

Review of DOE Computational Science Graduate Fellowship

November 1, 2011

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Charge Letter

“By this letter, I am charging the ASCAC to assemble a sub-committee to examine the effectiveness and impact of the CSGF, as compared to other educational activities, and the quality and breadth of the program over the past decade. The sub-committee should take into account the unique qualifications and skills of computational scientists and their role in the public and private sectors. It should also address the role of women and under-represented minorities, the projected need for trained computational scientists in the DOE laboratories and for continued US leadership in the computational sciences.”

Distilled Charges

- Address the **projected need** for trained computational scientists in the DOE laboratories and for continued US leadership in computational science.
- Examine the **effectiveness and impact** of the CSGF.
- Comment on the **quality and breadth** of the program over the past decade.
- Address the participation of **women and minorities** in the program.
- Compare to other **educational programs**.

Committee Process

- Information from ASCAR and Krell Institute
- Interviews at CSGF Annual Conference July, 22
(Dona Crawford, Jeff Hittinger , Bill Tang)
 - Jim Corones, Jeana Gingery, and Mary Ann Leung of Krell
 - Barb Helland of DOE-SC and Thuc Hoang of NNSA
- Teleconference July 7, Email Discussions

Projected Need

- Supported by Recent Reports
- Supported by Personal Experience

Projected Need

Reports Cited

- 2011 strategic plan for the U. S. Department of Energy (<http://energy.gov/downloads/2011-strategic-plan>).
- Brown, D. L. (Ed.); *Applied Mathematics at the U.S. Department of Energy: Past, Present and a View to the Future*, - Report by an Independent Panel from the Applied Mathematics Research Community, May 2008. <http://science.energy.gov/ascr/news-and-resources/program-documents/>
- *Nuclear Posture Review Report*, April 2010. <http://www.defense.gov/npr/>
- *High Performance Computing and U.S. Manufacturing Roundtable White Paper*, from the High Performance Computing Initiative of the Council on Competitiveness, February 25, 2010. <http://www.compete.org/publications/detail/1333/high-performance-computing-and-u.s.-manufacturing-roundtable/>
- Joseph, E; Conway, S; Wu, J; *IDC Special Study for DOE: HPC Talent and Skill Set Issues Impacting HPC Data Centers*, December 2010.
- Oden, J. T. (Ed.); *Simulation-Based Engineering Science: Revolutionizing Engineering Science through Simulation* – Report of the National Science Foundation Blue Ribbon Panel on Simulation-Based Engineering Science, February 2006. http://www.nsf.gov/pubs/reports/sbes_final_report.pdf

Projected Need Selected Quotes

- “DOE, NSF and other agencies should consider creating fellowship programs to train graduate students and postdocs in HPC modeling and simulation, and expanding the Presidential Early Career Awards in Science and Engineering (PECASE) program in this area.” (Council on Competitiveness)
- “At one laboratory, there is an ongoing hiring requirement for 30 computational scientists.” (DLC)

Projected Need: Conclusions

The Subcommittee has concluded that the need for well-trained computational scientists in government laboratories and in industry will far exceed the supply for the foreseeable future. This is especially true in the DOE laboratories. We conclude that the need for programs like the CSGF will increase over the next decade.

Projected Need

Recommendation:

The Subcommittee recommends that the Office of Science continue to view stimulation of the computational science workforce as important to its mission.

Effectiveness and Impact

Based on

- Effective Educational Process
- Impact
 - Alumni Outcomes
 - Impact on DOE
 - Broader Impact

Effective Educational Process

Program features

- Program of Study
- Practicum
- Annual CSGF Conference
- Alumni Outreach

Effective Educational Process

Program of Study

- Students required to propose a plan of study
- Plan must include the right mix of courses
 - Domain Science
 - Applied Math
 - Computer Science
- Treated as a contract

Effective Educational Process

Practicum

- Students spend at least one summer working in a DOE Laboratory.
- Additional practicum are encouraged
- Exposes student to Labs and real problems
- Establishes a network
- Gives Labs opportunity to evaluate students

Effective Educational Process

Annual CSGF Conference

- Required to present a poster
- Last required to give talk
- Teaches communication skills
- Develops network of Fellows

Effective Educational Process

Alumni Outreach

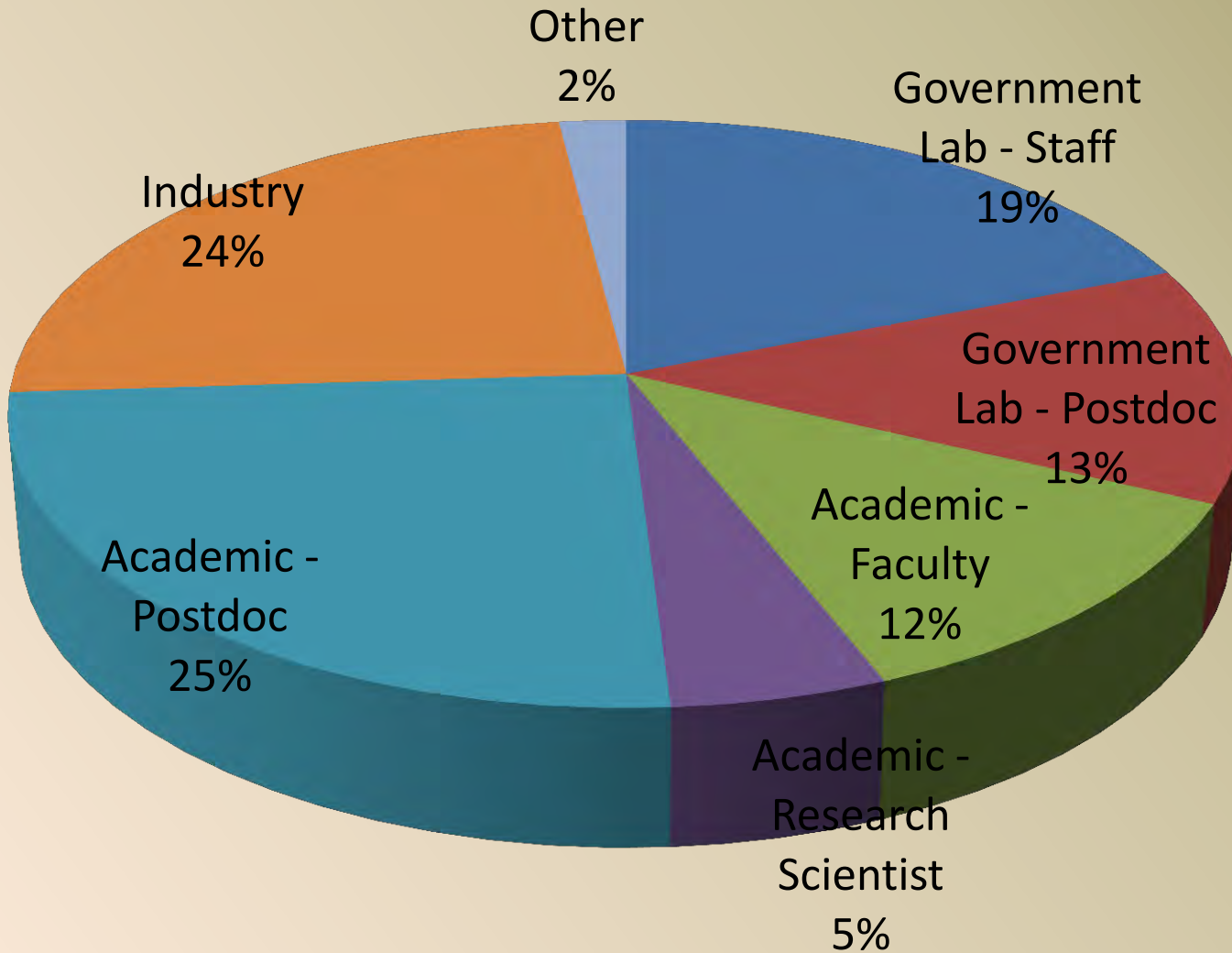
- Encouraged to mentor current Fellow practicum
- Invited to CSGF Annual Conference
- Receive CSGF Literature (DEIXIS)

Impact

Alumni Outcomes

- Graduation Rates:
 - Between 2001-2006, 96%
- Current positions
 - All but 1 out 102 in technical positions (01-09)
 - Academic, Industry, Government Labs
 - 27 Employed at some point in DOE Labs

Alumni Current Positions



Current Positions: Academic

Stanford,
Princeton,
Cornell,
Columbia,
Michigan,
Wisconsin,
Oxford,
KAUST,

NYU,
Harvard,
UC Berkeley,
Caltech,
Texas,
Illinois,
Cambridge,
Institut Pasteur

Current Positions: Industrial

Microsoft,

Shell,

Seagate,

Dataspora,

AREVA,

Google,

Exxon Mobil,

Amyris Biotechnologies,

British Petroleum,

Intellisis

Several Alumni have started new companies

Alumni at DOE Laboratories

ANL

- Jeff Hammond, Post Doc
- Stefan Wild, Post Doc
- Hal Finkel*

Bettis

- Stephen Vinay III

LANL

- Joshua Coe, Post Doc
- Ethan Coon, Post Doc
- William Daughton
- Jeff Drocco, Post Doc*
- Timothy Germann
- Aric Hagberg
- Nathaniel Morgan
- Sam Schofield
- Allan Wollaber

LBNL

- Jarrod Chapman, Post Doc
- Daniel Martin
- Anubhav Jain*

LLNL

- Teresa Bailey
- Thomas Epperly
- Brian Gunney
- Jeff Hittinger
- Matthew McNenley
- Elsie Simpson Pierce
- Brandon Wood

NREL

- Christina Payne, Post Doc

ORNL

- Mark Berrill, Wigner Fellow
- Kristine Cochran
- Gregory Davidson
- Steven Hamilton
- Judith Hill
- Richard Mills
- Matthew Norman
- Matt Reuter*

PNNL

- Christopher Gesh
- Kevin Glass
- Glenn Hammond
- Christopher Oehman

Sandia-CA

- Aron Cummings, Post Doc
- Alex Lindblad
- Michael Veilleux, Post Doc

Sandia-NM

- Nathan Crane
- Heath Hanshaw
- James Morrow
- Elijah Newren, Post Doc
- Laura Painton Swiler
- Michael Wolf, Post Doc
- David Rogers, Post Doc

* Starting in 2011

Alumni who have left DOE labs

Ames

- Heather Netzloff, Post Doc - > School

ANL

- Joseph Czyzyk, Post Doc ->Cent. Michigan Univ. Research Corp.
- Jaydeep Bardhan, Post Doc - > Rush Medical Center

LANL

- Eric Held, LANL/ORISE Fusion Fellow -> Utah State
- William Humphrey, Staff member -> NumeriX, LLC
- Mario Trujillo, Post Doc -> Penn State
- Scott Zoldi, Post Doc -> FairIsaac
- Dan Horner, Post Doc - > Center for Naval Analysis
- Charles Zeeb -> Deceased

LBNL

- Mary Dunlap, Post Doc -> University of Vermont
- Richard Propp, Post Doc -> Oracle
- Scott Stanley, Post Doc -> Hewlett-Packard

LLNL

- Allison Baker, Staff Member

ORNL

- Asegun Henry, Post Doc -> Northwestern

PNNL

- Collin Wick, Post-doc -> Louisiana Tech

Sandia - CA

- Edwin Blosch, Post-doc->CFD-FASTRAN
- Shilpa Talwar, Staff member -> Intel
- Obioma Uche, Post-doc->University of Virginia, Charlottesville

Sandia - NM

- Marcus Martin, Staff member -> Useful Bias (his own company)
- David Ropp, Post Doc -> SAIC
- Peter Wyckoff, Post Doc, -> Ohio Supercomputing Center
- Ahmed Ismail, Staff member - > RWTH Aachen University

Effectiveness and Impact

Subcommittee concludes that the DOE CSGF is an exceptionally effective program that has had a significant impact on the national Computational Science infrastructure.

As indication of direct benefit to the DOE, a large percentage of Fellows spend a portion of their early career in the DOE laboratories and an even larger portion continue interaction with the DOE laboratories as they pursue their careers in academia and industry.

Effectiveness and Impact

In light of the effectiveness and impact of this program and in the context of the growing projected need, the Subcommittee has concluded that funding for this program is not only well spent, but that additional funding should be provided.

Recommendation: *the Subcommittee recommends that the funding for this program be put on a path to double over the next 5 years.*

Budget History

Year	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010
Budget	5.0	6.5	5.5	5.5	5.5	5.5	6.0	6.8	6.8	7.8

Budget in \$M

Quality and Breadth

Quality

- Quality of Applicants and Awardees
- Selection Process
- Management of Fellowships

Breadth

- Applicants and Awardees by Field
- Outcomes

Applicants GRE Scores

Year	Number	Average UGPA	Average Percentile GRE Verbal	Average Percentile GRE Quantitative
2002	157	3.51	74	87
2003	312	3.60	75	85
2004	317	3.62	75	82
2005	337	3.59	73	83
2006	410	3.61	75	82
2007	396	3.68	75	85
2008	371	3.64	78	87
2009	349	3.60	79	86
2010	531	3.59	77	84
2011	628	3.64	77	85

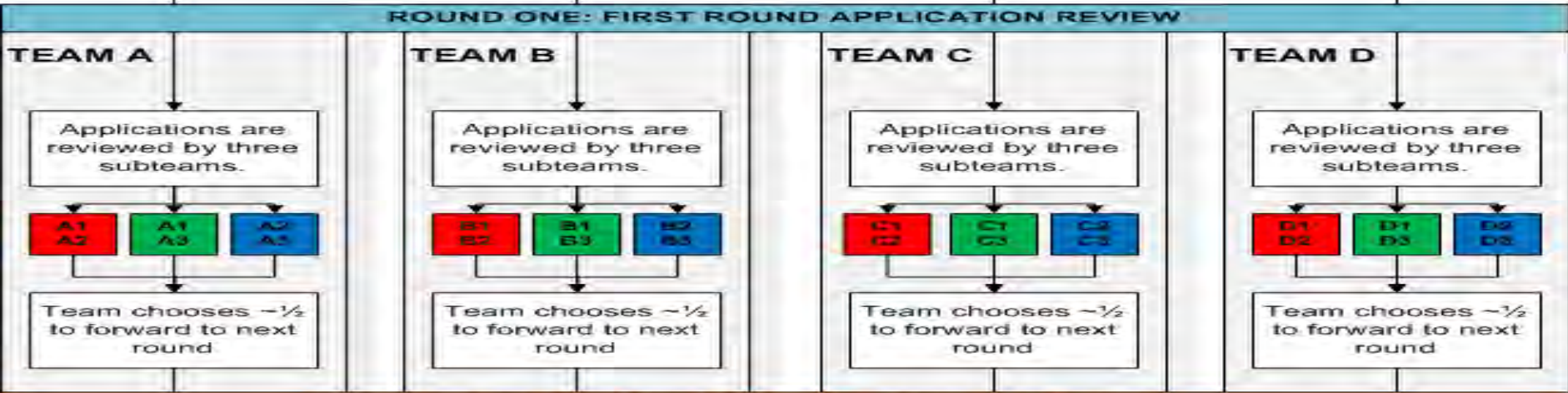
Awardees GRE Scores

Year	Average UGPA	Average Percentile GRE Verbal	Average Percentile GRE Quantitative
2002	3.72	77	90
2003	3.86	86	90
2004	3.90	83	88
2005	3.73	80	88
2006	3.92	85	89
2007	3.87	86	89
2008	3.80	86	91
2009	3.86	85	92
2010	3.81	87	91
2011	3.88	90	90

Selection Process

- Outreach
- Screening Committee
 - Triage on applications:
 - Noncompetitive
 - Competitive
 - Top tier
- Selection Committee
 - Complicated selection process

Applications are split amongst four teams



DEADLINE FOR FIRST REVIEW: FEBRUARY 25, 2011



DEADLINE FOR SECOND REVIEW: MARCH 21, 2011



AB

CD

ROUND THREE: MEETING MARCH 21-23, 2011, NEW YORK (CONTINUED)

TEAM AB

Team AB chooses ~½ of applications to go forward to next round

Team AB exchanges applications with Team CD

Team AB reads Team CD's applications

TEAM CD

Team CD chooses ~½ of applications to go forward to next round

Team CD exchanges applications with Team AB

Team CD reads Team AB's applications

ROUND FOUR (FINAL ROUND): MEETING MARCH 24, 2011, NEW YORK

TEAM ABCD

Team AB & CD Combine

Remaining 45-50 applications are reviewed by Team ABCD

Selection Process

- Quality of the selection process depends on the quality of the participants
- Committees consist of accomplished computational scientist from a broad range of application areas

Awards by Field

Area	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011
Bio & Bioeng	3	1	1	3	3	5	6	3	2	3
Math & CS	3	3	3	1	5	1	2	2	5	3
Engineering	15	8	4	7	3	5	6	6	6	4
Physical Sci	3	3	6	4	8	4	4	5	7	7
Social Sci	0	0	1	0	0	0	0	0	0	0
Did not report	1	1	0	0	1	1	0	0	0	0
Total	25	16	15	15	20	16	18	16	20	17

Selection Criteria

- Criteria not clearly documented
- Definition in application

“Computational science” involves the innovative and essential use of high-performance computation, and/or the development of high-performance computational technologies, to advance knowledge or capabilities in a scientific or engineering discipline.

Selection Process

Questions

- How does one weigh the application of existing technologies to advance science versus the development of new methods and techniques in this pursuit?
- Is there any preference for simulation over more data-centric scientific discovery, i.e., data mining and informatics?
- Is the goal to encourage non-computational scientists to enter into the field of scientific computing or to reward outstanding applicants already in the field?

Selection Criteria

- Kept intentionally vague
- Allows program to grow “organically”
- Sets few boundaries and relies on carefully chosen screening and selection committee
- Annual discussion to set priorities

Selection Criteria

Krell's interpretation based on program history and current grant proposal

- Fellowship proposal must be application driven
- Interpreted to mean application specific
- Excludes enabling science

Omission and Opportunity

- Excludes important part of the computational science endeavor.
- Krell (Jim Coronas) aware of this omission and has advocated for a new program to include enabling sciences.
- ASCR proposed Fellowship Programs in Applied Math and High Performance Computing in FY10 and FY11 at \$2M.

Conclusions

- Quality of the Fellows is exceptional.
- Quality of the management is exceptional.
- Program covers a broad range of scientific disciplines.
- Should be expanded to cover enabling sciences.

Recommendation

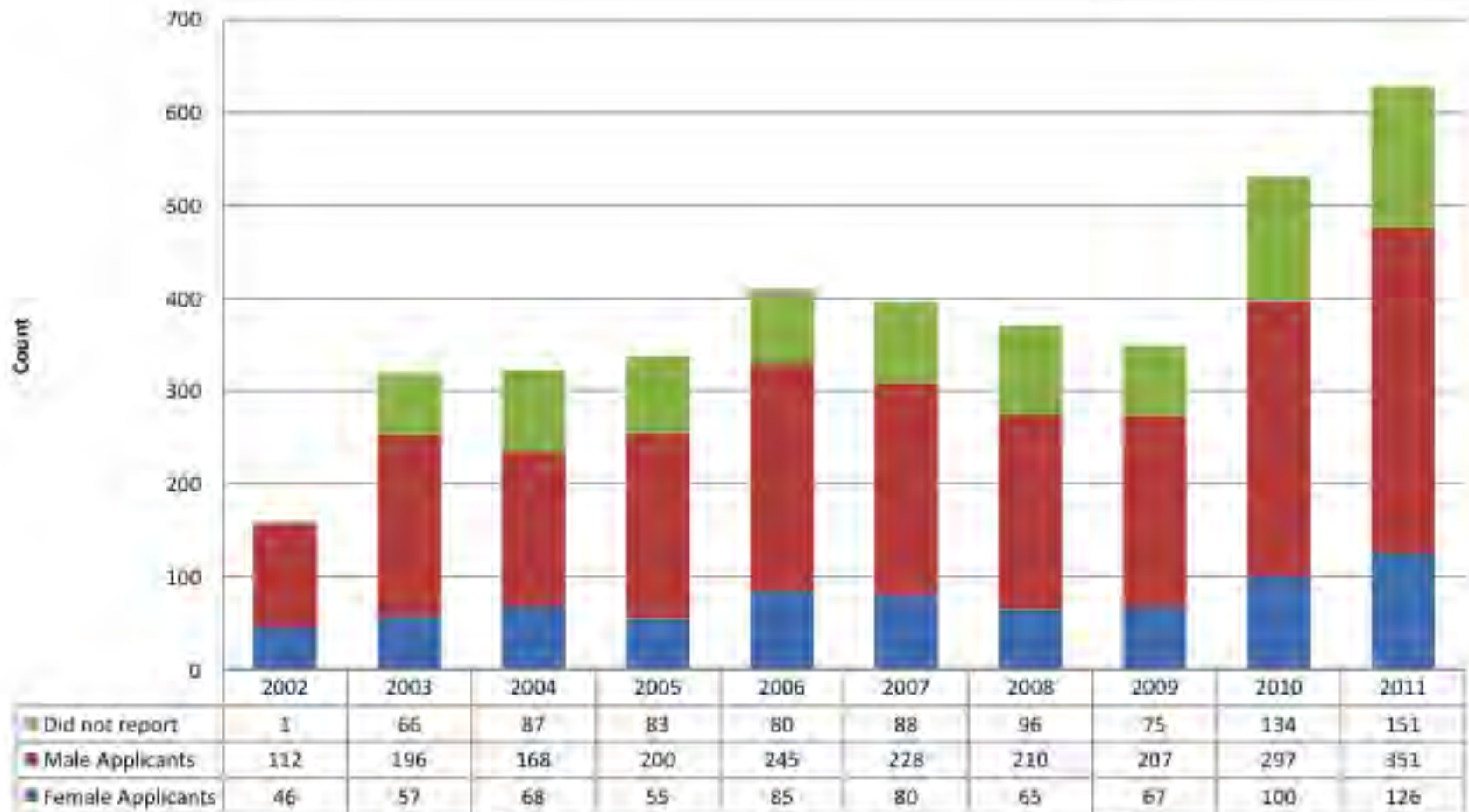
The Subcommittee recommends that the focus of the program be expanded to include enabling sciences, either through modification of the current program mandate or through the introduction of separate programs.

Women and Minorities

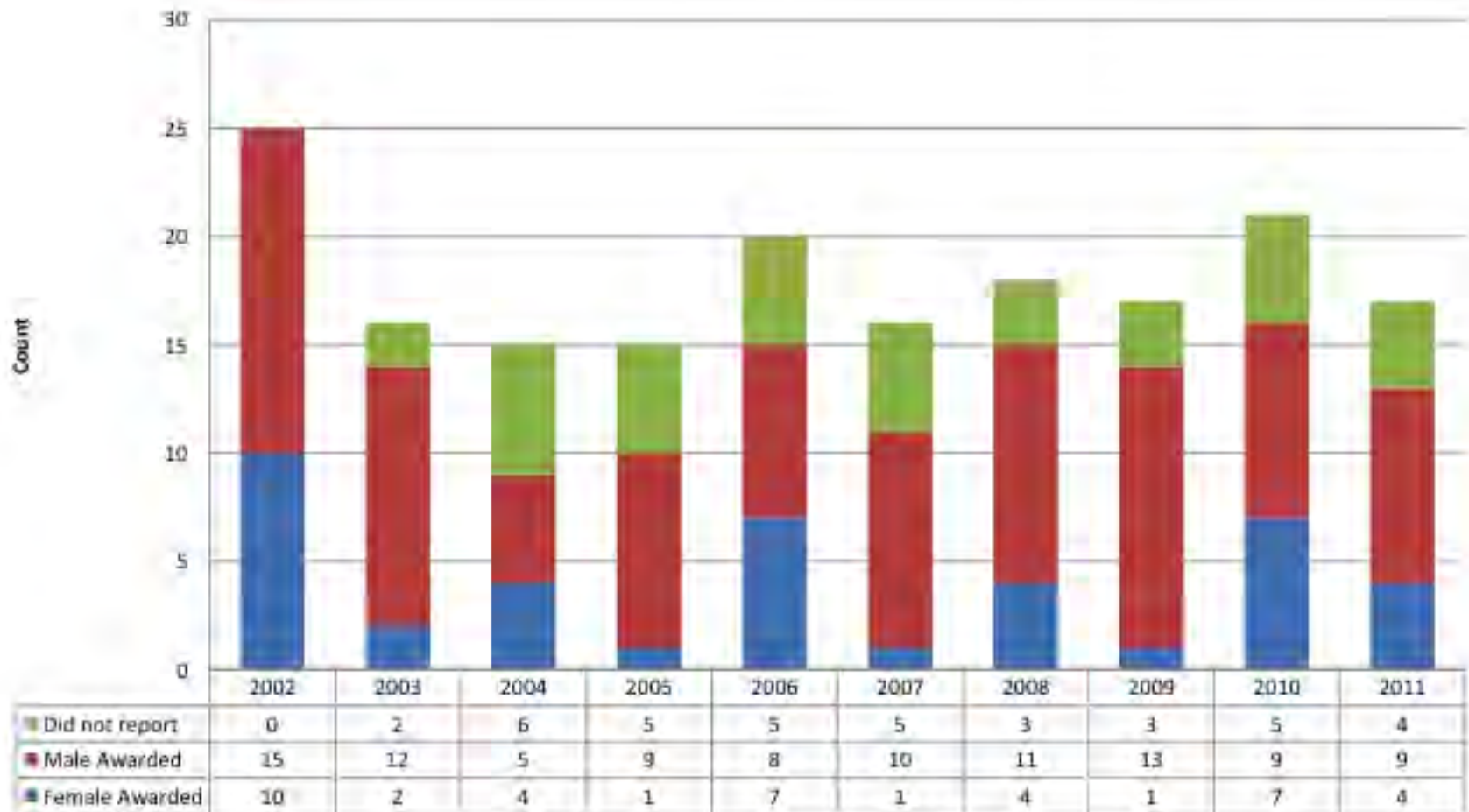
Based on

- Voluntary Data
- Outreach efforts

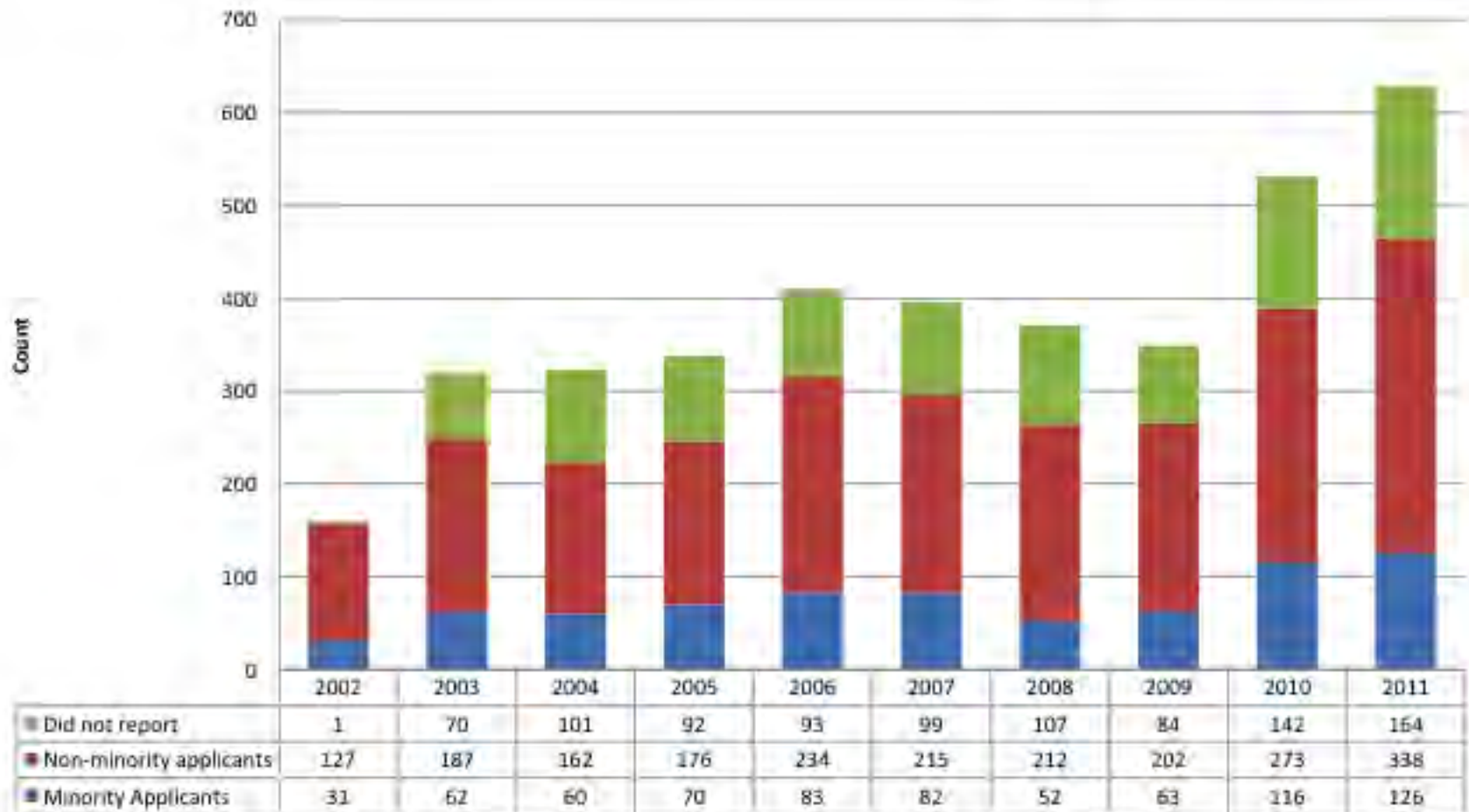
2002 – 2011 Applicants by Gender



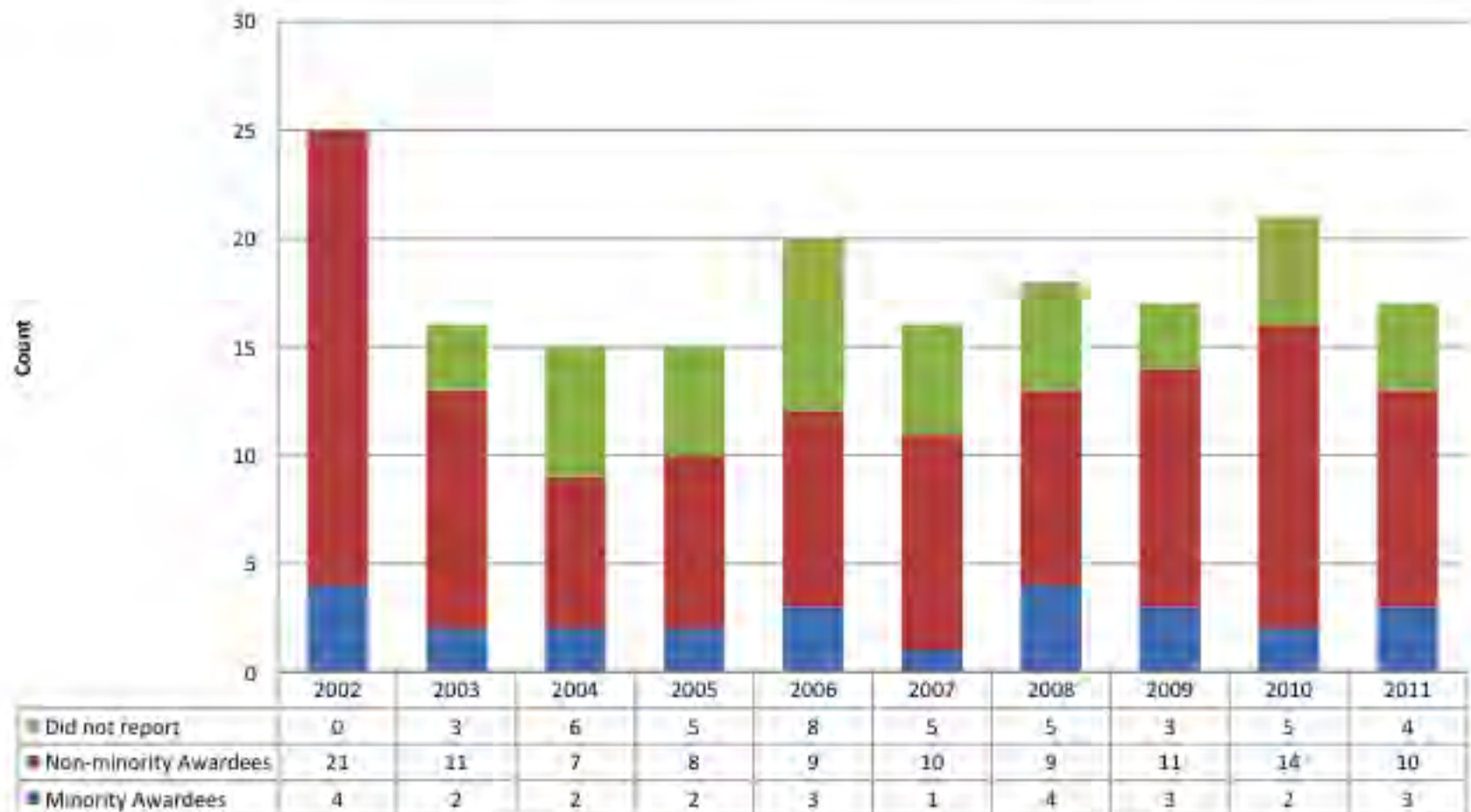
2002 – 2011 Awardees by Gender



2002 – 2011 Applicants by Minority



2002 – 2011 Awardees by Minority



Women

CSGF Data 2001-2010

- Applicants 26%
- Awardees 29%

SIAM statistics (Courtesy Jim Crowley)

- Non-student members 13%
- Student members 22%

Recent PhD (2009-2010)

- Math 31.4%
- Computer Science 18.8%

Minority

CSGF Self-reported Data (2001-2010)

- Applicants 26%
- Awardees 19%

No available data

Outreach Activities

Krell Staff attend conferences, booths handouts, plenary talks

- Women in Engineering Program Advocates Network (WEPAN),
- Association Minority Engineering Program Advocate (NAMEPA),
- Society of Women Engineers,
- Society for the Advancement of Chicanos and Native Americans in Science (SACNAS) ,
- Grace Hopper Conference Celebrating Women in Computing,
- Richard Tapia Celebration of Diversity in Computing Conference,
- SCxy Broader Engagement Program.

Outreach Activities

Mail printed material

- Diversity Careers,
- Association of Women in Science,
- Association of Women in Mathematics

Email material

- Women in Engineering,
- Systems
- Self-identified individuals

Conclusions

The Subcommittee feels that these efforts are commendable and no doubt lead to a higher participation of women and minorities than otherwise.

Recommendation: *The Subcommittee commends the Krell Institute on its efforts in this area and recommends that it continue these efforts.*

Other Educational Programs

- NSF GRFP

Other Programs

- DOD National Defense Science and Engineering Graduate Fellowship
- NASA Graduate Student Research Programs
- EPA STAR Graduate Fellowship
- USDA National Needs Graduate Fellowship
- NIH NRSA for Individual Pre-doctoral Fellowships

NSF GRFP

Awards Given

Year	2006	2007	2008	2009
CISE	53	52	82	102
DMS	28	23	63	62

No data available on number focused on Computational Science

Conclusions

The Subcommittee believes that the CSGF is unique in its focus on Computational Science. It provides features that other Graduate research Fellowships do not, such as the Plan of Study, the Practicum, the Annual CSGF Conference and efforts to keep alumni engaged. In this regard, the CSGF is an exceptional program that produces interdisciplinary scientists uniquely qualified to address current and future computational science challenges.

Recommendation

Recommendation: *The Subcommittee concludes that this is a unique educational program with features the DOE can best provide and recommends that the DOE continue stewardship of the program.*