National Science Foundation
4201 Wilson Boulevard
Arlington, Virginia 22230

NSF 14-027

Dear Colleague Letter: DMREF proposals of special interest to the Division of Mathematical Sciences in fiscal year 2014

January 6, 2014

Dear Colleague:

The Division of Mathematical Sciences (DMS) of the National Science Foundation (NSF) strongly encourages mathematicians and statisticians to participate in the 2014 NSF activity Designing Materials to Revolutionize and Engineer our Future (DMREF).

DMREF is the main program by which NSF participates in the Materials Genome Initiative for Global Competitiveness (MGI), a national materials initiative. MGI recognizes the importance of materials science to the well-being and advancement of society and aims to "deploy advanced materials at least twice as fast as possible today, at a fraction of the cost." It integrates all aspects of materials design, including materials discovery, development, property optimization, systems design and optimization, certification, manufacturing, and deployment, with each employing the toolset that is being developed within the materials innovation infrastructure. The toolset will integrate synergistically advanced computational methods and visual analytics with data-enabled scientific discovery and innovative experimental techniques, aiming to revolutionize the approach to materials research and engineering.

DMREF comprises well-coordinated activities involving the Directorates of Mathematical and Physical Sciences (MPS), Engineering (ENG), and Computer & Information Science & Engineering (CISE). For further details and participating divisions please see NSF 14-020, the broadly aimed Dear Colleague Letter about DMREF in fiscal year 2014. As described in that Letter, success in the initiative requires a collaborative, synergistic, iterative approach that shows interactions among theory, computation, and experiments. This approach is the central principle of MGI. DMREF proposals will be reviewed jointly by the appropriate participating divisions. Adherence to the aims and principles of MGI will facilitate this joint review.

DMREF proposals of specific interest to the Division of Mathematical Sciences must:

- seek new mathematical or statistical results that will advance the DMREF agenda;
- describe a research plan that meets the central Materials Genome Initiative principle of closely coupled, iterative interplay among theory, computation, and experiment;
- be submitted within the window 15 January - 18 February 2014, inclusive;
- be submitted to the Design of Engineering Materials Systems (DEMS/PD 12-8086) program; and
- deal with problems in the range of issues described in the DMREF Dear Colleague letter NSF 14-020.

In addition,

- the title of a DMREF proposal should begin with the word “DMREF.”

Proposals that do not seek new mathematical or statistical results may nevertheless fit well within

DMREF, and mathematical scientists are strongly encouraged to join any DMREF proposal that makes good use of their expertise. DMREF proposals may come from single investigators or from teams of investigators. However, successful proposals will offer evidence of that close, iterative collaboration among experts from different disciplines that is necessary to meet the central MGI principle on which DMREF is based. Letters of collaboration, which say what the collaborators will do for the proposed project and that affirm the collaborators' participation in the iterative interplay required for DMREF, are appropriate evidence.

In addition to the mathematical and statistical modeling and analysis that occur in the interactions among experiments, models, and simulations, DMREF topics of special interest to DMS include, but are not limited to:

- optimization of design in complicated, high-dimensional state spaces;
- effective data mining methods to uncover relationships important for predictive modeling and design (e.g. between microstructure and bulk properties, or among composition, processing, and bulk properties);
- first-principles understanding of materials;
- data-analytic tools and the interplay between data and predictive modeling;
- challenges presented not only by multiscale issues, but also by the problem of rapidly resolving differences between theory and simulation in the face of experimental data.

The last example is similar to data assimilation and data fusion problems encountered elsewhere, but here the possibilities offered by better data and closely coupled iteration create new opportunities for theoretical and algorithmic advances, on both the mathematical and statistical sides.

Participants interested in submitting proposals are strongly encouraged to first contact any of the program officers listed in the main DMREF Letter. For DMS, please confer with Michael Steuerwalt.

Henry Warchall
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