysis. He is particularly interested in investigating research issues involved in the software/hardware infrastructure, middleware and algorithmic support for extreme-scale computation and information extraction. Recently his research efforts have been on the development, deployment and evaluation of modern large-scale distributed computing infrastructures for this purpose.

Example research foci include the following: (1) exploiting massive parallelism at the algorithm level; (2) coping with software run-time errors from processing elements; (3) efficient large-scale inter-processor and processor-memory communications; and (4) reducing the power requirements for future hardware.