



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

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# DOE Applied Mathematics Committee of Visitors (COV) Response

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# Applied Mathematics COV Members

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- **Juan Meza** (Chair), Dean, School of Natural Sciences, University of California, Merced
- **Mary Ann Horn**, Program Director, Division of Mathematical Sciences, National Science Foundation
- **Padma Raghavan**, Director, Institute for CyberScience, Distinguished Professor of Computer Science and Engineering, The Pennsylvania State University
- **Homer Walker**, Professor, Mathematical Sciences Department, Worcester Polytechnic University
- **Alyson Wilson**, Associate Professor, Department of Statistics, North Carolina State University

## COV Summary Finding

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- The Applied Mathematics Program is ***highly effective*** in its process to solicit, review, recommend, and document proposal actions.
- The Applied Mathematics ***program managers*** do an ***excellent*** job of monitoring all aspects of their portfolios.
- The overall ***breadth and depth*** of the Applied Mathematics portfolio is ***excellent***.
- ASCR has a ***long tradition*** of supporting some of the ***best applied math research*** in the nation and also maintains an international leadership position in certain key mathematical areas.



# Applied Mathematics COV Charge

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Assess the efficacy and quality of the processes used to:

- Solicit, review, recommend, and document proposal actions
  - 4 Recommendations
- Monitor active projects and programs
  - 2 Recommendations

Within the boundaries defined by the DOE mission and available funding, comment on how the award process has affected:

- The breath and depth of portfolio elements
  - 3 Recommendations
- The national and international standing of the program with regard to other applied mathematics research programs
  - 2 Recommendations

# Solicit, review, recommend, and document proposal actions

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## **COV Recommendation (1 of 4):**

- A significant number of new investigators have been funded by the program in recent years. The COV recommends that the program managers continue to look for ways to enhance the program's ability to attract new investigators, while seeking to maintain the overall excellence of the program.

## **Program Response:**

- ASCR will continue to look for ways to attract new investigators. Currently, ASCR attracts new investigators through participation at DOE workshops and professional conferences such as Society for Applied and Industrial Mathematics (SIAM). Outreach to other professional societies such as American Statistical Association (ASA) has recently been initiated. Another mechanism to enhance awareness for researchers unfamiliar with ASCR is through participation on ASCR review panels and electronic reviews. Enhancing ASCR webpages can also help better inform new investigators regarding the DOE Applied Mathematics program.

# Solicit, review, recommend, and document proposal actions

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## **COV Recommendation (2 of 4):**

- The COV recommends that program managers be allowed to travel as needed to scientific meetings. Communicating with the research community is essential to maintaining the program's vitality and is especially important to attracting new investigators to the program.

## **Program Response:**

- ASCR agrees that program managers should travel to scientific meetings. Given that travel funds are limited, program managers provide a prioritized list of the conferences and technical meetings they would like to attend. ASCR senior management then manages the travel funds.

# Solicit, review, recommend, and document proposal actions

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## **COV Recommendation (3 of 4):**

- Regarding the CSGF program, the COV concurs with the 2011 report in recommending that the focus of the program be expanded and funding doubled over the next five years. The COV also recommends that the program remain within ASCR and not be moved to the National Science Foundation.

## **Program Response:**

- ASCR thanks the Committee for this comment.

## **COV Recommendation (4 of 4):**

- The COV recommends that award rates for Applied Mathematics Program solicitations be made publicly available. This information would be useful to prospective proposal submitters.

## **Program Response:**

- ASCR will update the Applied Mathematics web pages and provide this information for solicitations in 2013 and thereafter.

# Monitor active projects and programs

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## **COV Recommendation (1 of 2):**

- The COV recommends adding an annual center directors meeting in order to enhance linkages among the three Mathematical Multifaceted Integrated Capability Centers (MMICCs). The meetings could serve to highlight technical achievements and open problems could be shared to enable opportunistic collaborations. Additionally, it could serve as a forum to share lessons learned about effective center management.

## **Program Response:**

- ASCR agrees with this recommendation and will add an annual center directors' meeting.





# Monitor active projects and programs

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## COV Recommendation (2 of 2):

- The COV recommends instituting the use of a standard reporting format for the annual progress reports, including length and description of information to be provided.

## Program Response:

- ASCR agrees that a standard reporting format is useful. ASCR understands that a federal-wide standard format is being developed and will implement that format as quickly as possible.
- DOE laboratories progress reports (limited to 8 pages) include:
  - Technical progress (free format)
  - Any noteworthy changes in scope, schedule, budget, issues, or personnel in the last year or anticipated in future.
  - A brief (< 1 page) summary of your work plan for the next fiscal.
  - Bulleted list of key accomplishments, including relevance and impact to DOE
  - Transitions for past and future research. Comprehensive list of publications, presentations, or other noteworthy deliverables, e.g. software produced. (Not counted toward page limit)



# The breadth and depth of portfolio elements

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## **COV Recommendation (1 of 3):**

- The COV recommends that ASCR develop a short-term visitors program with the MMICCs, with concomitant funding, to enable promising researchers to develop collaborations with center members. Even with a relatively modest investment, such a program holds the potential for greatly increasing the scale and scope of new capabilities developed at an MMICC by leveraging research supported in large part through universities and other agencies. It may also help to bring new researchers into the Applied Mathematics Program.

## **Program Response:**

- ASCR will consider this recommendation. ASCR will discuss this with the MMICC center directors and also examine other visitors' program to determine an appropriate implementation of such a program and the associated costs. Assuming strong interest from the MMICCs and availability of funds, ASCR may implement this recommendation in FY15.



# The breadth and depth of portfolio elements

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## **COV Recommendation (2 of 3):**

- The COV recommends investigating the addition of a new interdisciplinary program of applied mathematics-statistics-computer science-facilities that could drive the next generation of fundamental research broadly applicable to the analysis of experimental/observational facilities data.

## **Program Response:**

- ASCR will consider this recommendation as part of ASCR strategic planning activities.



# Math / Stats for DOE Data Research Projects

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## **Active Subspace Methods for Data-Intensive Inverse Problems**

*Paul Constantine*, Colorado School of Mines, Wang (MIT), Youssef Marzouk (MIT), Tan Bui (UT Austin)

## **Combining Data and Simulation to Predict the Behavior of Complex Systems**

*John Bell*, Lawrence Berkeley National Lab (LBNL), Marcus Day (LBNL), George Pau (LBNL), Michael Kowalsky (LBNL), Jonathan Goodman (NYU), Ray Grout (NREL), Salman Habib (ANL)

## **Machine Learning Algorithms for Matching Theories, Simulations, and Observations in Cosmology**

*Jeff Schneider*, Carnegie Mellon University (CMU), Chris Genovese, Shirley Ho, Rachel Mandelbaum, Hy Trac, Peter Freeman, Barnabas Poczos, Chad Schafer (CMU)

## **Scalable Statistics and Machine Learning for Data-Centric Science**

*Prabhat*, Lawrence Berkeley National Lab (LBNL), Benjamin Bowen, Aydin Buluc (LBNL), Michael Mahoney, Michael Saunders (Stanford), Jon McAuliffe, Sommer (UC Berkeley)

## **Mathematical Modeling and Optimization for Automating Constrained Phase Retrieval**

*Stefan Wild*, Argonne National Lab (ANL), Sven Leyffer, Ian McNulty, Todd Munson, David Vine (ANL)

## **Spatio-Temporal Data Analysis at Scale Using Models Based on Gaussian Processes**

*Mihai Anitescu*, Argonne National Lab (ANL), Jie Chen (ANL), Michael Stein (U Chicago)



# A Snapshot of the ASCR Data Ecosystem

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- **Math / Stats for DOE Data**
- **Scalable Data Management, Analysis and Visualization (SDAV) SciDAC institute**
  - <http://www.sdav-scidac.org/>
- **ASCR / BES projects**
- **FY14 Computer Science solicitation “Scientific Data Management, Analysis and Visualization at Extreme Scale”**
- **Accelerating Scientific Knowledge Discovery**
  - [http://science.energy.gov/~media/ascr/pdf/program-documents/docs/ASKD\\_Report\\_V1\\_0.pdf](http://science.energy.gov/~media/ascr/pdf/program-documents/docs/ASKD_Report_V1_0.pdf)
- **ASCAC report on Synergistic Challenges in Data-Intensive Science and Exascale Computing**
  - [http://science.energy.gov/~media/ascr/ascac/pdf/reports/2013/ASCAC\\_Data\\_Intensive\\_Computing\\_report\\_final.pdf](http://science.energy.gov/~media/ascr/ascac/pdf/reports/2013/ASCAC_Data_Intensive_Computing_report_final.pdf)
- **Report on HEP / ASCR Data summit**
  - [http://science.energy.gov/~media/ascr/pdf/program-documents/docs/HEP\\_ASCR\\_Data\\_Summit\\_Report\\_April\\_2013.pdf](http://science.energy.gov/~media/ascr/pdf/program-documents/docs/HEP_ASCR_Data_Summit_Report_April_2013.pdf)
- **Data Crosscutting Requirements Review**
  - [http://science.energy.gov/~media/ascr/pdf/program-documents/docs/ASCR\\_DataCrosscutting2\\_8\\_28\\_13.pdf](http://science.energy.gov/~media/ascr/pdf/program-documents/docs/ASCR_DataCrosscutting2_8_28_13.pdf)



# The breadth and depth of portfolio elements

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## **COV Recommendation (3 of 3):**

- The COV recommends that ASCR continue its outreach efforts to professional societies and research communities through sponsored workshops and conference attendance, as these are critical to program development.

## **Program Response:**

- ASCR agrees with this recommendation and will continue to pursue outreach to the applied mathematics community pending available funds for travel and for DOE-sponsored workshops.

# The national and international standing of the program with regard to other applied mathematics research programs

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## COV Recommendation (1 of 2):

- The COV recommends that the review and annual reporting process for the MMICCs include a listing of awards and accolades received by the project participants with brief summaries indicating the associated technical achievements. This report can be used to highlight the leadership role of the MMICCs.

## Program Response:

- ASCR agrees with this recommendation. An annual review of the MMICCs was implemented around the same time as the COV. These recommendations will be incorporated into the annual reporting requirements of the MMICCs.
- Current annual MMICC reviews include:
  - A 2-3 page summary of center including (1) Motivation: Grand Challenge and Integrated Math, (2) Research Plan, (3) Coordination/Integration plans.
  - 5 year road map.
  - Presentations by MMICC researchers that is peer-reviewed.
  - A progress report (15 page limit) with following appendices:
    - An up-to-date, high-level organizational chart.
    - Presentations and publications:
      - A list of peer-reviewed papers published/accepted for publication directly related to this MMICC.
      - A list of conferences, workshops, and other external meetings you or your team members have attended directly related to this MMICC.
      - A list of invited presentations you or your team members have given directly related to this MMICC.



# The national and international standing of the program with regard to other applied mathematics research programs

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## COV Recommendation (2 of 2):

- The COV recommends that the Applied Mathematics Program develop a set of key mathematical areas that will have the greatest impact on the DOE mission and in which they can either currently claim or plan to develop international leadership.

## Program Response:

- Since the COV, ASCR Applied Mathematics has defined a set of key mathematical areas, e.g. core strengths, which we consider to have to the greatest impact on the DOE mission.
- Core strengths:
  1. **Numerical PDEs:** Recognized leader with decades of investments and high DOE impact, e.g. Adaptive Mesh Refinement, Level Set Methods, Fast Multiple Methods
  2. **Linear Algebra & Scalable Solvers:** Recognized leader with decades of investments. Numerous solvers utilized within DOE and computational science community, e.g. PETSc.
  3. **Multiscale, Multiphysics & Multicomponent Methods and Models:** Recognized leader for real-world complex systems with a decade of investments.
  4. **Optimization:** Recognized leader in optimization of complex systems with a decade of investments. Strong interest within DOE applied programs.
  5. **Stochastic Systems & Uncertainty Quantification:** Establishing leadership. Almost a decade of investments.
  6. **Mathematics and Statistics for DOE Data:** Relatively new thrust area. Critical to achieving next-generation scientific discoveries at DOE facilities given exponential growth and complexity of experimental, observational and simulation data.