Proposal to the DMS Workforce Program

Fellows in Theoretical and Mathematical Science

A Postdoctoral Program for Science at the Interface

Project Description

1. Senior Participants and Central Goal

Principal and Co-Principal Investigators: Jonathan Mattingly (PI, Department of Mathematics), Alan Gelfand (co-PI, Department of Statistical Science), Berndt Mueller (co-PI, Department of Physics), Weitao Yang (co-PI, Department of Chemistry)

Other Senior Personnel: Harold Baranger (Physics), David Beratan (Chemistry), Patrick Charbonneau (Chemistry), James Clark (Environmental & Earth Sciences), Steven Cummer (Electrical & Computer Engineering), Gabriel Katul (Environmental & Earth Sciences), Katia Koelle (Biology), Mauro Maggioni (Mathematics), Sayan Mukherjee (Statistical Science), Kamesh Munagala (Computer Science), Frederik Nijhout (Biology), Dalia Patino-Echeverri (Environmental & Earth Sciences), David Schaeffer (Mathematics), Joshua Socolar (Physics), Carlo Tomasi (Computer Science), Stephanos Venakides (Mathematics), Thomas Witelski (Mathematics), Rebecca Willett (Electrical & Computer Engineering), Robert Wolpert (Statistical Science)

We propose to create and administer a formal Fellows program that encourages talented postdocs with mathematical or theoretical science expertise to work on topics arising in a variety of disciplinary contexts and to benefit from interactions with peers and established faculty research groups. A number of senior faculty spanning a broad range of mathematical, physical, biological, and engineering sciences are prepared to mentor a group of postdoctoral fellows and actively participate in a community that will seek common themes and opportunities for research the crosses traditional disciplinary boundaries. Our primary goal is to train broad-minded mathematical scientists capable and willing to move between disciplines and problem domains during their careers. We also expect benefits for the Mathematical Sciences network at Duke and beyond, as Fellows with this type of training make connections between scientists that may not have recognized the ways in which their interests intersect.

2. Motivation and Background

2.1. Context and Motivation.

As mathematics extends its reach into new disciplines; as theoretical approaches become increasingly important with enhanced computational power; as technology penetrates breath-takingly quickly new corners of everyday life; the need for broadly trained transdisciplinary theoretical scientists becomes increasingly important. They provide the horizontal layer across subject areas and departments which facilitate the transfer of mathematical methods and techniques. They are nimble enough to move into emerging areas transplanting ideas developed elsewhere or forming an entirely new synthesis from disparate parts. There is hardly a major NSF initiative which does not require an interdisciplinary team of scientists including almost always a number of mathematical or theoretical scientists.

The importance is evident, but how does one form and train such a group? Is it an organic process that one leaves to chance, particularly the training? How does one consciously create the environment and cross-disciplinary intersections which fortuitously formed the trans-disciplinary scientist who exists in many faculties? The questions of organization and training are necessarily intertwined. While this proposal concentrates on the latter, it is informed by the former. Furthermore, the proposal's efforts to vertically integrate reinforces the organizational structure we see as appropriate. Hence, it is appropriate to discuss the organization briefly.

Though the exact definition is in constant flux, there is a discipline of applied mathematics. There are programs and departments of applied mathematics or mathematical sciences which train students and conduct research in this intellectual space. Duke has a very active, substantial, and nationally recognized applied mathematics group in its Mathematics Department. It has a strong and nationally recognized statistics group whose educational mission was recently expanded by the formation of the Department of Statistical Science. There are strong theory groups in established disciplines such as Chemistry and Physics. In many respects organizational lines between these groups are historical and arbitrary. Fluidity should be encouraged not stifled.

With the increased quantitative emphasis in Biology and Medicine, every science department on campus has a component conducting theoretical and mathematical research. Every major university initiative in the sciences has a theoretical component with heavy mathematical content. This leads to a fragmentation of mathematical science around the university. It is in fact desirable to have applied mathematicians and theoretical mathematicians embedded in all of the sciences and engineering departments. This tethering keeps the discipline intellectually honest and relevant. However, the dispersion needs to be balanced by an organizational structure that creates a common forum for all mathematical and theoretical scientists, who aspire to look beyond their own narrow area of specialization for new applications or intellectual stimulation. The Center for Theoretical and Mathematical Sciences described below attempts to fulfill this function by building and organizing this community in a way that is complementary, supportive, and inclusive of the applied mathematics group headquartered in the Mathematics Department.

But still, how does one train a new generation of mathematical scientists ready to move into emerging areas transplanting ideas developed elsewhere or forming an entirely new synthesis from disparate parts? It seems that an important moment of opportunity lies in the postdoctoral years. These are naturally the time of broadening after the task of assimilation of and indoctrination into a single field is formally completed with the award of a doctorate. By exposing postdocs to the wealth of techniques and domains of applications of the mathematical and theoretical sciences, we hope to create broad-minded mathematical scientists capable and willing to move between disciplines and problem domains during their careers. By including them in a community of mathematical scientists spanning horizontally across many fields, we hope to spread and build that culture as they move forward in their careers. By strengthening the Mathematical Sciences network across the university, we hope to enrich the set of problems considered by applied mathematics groups. One must both expose the mathematically inclined to more applications and increase the mathematical sophistication and perspective of those who started with a more problem specific perspective.

2.2. **Institutional background.** In order to take advantage of emergent opportunities for theoretical collaboration and exchange of ideas and methods across disciplines, Duke University established a trans-disciplinary *Center for Theoretical and Mathematical Sciences* (CTMS) in 2008 [2]. The mission of the Center is (*i*) to strengthen the communication and exchange of ideas among members of the theory and mathematical sciences community across departmental and school lines; (*ii*) to work with departments and institutes to attract broadly interested, outstanding theorists in scientific priority areas; and (*iii*) to germinate new programmatic collaborations among theorists or between theorists and experimentalists in forefront areas of research. From its inception, the CTMS has been jointly shaped and modeled by researchers in Applied Mathematics, Physics, Chemistry and Biology. This diversity distinguishes it from other such entities.

To pursue its mission, the CTMS strives to build an open community of scholars practicing scientific research of a predominantly theoretical and mathematical nature who are interested in applying their skills beyond the traditional confines of their discipline and/or in collaborating with scientists from other disciplines. The Center organizes lectures of broad interest, bi-weekly informal "brown bag" lunch discussions nicknamed *The Marketplace of Ideas*, and focused workshops on mathematical topics of wide interest. It hosts visiting scholars whose interests extend beyond a single discipline or who are more method- than problem-oriented. The CTMS also facilitates interactions among scholars and students in different disciplines, at all levels, by providing web-based information on relevant courses and research activities, brings experimentally working scientists and students in contact with theorists and applied mathematicians who could advance their research, and works with departments and deans to identify possible areas for faculty development.

The Center does not exclusively cater to theoretical scientists who are routinely engaged in interdisciplinary research. In many, though not in all, cases these already have their own self-organized communities of like-minded scholars in which they discuss and exchange ideas. The Center is designed to go beyond that by providing a forum for those theorists who mostly work within their discipline, but branch out from time to time to address important problems elsewhere, when the scientific tools at their disposal are conducive to the problems' solution, and then prefer to return to their more narrowly defined research. For this reason, the community built and served by the Center must remain an open one. As an example of this openness, the Center sponsors a theoretical component of an experimental thesis project on a competitive basis. In many disciplines, research of a theoretical or mathematical kind is not usually supported by the funding agencies.

2.3. **The CTMS Fellows Program.** The proposed *Postdoctoral Fellows Program in Theoretical and Mathematical Science at the Interface* will be an integral part of the CTMS. It will complement the existing CTMS structure to create an innovative, integrative science program involving scientists at all levels of the academic hierarchy. The core goal of the CTMS Fellows Program is to educate a cohort of highly talented mathematical scientists and theorists who have extensive experience in self-determined trans-disciplinary research and will be strong candidates for faculty positions in a broad range of disciplines, from applied mathematics, to physics, chemistry, biology, and even engineering or environmental science. In doing so, we will create a group of strong mathematical scientists with experience working in interdisciplinary contexts and interacting directly with frontier researchers in different fields. In addition to the training benefits to the Fellows, the CTMS Fellows Program will help researchers at Duke extend the reach of mathematical sciences to new areas, bring into focus common problems facing scientists in traditionally distinct disciplines, and enrich existing applied mathematics by bringing new topics to their attention. We propose to draw from both the mathematcians looking to better connect with applications and the more disciplinary trained scientists looking to increase their mathematical and theoretical sophistication and perspective.

A dedicated program of this kind will be able to avoid constraints from traditional institutional and funding structures that make it difficult for many scientists at academic institutions to take on postdoctoral fellows who do research between disciplines and are not constrained to work on narrowly defined projects. Funding for postdoctoral researchers in the physical and biological sciences is usually based on individual PI or group grants which are programmatically well defined and address a specific scientific problem. Mechanisms available for graduate student education, such as interdisciplinary training programs and grants, are rarely, if ever, available for postdocs. The proposed CTMS Fellows program is aimed at counteracting this deficit. We often speak of the need for broad minded interdisciplinary mathematical scientists. The postdoctoral period is a natural moment for such broadening, before the rigidity of disciplinary boundaries is set. Yet, there are very few mechanisms to encourage this in the at the institutional level.

A guiding exception to this are the "term-limited assistant professorships"[1] that exist in some mathematics and applied mathematics departments. These prestigious positions afford the post-doctoral fellows a high degree of intellectual freedom to interact with a number of faculty and build their own research programs while benefiting from a first rate research environment. The Duke mathematics department has a steady-state of six such "Assistant Research Professors." However

[1]Also often called "named" assistant professors. Examples include Szegö assistant professors at Stanford. Benjamin Pierce instructors at Harvard, Doob assistant professors at UIUC, Bing assistant professors at Texas, Prager Assistant Professor at Brown applied mathematics.

usually at most three of these are dedicated to applied mathematics, analysis and probability. In the past, the mathematics department has used these positions to hire postdoctoral fellows who worked closely between mathematics faculty and faculty in Physics, Biology, Statistics, and Computer Science. Greater numbers will allow the formation of a stronger, more cohesive community. By expanding the scope to beyond mathematics, it will allow for a more diverse and rich community. At once exposing a greater community to applied mathematics and applied mathematics to a large body of problems and techniques. The culture and teaching structure of Mathematics allows for these positions to be funded largely through teaching a full faculty load of three courses a year. This is less feasible in other disciplines where the structure of teaching and transitions postdoctoral education make heavy teaching loads impractical and non-competitive in the open market. Furthermore, the extremely interdisciplinary nature of the proposed fellowship program requires Fellows with sufficient time to interface and assimilate multiple academic traditions and skill-sets.

The CTMS Fellows program will also create a mechanism for continuously infusing new intellectual topics at the interface of theoretical science and applied mathematics. By teaching a graduate topics class or seminar, the Fellows will not only strengthen their own academic credentials and increase their future chances of securing a faculty position, but they will also provide a constantly renewing source of cutting edge mathematical tools and techniques for other members of the campus community. While CTMS Fellows will generally (but not exclusively) be hired with specific groups in mind, they will not be tied to a particular project. Furthermore, the Fellows will form a community that bridges across disciplines and provides for each of its members an environment that is intellectually broader and richer than that which any single research project or group could provide.

These three points together form the core of our rationale for creating the CTMS Fellows program. A group of interacting postdocs working in diverse but communicating fields will be a richer environment for career development than one or two post-docs working on a single grant. The freedom to follow their own course of intellectual growth while being mentored by senior scientists will produce a seasoned group of researchers who innovate at emerging interfaces without fear of crossing disciplinary boundaries. These are the characteristics of the best applied mathematics groups and large disciplinary research groups, but with a more limited scope. This model of community building has proven very successful among the Assistant Research Professors in the Mathematics department at Duke. A model needs to be found to strengthen the related community of postdoctoral fellows in the mathematical and theoretical Sciences. We propose to develop such a program.

2.4. **Timeliness and workforce relevance.** The proposed CTMS Fellows program will provide outstanding opportunities for broadly interested and talented, young applied mathematicians and theoreticians to develop their careers in a time when faculty positions are temporarily rare due to the cut-backs of searches by almost all academic institutions in the United States. From a longer term perspective, we view agency funding for such a program as "seed money" for a permanent trans-disciplinary postdoctoral fellows program in the theoretical and mathematical sciences that is supported by a combination of sources including a core of internal funds. We hope that it might serve as a model that could be duplicated at other institutions as a way to foster a more integrated and cooperative applied mathematics and theoretical science community across the university.

2.5. **Why at Duke University?** A workforce proposal such as this one needs to address the question: Why should this postdoctoral fellows program be sited at Duke University and not elsewhere? We believe that our institution is ideally positioned to explore the full potential of a broadly constructed, trans-disciplinary postdoctoral fellows program. The necessary organizational infrastructure, provided by the recently founded Center for Theoretical and Mathematical Sciences, is in place and functioning. The university has a long-standing commitment, recently re-confirmed and buttressed by the 2006 Strategic Plan *Making a Difference*, to interdisciplinary research unconstrained by departmental and school boundaries. Collaboration across these boundaries is not just a goal, it is happening at all levels of the professorial hierarchy.

The broad scope of the CTMS is a partial outgrowth of the vision of applied mathematics held in Duke's Mathematics department. The department enjoys very amicable relations between pure and applied mathematics with many faculty members claiming membership in both camps. The department has resisted forming a separate applied mathematical science department or program, preferring to keep it integrated with mathematics. This naturally has led the department to foster strong relations through collaboration with other allied departments and encourage the more disciplinary mathematical sciences to be embraced by partner departments. This results in a broad community ideally suited to nurture interdisciplinary post-doctoral fellows in the mathematical sciences.

Duke University also has strengthened its institutional support for postdoctoral fellows by creating an *Office for Postdoctoral Services* which offers individual career counseling, advice on application materials, mock interviews, career development workshops and symposia, and information about other services relevant to postdocs (e.g., international office, child care services, etc.). Duke's recent campus-wide Postdoctoral Policy defines rigorous benchmarks for compensation, mentoring, leaves and other benefits.

3. Program Structure

Primary Fellows: The program will consist of 9 Fellows spread over 6 years each with an appointment of 3 years. We feel that three years is the correct length of time to develop and make serious progress on an interdisciplinary project given that the Fellows will be interacting with established groups at Duke. The funds for 7 1/3 of the Fellows will come from this grant while 1 2/3 will be funded with university funds. In particular, university funds will be used to extend the effect of the grant in to a sixth year. The program ramps up over three years. Appointments will be for three years. New Fellows supported by the NSF will be hired in years 1-4. An entirely Duke supported Fellow will be hired in year 2. The two Fellows hired in year 4 will be funded by the NSF during the first 2 years (year 4 and 5) and by Duke during the 6th year.

	NSF Funded Fellows		Duke Funded Fellows		Total Fellows
	New	Total	New	Total	in residence
Year 1	2	2	0	0	2
Year 2	2	4	1	0	5
Year 3	2	6	0	1	7
Year 4	2	6	0	1	7
Year 5	0	4	0	0	4
Year 6	0	0	0	2	2

Table 1. Timetable new hires and total number of Fellows in the program, by funding source.

A program review in the 3nd year will help identify any structure problems with the program and help assess its long-term viability. We hope that other, sustainable funding sources will be found after year 3 so that the program can continue at full strength beyond year 4.

Associate Fellows: In addition to the main group of fellows, the program will name 2 *Associate Fellows* per year. These Associate Fellows will be individuals who were hired outside of the CTMS Fellows Program, but who once at Duke were deemed appropriate to participate in the program, though at lower level that is described in the next section. This will allow like minded postdocs who arrive at Duke by other means to be included in the CTMS Fellows community. This will greatly expand the reach of the flellowship program. This will also ensure that the community reaches critical mass. Initially it will also provide some more senior and experienced leadership in the Fellows cohort as the program begins. The Associate Fellows will be chosen by the leadership of the CTMS based on letters of nomination from their faculty mentors.

3.1. **Selection process.** Positions will be broadly advertised, including though all of the standard channels used by the participating disciplines. The Fellows will utilise the web-base application site "AccademicJobsOnline.org" which is derived from the highly successful "Mathjobs.org". Both were developed at Duke in the Mathematics department and have been used by mathematics departments across the coutnry and other departments across Duke.

Selection committee composed of faculty from all relevant scientific areas drawn from the PIs and the Faculty associates will review applications. A short list, selected principally on the candidates intellectual and research quality, potential interdisciplinary, compatibility with research at Duke, and diversity concerns will be invited to campus for interviews. While some attention to potential faculty mentors will be made, the matching will primarily take place once the candidate visits for an on campus interview. After the interviews, final decisions will be made. Only candidates with a willing and enthusiastic mentor with be offered a fellowship. Our target is that at least 30% of the Fellowships will go to Woman and under represents minorities. With this in mind, each short list will have a composition reflecting our target of Woman and under represented minorities. [74, 1]

3.2. **Duties of the Fellows.** The central goal of the CTMS Fellows program is to develop tomorrow's leaders in Theoretical and Mathematical science and to ensure that they are well equipped to make transformative contributions to their current fields the new fields we can not for see. Hence, the Fellows must be practiced the art of interacting with theoreticians in other fields and be aware of the toolbox under use in other fields. They must begin to acquire the skills needed to teach across disciplines and mentor students and colleagues. Lastly, if they are to lead, they must have some appreciation for how research in general and their research fits in the broader university and society as a whole.

All of the Fellows (both Primary and Associate) will be expected to:

- Engage in research on topics transcending a single discipline.
- Participate in biweekly CTMS Fellows research meetings.
- Engage in CTMS activities, especially "Marketplace of Ideas" and yearly CTMS retreat.
- Write an annual report to mentor and PI committee on activities and achievements (with feedback).

In addition the Primary Fellow will be expected to:

- Upon arrival at Duke, present a seminar in one of the CTMS forums to introduce the fellow scientifically to the community.
- Typically in year 1, teach one high-level (graduate and postdoc-level, 3 hrs./week) course on a frontier topic related to their research.
- Invite 4-5 speakers to the CTMS Fellows seminar to speak on topics related to their research and complimentary the Fellow's topics course.
- Attend the grant writing workshop and, by the appropriate deadline in second year, write a research grant suitable for summation to the NSF.
- Give a general lecture on their field. This could be in the from of a lecture targeted at undergrads or high-school students or in one of the general audience forms at Duke which mix the sciences, humanities and social sciences together.

In addition the Associate Fellows will be expected to:

- Attend the grant writing workshop.
- Invite 2 speakers to the CTMS Fellows seminar whose work is pertinent to their research.

CTMS Fellows research meetings: At each of these bi-weekly meetings, a different Fellow will present the current state of their work and receive feedback from the group. These informal sessions are a vehicle for the Fellows to exchange ideas and techniques. The Fellows will be expected to provide a suggested reading list. At least some of the reading should be appropriate to provide the needed background to a general mathematical scientist uninitiated in the specific field. A different faculty member will chair the meetings each semester. In addition, the Fellow's mentor will attend on the days when their mentee is presenting. We believe that instruction and mentorship by one's peer-group is invaluable and important to cultivate through out one's career.

Graduate Topics Course: Each Fellow will teach a topics graduate course, typically during the first year of the fellowship. The course will be centered on the themes of research which interest the Fellow. This course could take the form of a directed reading seminar with the group reading through and presenting important papers in the field. Or, it could be a more traditional lecture class with the Fellow giving lectures providing the needed background to enter into the field. The goals of the course are many fold. First, it will be an introductory vehicle to draw others at Duke into the fellows field and provide others with the common language needed to interact with the Fellow scientifically. Second, running a course centered on one's research has an uncanny tendency to improve one's own understanding and sharpen the questions one asks. Third, the courses given by the CTMS fellows will provide a constant stream of fresh topics perspectives into the local scientific environment. Students and researchers from the neighboring institutions (University of North Carolina, NC State University) regularly attend advanced classes and lectures at the other intuitions. Hence, the courses will enrich the intellectual fiber of the entire region. Lastly, since the fellows will be fresh from other top research environments, it will be an effective way to disseminate and spread the understanding developed in other institutions to Duke.

CTMS Fellows Seminar: The CTMS fellows will run a seminar series featuring talks by leading researchers from other universities. In a semester following the topics course, each fellow will be responsible for inviting a block of speakers related to their interests. In many ways, this will be a continuation of the topics course. It will further expose the community to the fellows research area and interests, hopefully further stimulating activating in the community around the Fellow's interests. Lastly, serving as host for the invited speakers will provide the Fellow with an invaluable chance to network and obtain exposure to the leaders in the field.

Grant Writing Workshop: The Duke mathematics department for many years has run a successful one afternoon workshop on how to write a grant. The CTMS will run its own session at the workshop, coordinating with the Mathematics department, to add information on writing grants beyond the DMS and the NSF in general. This will also be helpful for the applied mathematics postdoctoral fellows in the mathematics department. The CTMS fellows will be expected in there second year to write a grant in consultation with their mentor. The rational being, that grant writing is a good exercises in sharpening, defending, and prioritising one's research agenda. If the proposal is deemed worthy, the Fellow will be encouraged to submit it. This may allow the Fellow to obtain their own funding source. This is both invaluable in procuring a tenure track position as well as freeing CTMS funding to hire another Fellow in subsequent years.

Summer Mentorship Experience: Developing mentoring skills is important as one transitions from Postdoctoral Fellow to junior faculty or staff researcher. In a research setting, postdoctoral researchers naturally aid with mentoring graduate students. However, it is quite different to plan and supervise a project completely. To do so can be an important learning experience. During one of the summers, each of the Fellows with participate as a mentor in one of the many high school and undergraduate research programs run at Duke. These programs typically last 5-7 weeks during the summer. The students are in residence at Duke and work on a project designed by the Mentor. Among the programs to choose form are the PRUV program in Mathematics, the Instutute for Genome Science and policy (IGSP) Summer Fellows program (in Genomics and System Biology), and a number of REU run by individual faculty in the sciences at Duke. In addition, the chemistry department participates in the highly successful SEED program for mentoring high school minority students.

General Audience/Outreach Lecture: It is important to have an appreciation for how one's subject fits in to the greater landscape of society. Even with this understanding, the ability to communicate this is a skill which must be cultivated. As the world becomes more driven and saturated with technology the ability of broad minded scientists to communicate to a larger audience is evermore important. Hence it is critical to express to young researchers that these skills are valued so that they might, from the beginning of their careers, cultivate them. During the last year of the fellowship each fellow will give either a public outreach lecture or a lecture aimed at a diverse general academic audience. There are a number different venues in which this could happen. Most of the science departments have undergraduate clubs that welcome general talks. Similarly, the North Carolina School of Science and Mathematics, a state magnet high school, is only one block from Duke and welcomes such talks. The PI is a graduate of this school. There are also a number of forums at Duke, such as the Institute for Genome Science and Policy, which mix natural scientists, social scientists, and Humanists together in one lecture series.
Undergraduate Instruction: In many disciplines, it is important and standard for post-doctoral fellows to act as the primary instructor for a number of undergraduate classes during their post-doctoral years. In math, it is the norm and essentially required to secure a tenure-track position. In Physics, Statistics, and Computer science it is not unheard of for post-doctoral fellows to teach a class. It is less frequent in other subject. The CTMS Fellows will be encouraged teach at least one undergraduate course, usually during their second year. Due to the differences in the cultures in different disciplines, this will not be required. However, when it is the norm or if the fellow desires it, they will be strongly encouraged to teach an undergraduate class. When this happens, the Fellows program will recoup a portion of the Fellows salary from the department. If enough Fellows opt for this option the program will be able to hire additional Fellows and extend the length of the program without additional funds.

3.3. **Community aspects.** Though relatively young, the CTMS has been very successful through its retreats, lunch and afternoon seminars, and workshops at increasing the sense of community in the mathematical sciences across the university. This horizontal integration, across different subject areas and problem-specific collaborative groups, is one of its main goals. This cross talk is critical for the communication of scientific idea and success at the theoretical edge of science. Though working in different domains, the members of the CTMS have found they have as much in common with each other as with the more problem-centered applied researchers working in their domain. Both communities are important and critical for the success of the theoretical enterprise. Too often, the emphasis is on the problem specific community and not on the trans-disciplinary. The later is often responsible for transferring ideas from one domain to the other and identifying new and emerging problems.

The CTMS fellowship program is an attempt to duplicate this success at the post-doctoral level. It will build an community of postdoctoral researches working in the theoretical and mathematical sciences integrated horizontally across problem areas and integrate it vertically with the horizontally integrated faculty cohort. The biweekly Fellows meetings are designed to build a community of Fellows. The courses and research seminars will also building the postdoctoral community will integrate the Fellows into the community of researchers at Duke. This integration will be both vertically in their research area and vertically with the generally broadly interested members of the CTMS faculty.

3.4. **Postdoctoral Conference.** We suspect that the successful elements for the program will be duplicated at other institutions. However, we plan to have a more national effect from the start. We will run two postdoctoral fellows conferences in the during the duration of the grant. They will happen in years 2 and year 5. The CTMS Fellows program will weave together a group of Duke postdoctoral fellows from disparate disciplines. To increase the national impact, the Fellows will organise a conference bringing together strong junior researchers from the domains they know to

Duke for a multi-day conference. This will bring together the disciplinary cohort at the national level of each of the Fellows and create connections between them and between the different fellow's cohorts. We envision the funds requested to bring pay for around 20 junior researchers to come to Duke. We hope that other will also attend using there own funding or other funds the CTMS secures.

3.5. **Exposure to Industrial and government careers.** It is important that postdoctoral Fellows are exposed to the diverse paths their career could take. In addition to the many possible academic possibilities, there are also opportunities in the private sector and the government. The postdoctoral years are the natural time to make such explorations. Duke is situated in the vicinity of the Research Triangle Park which contains a wealth of diverse industrial and government labs and institutes including the Research Triangle Institute, the Environmental Protection agency, and the Statistical and Applied Mathematical Sciences Institute. Duke also has formal connections with Oakridge National Labs. As part of the CTMS Fellows program, we will during the year invite a number of representatives from various industrial and government labs to lunch and interact with the Fellows. The exact makeup of the invitees will be colored by the fields of the current Fellows. The mentors of the current Fellows and the CTMS leadership will be responsible for identifying appropriate guests.

3.6. **Mentoring.** Mentoring procedures include the assignment of a primary faculty mentor, the annual evaluation of the progress of each Fellow based on a written progress report, a supervised grant writing effort, and several peer mentoring components. The details of the mentoring plan are described in a one-page supplementary document.

4. Research Themes

Although we believe that the selection of Fellows should not be constrained by topical considerations, but only be based on their individual excellence and interest in conducting research at disciplinary interfaces, we highlight a number of areas in which considerable strength exists among the Duke faculty and which may be particularly attractive to applicants for these postdoctoral fellowships:

Stochastic modeling and simulation: Stochastic modeling use has dramatically increased in the past decades. Driven by our increased ability to simulate and our enhanced mastery of stochastic analysis, the desire and effort has grown to understand how random systems evolve and uncertainty propagates. This requires both increased transfer of sophisticated methods from stochastic analysis to applied investigations and more nuanced understanding of the modeling framework by stochastic modelers. Analytic methods alone are usually insufficient and need to be coupled with numerical methods which are informed by the structure of the stochastic dynamics. There is need for more efficent stochastic methods for simulations of stochastic differential equations and random processes. There are basic processes such as heat conduction in non-linear materials which require the marriage of sophisticated stochastic analysis and nonlinear dynamics. The understanding of front propagation and wave transition in disordered medium is important in many models and still poorly understood. Increasingly sophisticated Bayesian models require the understanding and intelligent simulation of increasingly complicated and hierarchical models including probabilistic models used in environmental and genomic modeling. (Primary Duke faculty: Bass, Charbonneau, Chandrasekharan, Gelfand, Mattingly, Mukherjee, Nolen, Porporato, Schmidler, West, Wolpert) (see [32, 67, 50, 68, 13, 14, 64, 63, 16, 87, 39, 9, 85, 86, 23])

Multi-scale modeling, numerics and analysis: The analysis and simulation of systems spanning many scales present their own challenges. The modeling, analysis, and simulation of multi-scale problems is spread across many disciplines and traditional toolset boundaries. It requires the combination of deep insight into the processes being modeled, mastery of sophisticated modern mathematical techniques, and understanding of algorithmic and numerical trade-offs. (Primary: Albertson, Bass, Katul, A. Layton , Maggioni, Mueller, Nolen, Witelski, Yang) (see [37, 62, 21, 20, 31, 34, 49])

Geometry, structures and inference in large data sets: In the past decade the analysis of massive, high-dimensional data sets has become a necessity for many researchers in a wide range of disciplines; examples of such fields represented at Duke include: analysis of gene arrays and biological assays, molecular dynamics, social networks, image analysis, high-dimensional point clouds in machine learning. In addition, there is extensive experience with very large data sets in high energy physics.

Existing data processing algorithms are unable to compete with this volume, in particular, since much of the data is very high-dimensional with complicated underlying structure. Innovative algorithms are needed to process this data, determine the relative significance of different data subsets, and extract structures that help us better understand underlying physical phenomena. For instance, understanding the manifold structure underlying large, high-dimensional data can lead to improved compression, classification, filtering strategies. Similarly, online algorithms which are robust to statistical dependencies between successive data points or data corruption are critical to rapid and accurate processing of streaming data .

Mounting evidence suggests the ubiquitous existence of geometrical structures in the data which can be exploited for improved prediction and information extraction. These geometric structures may be analyzed with different tools: from a topological perspective, from the point of view of high-dimensional geometric measure theory and multiscale analysis, from the point of view of large graphs modeling the relationships between the data points, as realizations of parametrized families of statistical models in high dimensions, and from a dynamical systems perspective. New broadly applicable theoretical paradigms, algorithms, and computational tools are needed in this field, as is their integration and tuning for each field of application. (Primary Duke faculty: Edelsbrunner, Harer, Maggioni, Mukherjee, Wolpert, Willett) (See [21, 40, 56, 57, 58, 59, 60, 76, 69, 30, 75])

Dynamics and regulation of biological networks: This field at the intersection of mathematics and biology aims at the characterization and analysis of highly nonlinear biological networks in genetics, metabolism, physiology and development, including both the dynamics of network states and the dynamics of network structures as they change during development and evolution. Achieving progress in systems biology requires the close working relationship between theoretical and experimental scientists. Many different approaches, including large-scale simulations, sophisticated statistical methods, graph and network theory, dynamical systems theory and computational geometry and topology are being brought to bear on the problem. (Primary Duke faculty: Greenside, Harer, Hartemink, Mattingly, Mukherjee, Nijhout, Reed, Schaeffer, Socolar, Schmidler) (See [61, 5, 83, 26, 4, 24, 11, 15, 29, 25, 72, 82, 79, 81, 10])

Molecular description of quantum complex systems and processes: Applications of theory to basic and applied challenges in molecular biology, biomedicine, and materials science are growing at a rapid pace. Indeed, theoretical and computational chemistry approaches that are based on physical principles describing complex phenomena at multiple length, time, and energy scales are becoming invaluable research tools across disciplines. There are many exciting frontiers: molecular descriptions of photosynthesis and energy transduction, the design of optimal combinatorial chemical libraries for drug discovery, the design and analysis of molecular-scale transistors, and descriptions of biological machines, including molecular motors and DNA processing machinery. At the mesoscopic scale, a better understanding of molecular self-assembly plays a major role in expanding the variety of materials that can be designed. Whether for protein crystallization, nanowire and photonic crystal assembly, or metallic glass formation, the theoretical and mathematical linking of microscopic details to mesoscopic structures helps broaden the synthetic toolset. (Primary Duke faculty: Beratan, Charbonneau, Yang) (See [36, 35, 73, 54, 19, 52, 42])

Correlated Quantum Systems: Materials in which the electrons are strongly correlated are becoming ubiquitous in chemistry, physics, and materials science. Quantum states involving such strong correlations are the basis for a rich variety of novel phases of matter, such as the magnetic and superconducting phases of complex oxides or interaction-induced insulating behavior. In a less dramatic but no less important way, correlations between electrons are a critical issue in the molecular description of complex phenomena and in combinatorial searches for new materials. Theory in this area faces the severe challenge of dealing with a large number of interacting (fermionic) particles. Dramatic improvements are needed, such as the development of accurate density functional theories or vastly improved quantum Monte Carlo algorithms, in order to tackle the key issues posed by the many new materials discovered. (Primary Duke faculty: Baranger, Beratan, Curtarolo, Yang) (See [18, 43, 55, 53, 22, 28, 65, 47, 33, 19])

Energy science: The grand challenges presented by modern energy science require input from a wide range of theoretical and mathematical sciences. From the theory of complex social networks, to the development of new physical descriptions for multi-carrier generation in nanoparticles, to multi-scale modeling of bio-molecular machines and solar energy conversion structures, mathematical modeling will pervade successful breakthroughs in energy research. At Duke, and through partnerships with the Research Triangle Park Institute and neighboring universities, important new energy research centers are being formed that involve major elements of theoretical research contributed by teams of CTMS researchers. For example, Duke's emerging initiative on Energy and the Environment emphasizes cross-disciplinary education related to the challenge of meeting the current and future worlds energy needs in a sustainable way. Dukes Nicholas Institute for Environmental Policy Solutions and the Climate Change Policy Partnership engage in research projects that pose difficult and complex questions on the decarbonization of the electricity and transportation systems, providing a good opportunity for CTMS Fellows to be exposed to complex problems such as environmental market design, decision making under uncertainty, and risk management in the energy/climate domain. The University of North Carolina at Chapel Hill's recently funded Department of Energy Energy Frontier Research Center focuses on solar energy and supports faculty partners from Duke's CTMS who will focus on theoretical aspects of energy capture and transport in organic films. As well, a group of local universities including Duke has teamed up with the Research Triangle Institute to form the new "Research Triangle Energy Consortium" [3] to explore further interdisciplinary collaborations that address complex frontier challenges in energy science. These specific enterprises will define exciting new interdisciplinary research challenges for the CTMS fellowship candidates and will contribute to the rich training environment.

New challenges in nonlinear dynamical systems: The dynamics of many complex physical systems pose important mathematical problems that do not simply fit into the classical framework of bifurcation theory and weakly nonlinear analysis. A notable subclass of such problems involve piecewise-smooth dynamics, in which evolution is controlled by an interplay of smooth dynamics and discrete mappings. Such problems arose first in control engineering, more recently they have appeared in cardiac dynamics and genetic networks, and they are central to coarsening dynamics in thin films. In analyzing networks of time-delay differential equations or autonomously updating Boolean gates connected by links with associated propagation delays, traditional techniques of time-series analysis or numerical determination of Lyapunov exponents must be modified, and possible sources of complex behavior are not yet well understood. We believe that the interdisciplinary approach of the CTMS—combining theory, simulations, and experiments in the study of problems from several application areas simultaneously by researchers in close contact with one another–offers the promise of pushing back the frontier of our understanding. (Primary: A. Layton, Behringer, Nolen, Porporato, Schaeffer,Socolar, Witelski) (See [38, 31, 77, 12, 48, 70, 66, 88, 8])

Spatial and temporal scales in ecology: Ever increasing interest has focused on understanding the role of spatial and temporal scales in shaping the emergent population-level, community-level, and ecosystem-level patterns observed in ecological systems. Research on spatial scales has focused on how local interactions, either in physical space or through networks of interaction, change the structure and function of the aggregate under study. Larger-scale patterns that arise from these localized interactions frequently exhibit properties well-described in other theoretical sciences: aggregative patterns with power-law characteristics, self-organized criticality, threshold effects (frequently with hysteresis), and regions of robustness. Understanding these ecological patterns from a mathematical/theoretical perspective is critical not only from a basic science perspective, but also will help guide policy, including where to place conservation emphasis. Research focusing on temporal scales also will benefit from a further interface with mathematical and theoretical perspectives. Historically, ecological analyses have assumed a separation of timescales to simplify problems. However, long-term ecological research data now frequently indicate that this traditionally assumed separation of timescales may not be a valid assumption. This is especially the case when considering the interaction of ecological and evolutionary dynamics (for example, for Darwin's finches, heavily harvested fish populations, and viral pathogens), for which the evolutionary dynamics of a population affect its ecological dynamics. ecology. (Primary Duke faculty: Clark, Katul, Koelle, Mukherjee, Nijhout,Porporato, Uyenoyama) (See [41, 7, 71, 17, 44, 45, 46])

Inferential Ecosystem Model: From Network Data to Prediction: Data are collected with the aid of models and are also used to inform models. Wireless sensor networks provide an ideal setting for exploring this duality. Such networks are being increasingly used for monitoring environmental processes such as soil moisture, light availability and sap flux. With such networks, battery life is critical. Hence, efficient networks require ecosystem models that can weigh the inferential value of an observation against the cost of transmission of the observation. In this regard, network control must be dynamic, driven by models capable of learning about both the environment and the network. We witness a barely studied interplay between modeling for network data collection and communication along with modeling for complex space-time ecological systems. Each model demands challenging formulation with theoretical needs to understand behavior and theoretical investigation of the joint model behavior is completely lacking. However, better understanding of this interplay is vital for national environmental research platforms such as NEON (National Environmental Observation Network) and CLEANER (Collaborative Large-scale Engineering Analysis Network for Environmental Research). (Primary Duke faculty: Clark, Gelfand, Wolpert) (See [16])

Integrating Algorithmic and Stochastic Modeling for Environmental Prediction: Predicting biodiversity, i.e., abundance of species, in response to climate change is a goal of environmental change research. Despite recent valuable advances in understanding biodiversity and climate, the current grasp is limited. There are two widely recognized obstacles: first, because of the complexity of the underlying processes, the existing models intended for understanding and prediction are not (computationally) scalable. Second, the coarse-scale environment models fail to capture fine-scale interactions among species, which control biodiversity, and second, the models based on fine-scale, short-term observations are unable to make long-term predictions. Research is needed to develop a computationally scalable prediction framework that coherently combines broad-scale pattern data with fine-scale data on species interactions. The focus will be on prediction at the geographic scale and in using geographic-scale data to better understanding at the scales where species interactions occur. The proposed research requires formulating a multi-scale modeling framework and designing algorithms that make environmental models computationally scalable. The approach hinges upon strong interplay of algorithmic and statistical techniques. Statistical inference brings stochastic modeling sophistication in space and time, and yields improved characterization of the process and the possibility of full inference. Sophisticated algorithms will make models and processes scalable and provide trade-offs between accuracy and efficiency. (Primary Duke faculty: Clark, Gelfand, Agarwal).

4.1. **Relation to other University Centers.** Duke University hosts a number of centers with a multi-disciplinary yet programmatic focus which comprise theoretical and mathematical components. These include the Duke Institute for Genome Sciences and Policy (IGSP), the Duke Institute for Brain Sciences, the Center for Systems Biology (part of the IGSP), the Fitzpatrick Institute for Photonics, the Center for Nonlinear and Complex Systems, and the Center on Global Change. We anticipate a productive symbiosis between these programmatically oriented centers and the proposed CTMS Fellows Program. Depending on the research interests of the CTMS Fellows, these centers may serve as natural "home bases" with an interdisciplinary culture for some of the postdoctoral fellows. In turn, the Fellows will enrich the environment of these other centers. Finally, Duke University is a member institution of the nearby Statistical and Applied Mathematical Sciences Institute (SAMSI). While we conceive the CTMS Fellows program as primarily campus based, SAMSI will act as an additional attraction for potential applicants to the Fellows program, and as an important intellectual resource for the resident Fellows.

5. Broader Impact

5.1. **Impact on the national scientific workforce.** The postdoctoral training phase represents a peculiar bottleneck in the development of the nation's academic workforce in the sciences. On the one hand, postdocs are expected to function, as much as possible, as independently thinking and researching scientists, on the other hand they are usually not, unlike faculty, part of a recognized peer group with significant networking opportunities. Mentoring is often haphazard and dependent on the good-will of a single faculty member. Research objectives are in most cases rigidly defined by the objectives of the grant supporting the position; at the same time the pressure to perform is extreme due to the temporary nature of the appointment and the perceived risk of getting "too old" for a entry-level faculty job.

Mathematics has always had a small number of prestigious "term-limited" assistant professorships that attracted the best and brightest. The tightening of the job-market in the mid 90's lead to the creation of even more such positions. Their relative freedom made them very competitive which helped to alleviate any stigma associated with a longer post-doctoral period. While initially solving the employment dilemma of the moment, departments have found these groups of researchers to be a valuable resource of new problems and interactions. We hope to export this successful model to the broader mathematical science community. The NSF increasingly pushes research groups to be interdisciplinary. Duke University, with an outwardly looking mathematics department and the CTMS drawing various groups together, is an ideal environment to incubate an educational component to train researchers to be more trans-disciplinary from the start of their career. It is reasonable to expect that if successful the program will be copied. This was the case with the "term-limited" assistant professorships in mathematics.

Transitionally, the postdoctoral stage is the loneliest phase of the academic career of most scientists. This fact discourages underrepresented minorities and women from pursuing an academic research path requiring an extensive postdoc experience, as most faculty positions in the sciences at major research universities do. We believe that building a more cohesive postdoctoral cohort, we can better support and launch them to successful careers. Furthermore, empirically since the mathematical sciences have been less populated by women and minorities, we hope that the Fellows program might be a vehicle by which students with a PhD in an allied field might be drawn into the more mathematical science in there post-doctoral years.

The traditional postdoctoral approach also discourages young scientists at that stage in their careers, when they develop their own research style, from thinking broadly and considering to apply their knowledge to problems outside their present horizon. This presents a missed opportunity especially in the (applied) mathematical and theoretical sciences where methods and tools, such as computational approaches or structural concepts, can often be easily and successfully transported from one field of science to another, leading to quantum jumps in scientific insight or opening up completely new research opportunities.

There are few programs in existence that attempt to implement systematic career development at the postdoctoral career stage within an intellectual environment that encourages individuals to apply their knowledge to problems outside their traditional comfort zone. Existing interdisciplinary postdoctoral training programs in the sciences usually focus on what may be termed "bilateral" interdisciplinarity, such as mathematical or computational biology, or particle astrophysics. While these programs serve specific, already determined and widely recognized needs, they do not aim at creating a generation of research scientists who feel comfortable venturing outside those predetermined intellectual paths and charting their own trans-disciplinary research directions. This is what the CTMS Fellows Program aims for.

5.2. **Synergy with programmatic research.** A tangible, immediate benefit to the funding agency is that the research activity of the CTMS Fellows is expected to forge new and/or cement existing trans-disciplinary collaborations among scientists, and thus to further invigorate the research programs of research groups many of whom are supported by grants from various Divisions in the Physical and Mathematical Sciences and the Biological Sciences Directorates of the NSF. Postdoctoral fellows have more time available to dedicate to research than the typical faculty member and are thus more easily able to learn new methods or assimilate the knowledge of a new application area. This allows them to act as agents capable of stitching together new interactions among faculty from different disciplines, that remain in place when the postdoc departs to take another job.

5.3. **Model function.** If the proposed Fellows program proves to be successful, it will serve as a model that other academic institutions may be motivated to adopt. We do not know of other trans-departmental fellows programs in the mathematical and theoretical sciences. We fell strongly that such an initiative is needed and timely. It is a natural complement to the efforts of an applied math group. It is our hope and expectation that once the program has been shown to be successful similar programs will be adopted at other institutions.

5.4. **Diversity related considerations.** A well structured community component can help attract and retain minorities in the scientific workforce. Especially women, who are traditionally underrepresented in theoretical and mathematical science, often cite a lack of a supportive social environment, including peer group and mentor support, as a reason for pursuing other careers. In addition, less specialized, more integrative research areas in the sciences have a record of attracting a larger pool of talented women. We therefore believe that the CTMS Fellows Program, as it is described here, will be especially attractive for exceptionally gifted women and minority scientists. A core rationale for the university's offer to provide several matching positions is to ensure that highly talented minority and women candidates can be attracted to the program even if they do not satisfy all the conditions associated with the NSF workforce development program.

6. Assessment

Since we are proposing a new type of postdoctoral program, assessment is important both to provide information that can be used to adjust the program mid-course and to track the success of the Fellowship program over time.

On going assessment: Duke has a sophisticated "Faculty Database System" that was grown in-house and is used to generate all of the faculty webpages in Arts and Science, the Law School and the Medical School. We will use the database system to collect information on scientific interactions, talks given, talks attended, papers written. The data can be entered incrementally using a simple web interface. Specifically we will collect:

- Scientific interactions: (Name, Discipline and Type) Type is either: (1) brief: consisting of one or two meetings; (2) Substantive: Multiple meetings, but not necessarily involving formal collaboration. This could include, but will not be limited to, regularly participating in a research team's "group meetings"; (3) Extended: Collaboration.
- Talks attended (speaker and general discipline of talk/meeting/seminar series).
- Talks Given (title and discipline of seminar series or meeting).
- Papers written (discipline of collaborators).

At each semester's end, we will ask each Fellow to ensure that the semester's information is complete. While this is slightly onerous, it is a small price for the academic freedom and light teaching load they will be given. The Faculty Database system can automatically generate reports from the information entered by the Fellows. The publication and talks given information entered by the Fellows will automatically update their webpage and CV. This serves as an incentive to keep the information up-to-date. All faculty at Duke are required to submit an end-of-year report on their scientific activities. The CTMS Fellows will be asked do the same. This report is also entered electronically through the Faculty Database System. The CTMS Fellows form will require a summary of research performed and a description of the direction the Fellow intends to pursue in the next year. The Fellows will also be asked to comment on which groups they interact most with, what activities they found the most useful, and suggestions for the future.

Mid-course report: In the fall of the third year, we will collect all of the information gathered, evaluate how the program is performing in the following areas and report our findings to the NSF along with plans to alleviate any perceived shortcomings. We will specifically comment on the following issues:

- The range of fields and topics covered by the Fellows activities.
- The level of interdisciplinary of the Fellow Cohort.
- The degree to which the Fellows seem to be mentoring each other.
- The effectiveness of the faculty mentoring.
- The results of the Fellows mentoring of undergraduates and high school students.
- The success of the Fellow courses and seminar series of drawing a diverse population.
- Diversity issues in the Fellows makeup and recruiting.

To aid in the collecting of information, we will engage a small panel of Mathematical Scientists (2-3) from outside of Duke to meet with the Fellows during an afternoon and write a brief report summarizing the feelings of the fellows and the success of the program. This report will be forwarded unedited to the NSF.

End of Grant Report and continued tracking: After the sixth year, we containing all of the elements of the mid-course report as well as placement information. As since most will have left Duke, the Fellow's comments will be solicited by mail rather than a visiting committee. The Faculty Database article and talk archive function will be made available to the Fellows for "as long as they wish" to use it. This will allow the CTMS to better track their publication record and fields after they leave Duke. It is realistic to expect that many will continue to use the system as a number of former Duke Mathematics faculty have continued to use the systems after they left Duke. From those who do not contiune to use the Faculty Database, we will request a yearly update of the research activities and publications after they leave Duke so they we may measure the level of interdisciplinary in their reseach programs.

Long-term perspective: While presently we cannot make any firm statements about the Fellows program's long-term prospects; if the program is as successful as we expect it to be, we intend to work with university leaders to identify appropriate mechanisms and resources to assure the program's continuation. This will likely come from a mixture of university funds and funds raised from outside sources. However since there are few examples of such a program, we need to establish a track record to allow us to raise funds. This is the one of the main purpose of this funding request.

References

[1] National Acadamies. *Gender difference at critical transitions in the careers of science, engineering, and mathematics*, 2009. Committee on Gender Differences in Careers of Science, Engeneering, and Mathematics Faculties.

[2] See `http://ctms.aas.duke.edu` for a more detailed description of the goals, activities, and organization of the Center for Theoretical and Mathematical Sciences at Duke University.

[3] See `https://www.rtec-rtp.org/` for a description of the structure and goals of the Research Triangle Energy Consortium.

[4] CR Acharya, DS Hsu, CK Anders, A Anguiano, KH Salter, KS Walters, RC Redman, SA Tuchman, CA Moylan, S Mukherjee, WT Barry, HK Dressman, GS Ginsburg, KP Marcom, KS Garman, GH Lyman, JR Nevins, A Potti *Gene expression signatures, clinicopathological features, and individualized therapy in breast cancer.* J. Am. Med. Ass., 299, 13, 1574–87. 2008.

[5] David F. Anderson, Jonathan C. Mattingly, H. Frederik Nijhout, and Michael C. Reed. Propagation of fluctuations in biochemical systems. I. Linear SSC networks. *Bull. Math. Biol.*, 69(6):1791–1813, 2007.

[6] David Anderson and Jonathan C. Mattingly. A Second order method for the SDEs associated with Biochemical Networks *Submitted*, 2009.

[7] Claudia Angelini, Daniela Cava, Gabriel Katul, and Brani Vidakovic. Resampling hierarchical processes in the wavelet domain: a case study using atmospheric turbulence. *Phys. D*, 207(1-2):24–40, 2005.

[8] Soumitro Banerjee, M. S. Karthik, Guohui Yuan, and James A. Yorke. Bifurcations in one-dimensional piecewise smooth maps—theory and applications in switching circuits. *IEEE Trans. Circuits Systems I Fund. Theory Appl.*, 47(3):389–394, 2000.

[9] James O. Berger, Brunero Liseo, and Robert L. Wolpert. Integrated likelihood methods for eliminating nuisance parameters. *Statist. Sci.*, 14(1):1–28, 1999.

[10] R Berger, PG Febbo, PK Majumder, JJ Zhao, S Mukherjee, T Campbell, WR Sellers, TM Roberts, M Loda, TR Golub, WC Hahn Androgen-Induced differentiation and tumorigenicity of human prostate epithelial cells. Cancer Research, 64, 8867–8875. 2004.

[11] H Bonnefoi, A Potti, M Delorenzi, L Mauriac, M Campone, M Tubiana-Hulin, T Petit, P Rouanet, J Jasem, E Blot, V Farmer, S André, CR Acharya, S Mukherjee, D Cameron, J Bergh, JR Nevins, RD Iggo (2007). Validation of gene signatures that predict the response of breast cancer to neoadjuvant chemotherapy: a substudy of the EROTC 10994/BIG 00-01 clinical trial. Lancet Oncol., 8, 12, 1071–1078.

[12] Anne Bourlioux, Anita T. Layton, and Michael L. Minion. High-order multi-implicit spectral deferred correction methods for problems of reactive flow. *J. Comput. Phys.*, 189(2):651–675, 2003.

[13] Patrick Charbonneau and D. Frenkel. Gas-solid coexistence of adhesive spheres. *Journal of Chemical Physics*, 126:196101, 2007.

[14] Patrick Charbonneau and D. R. Reichman. Phase behavior and far-from-equilibrium gelation in charged attractive colloids. *Physical Review E*, 75(5):050401(R), 2007.

[15] JT Chi, EW Rodriguez, Z Wang, DSA Nuyten, S Mukherjee, M van de Rijn, MJ van de Vijver, T Hastie, PO Brown (2007). Gene Expression Programs of Human Smooth Muscle cells: tissue-specific differentiation and prognostic significance in breast cancers. PLoS Genet., 3, 9, e164.

[16] Merlise A. Clyde and Robert L. Wolpert. Nonparametric function estimation using overcomplete dictionaries. In *Bayesian statistics 8*, Oxford Sci. Publ., pages 91–114. Oxford Univ. Press, Oxford, 2007.

[17] Cobey, S., Koelle, K. *Capturing escape in infectious disease dynamics.* Trends in Ecology and Evolution. 23(10), pp.572-577. 2008.

[18] A. J. Cohen, P. Mori-Sanchez, and W. T. Yang. Insights into current limitations of density functional theory. *Science*, 321(5890):792–794, Aug 2008.

[19] Aron J. Cohen, Paula Mori-Sanchez, and Weitao Yang. Insights into current limitations of density functional theory. *Science*, 321:792–794, 2008.

[20] R.R. Coifman, M. Maggioni, *Diffusion wavelets*, Appl. Comp. Harm. Anal., 21 (2006), pp. 53–94.

[21] R. Coifman, I. Kevrekidis, S. Lafon, M. Maggioni, and B. Nadler, *Diffusion maps, reduction coordinates and low dimensional representation of stochastic systems*, SIAM J.M.M.S. 7(2) (2008), pp. 842–864.

[22] S Curtarolo, D Morgan, K Persson, J Rodgers, and G Ceder. Predicting crystal structures with data mining of quantum calculations. *Phys. Rev. Lett.*, 91, 2003.

[23] Edoardo Daly and Amilcare Porporato. State-dependent fire models and related renewal processes. *Phys. Rev. E (3)*, 74(4):041112, 9, 2006.

[24] E Edelman, J Guinney, JT Chi, PG Febbo, S Mukherjee (2008). Modeling Cancer Progression via Pathway Dependencies. PLoS Comput. Biol., 4,2, e28.

[25] E Edelman, A Porrello, J Guinney, B Balakumaran, A Bild, PG Febbo, S Mukherjee (2006). Analysis of sample set enrichment of sets of genes for individual genome-wide expression profiles. Bioinformatics, 22, 14, 108–116.

[26] KS Garman, E Edelman, CR Acharya, M Grade, J Gaedcke, S Sud, K Walters, G Ginsburg, W Barry, AM Dieh, D Provenzale, BM Ghadimi, T Ried, D Hsu, JR Nevins, S Mukherjee, A Potti *A genomic approach to dissecting colon cancer progression yields biologic insights into therapeutic opportunities.* Proc. Natl. Acad. Sci. U.S.A., 105, 49, 19432–19437. 2008.

[27] L. Glass and S. Kauffman, *The logical analysis of continuous, nonlinear biochemical control networks.* J. Theor. Biol., vol. 39 pp103–129. 1973.

[28] A. Ghosal, A. D. Güçlü, C. J. Umrigar, D. Ullmo, and H. U. Baranger. Correlation induced inhomogeneity in circular quantum dots. *Nature Physics*, 2:336–340, 2006.

[29] L Goh, SK Murphy, S Mukherjee, TS Furey (2007). Genomic sweeping for hypermethlyated genes. Bioinformatics, 23, 3, 281-288.

[30] P Golland, F Liang, S Mukherjee, D Panchenko *Permutation tests for classification.* In Proceedings of the Conference on Learning Theory (P Auer and R Meir), Springer-Verlag, Heidelberg, 501–515. (2005).

[31] M. B. Gratton and T. P. Witelski. Coarsening of unstable thin films subject to gravity. *Phys. Rev. E (3)*, 77(1):016301, 11, 2008.

[32] Martin Hairer and Jonathan C. Mattingly. Slow energy dissipation in anharmonic oscillator chains *Comm. Pure and Applied Math*, 2008.

[33] A. R. Harutyunyan, N. Awasthi, A. Jiang, W. Setyawan, E. Mora, T. Tokune, K. Bolton, and S. Curtarolo. Reduced carbon solubility in Fe nanoclusters and implications for the growth of single-walled carbon nanotubes. *Phys. Rev. Lett.*, 100, 2008.

[34] Ryan P. Haskett, Thomas P. Witelski, and Jeanman Sur. Localized Marangoni forcing in driven thin films. *Phys. D*, 209(1-4):117–134, 2005.

[35] H. Hu, A. Boone, and W. T. Yang. Mechanism of omp decarboxylation in orotidine 5 '-monophosphate decarboxylase. *Journal of the American Chemical Society*, 130(44):14493–14503, Nov 2008.

[36] H. Hu, Z. Y. Lu, J. M. Parks, S. K. Burger, and W. T. Yang. Quantum mechanics/molecular mechanics minimum free-energy path for accurate reaction energetics in solution and enzymes: Sequential sampling and optimization on the potential of mean force surface. *Journal of Chemical Physics*, 128(3):034105, Jan 2008.

[37] H. Hu and W. T. Yang. Free energies of chemical reactions in solution and in enzymes with ab initio quantum mechanics/molecular mechanics methods. *Annual Review of Physical Chemistry*, 59:573–601, 2008.

[38] Hyung Ju Hwang and Thomas P. Witelski. Short-time pattern formation in thin film equations. *Discrete Contin. Dyn. Syst.*, 23(3):867–885, 2009.

[39] Katja Ickstadt and Robert L. Wolpert. Spatial regression for marked point processes. In *Bayesian statistics, 6 (Alcoceber, 1998)*, pages 323–341. Oxford Univ. Press, New York, 1999.

[40] P. Jones, M. Maggioni, R. Schul, *Manifold parametrizations by eigenfunctions of the Laplacian and heat kernels*, Proc. Nat. Acad. Sci. 105(6) (2008), pp. 1803–1808.

[41] Gabriel Katul, Fabrizio Ruggeri, and Brani Vidakovic. Denoising ozone concentration measurements with BAMS filtering. *J. Statist. Plann. Inference*, 136(7):2395–2405, 2006.

[42] S.-H. Ke, W. Yang, S. Curtarolo, and H. U. Baranger. Thermopower of molecular junctions. *Nano Lett.*, 9:1011–1014, 2009.

[43] S. H. Ke, W. T. Yang, and H. U. Baranger. Quantum-interference-controlled molecular electronics. *Nano Letters*, 8(10):3257–3261, Oct 2008.

[44] Koelle, K. Cobey, S., Grenfell, B., and Pascual, M. *Epochal evolution shapes the phylodynamics of interpandemic influenza A (H3N2) in humans.* Science. 314. pp. 1898-1903. 2006

[45] Koelle, K., Pascual, M., and Yunus, M. *Serotype cycles in cholera dynamics.* Proceedings of the Royal Society, Series B, Biological Sciences. 273. pp. 2879-2886. 2006

[46] Koelle, K., Pascual, M., and Yunus, M. *Pathogen adaptation to seasonal forcing and climate change.* Proceedings of the Royal Society, Series B, Biological Sciences.272. pp. 971-977. 2005.

[47] Aleksey N. Kolmogorov, Matteo Calandra, and Stefano Curtarolo. Thermodynamic stabilities of ternary metal borides: An ab initio guide for synthesizing layered superconductors. *Phys. Rev. B*, 78, 2008.

[48] Anita T. Layton. Role of UTB urea transporters in the urine concentrating mechanism of the rat kidney. *Bull. Math. Biol.*, 69(3):887–929, 2007.

[49] Anita T. Layton. An efficient numerical method for the two-fluid Stokes equations with a moving immersed boundary. *Comput. Methods Appl. Mech. Engrg.*, 197(25-28):2147–2155, 2008.

[50] F Liang, S Mukherjee, M West *Understanding the use of unlabelled data in predictive modelling.* Statistical Science, 22, 2, 189-205. 2007.

[51] Jonathan C. Mattingly, Toufic Suidan, , Eric Vanden-Eijnden . Simple systems with anomalous dissipation and energy cascade. *Comm. Math. Phys.* 276 (2007), no. 1, 189–220.

[52] J. A. van Meel, D. Frenkel, and P. Charbonneau. Geometrical frustration: A study of four-dimensional hard spheres. *Phys. Rev. E*, 79, 2009.

Mentoring Plan

Our mentoring plan for the CTMS Fellows is building on the mentoring processes of the Duke Department of Mathematics, which has a strong and successful record of mentoring its postdoctoral fellows. The Department has six University funded postdocs called Assistant Research Professors (ARPs) who appointments are normally for three years. The ARPS are generally excellent researchers, but a main criterion in hiring is the commitment of a senior faculty member (or two) to be the mentor. No ARP is hired without such a commitment. While building on this practice, our mentoring plan is adapted to the wider, interdisciplinary action range of the CTMS Fellows program and takes into account that the Fellows will seek employment in a much broader range of disciplines and career avenues.

Following the ARP pattern, the CTMS Fellows to be supported by funds requested in this proposal will only be hired if there is a meaningful match in research interests between the postdoctoral fellow and one or more of the faculty members interested in or already engaged in trans-disciplinary research areas (see the project description for examples of such areas with significant strength at Duke). We will also require one faculty member to commit to the role of mentor, who is responsible for facilitating connections to various other researchers at Duke, giving advice of research topics and directions, student teaching and mentoring, and career related issues. The Fellow may, but does not have to, engage in joint research projects with the primary mentor.

At the end of each appointment year, the Fellow will submit an activity report and self-assessment of achievements and career development progress to the mentor, who will share it with the PI's together with his or her comments. After the evaluation of all reports and comments, each Fellow will receive a written response, which will be transmitted in a conversation with the mentor.

An important component of our mentoring plan is faculty guided peer mentoring. It is a well known fact that, at any career level, people learn best by interacting with their peers in an environment that is conducive to peer learning. For this reason, the CTMS Fellows will attend bi-weekly lunch meetings, during which individual fellows will report in the presence of their faculty mentor about their research projects or talk about novel developments in their fields that are of potential broader interest. These meetings will also permit the Fellows to exchange experiences with regard to job searches, teaching activities, and so on.

While the primary focus of the CTMS Fellows program is on trans-disciplinary research, we also want the Fellows to develop the teaching record and skill that makes them competitive for faculty positions. They will required to teach a (graduate) specialty course of self-defined content in their first year in the program and a graduate/postdoc level seminar during their second year. In the third year, each Fellow will be asked to give a "public" lecture to undergraduate or high-school students, parents, or in some other appropriate venue. If a Fellow desires, we will arrange for the opportunity to teach a regular college course, with teaching funds defraying part of the Fellow's salary. Furthermore, CTMS Fellows will be encouraged to mentor and work with an undergraduate or high school student during one of the summers with an emphasis on students from underrepresented groups in STEM field. There are several support mechanisms available for such mentoring relationships.

The Department of Mathematics has various established training activities for postdocs like the annual Grant Writing Workshop. The CTMS Fellows will be required to participate in this workshop and write a grant proposal during their second year in the program. If the proposal is by the mentor (and other faculty members the mentor may consult) as appropriate, the Fellow will be encouraged to submit it to a funding agency. A wide range of career related mentoring services is also available to the CTMS Fellows through the Duke Office for Postdoctoral Services.

7. Associated CTMS Faculty

The following is a list of the names of Duke faculty members who are associated with the Center for Theoretical and Mathematical Sciences, but are not included as Senior Personnel on this proposal. Nevertheless, these faculty members are potentially available to serve as primary mentors for CTMS Fellows:

Pankaj K Agarwal (Computer Science / Mathematics)
John D. Albertson (Civil and Environmental Engineering)
Paul S Aspinwall (Mathematics / Physics)
Steffen A Bass (Physics)
Bob Behringer (Physics)
J. Thomas Beale (Mathematics)
James O Berger (Statistical Science)
David J Brady (Electrical and Computer Engineering)
Shailesh Chandrasekharan (Physics)
Benoit Charbonneau (Mathematics)
James S. Clark (Environment / Biology / Statistical Science)
Vincent Conitzer (Computer Science)
Bruce R Donald (Computer Science)
Earl H Dowell (Mechanical Engineering and Materials Science)
Herbert Edelsbrunner (Computer Science)
Silvia Ferrari (Mechanical Engineering and Materials Science)
David Fitzpatrick (Neurobiology)
Henry Greenside (Physics)
John Harer (Mathematics)
Alexander Hartemink (Computer Science)
Craig S Henriquez (Biomedical Engineering)
Mark Huber (Mathematics / Statistical Science)
Prasad S Kasibhatla (Civil and Environmental Engineering)
Anita T Layton (Mathematics)
Harold Layton (Mathematics)
Anne A Lazarides (Mechanical Engineering and Materials Science)
Jian-Guo Liu (Physics)
Qing H. Liu (Electrical and Computer Engineering)
Paul M Magwene (Biology)
Roummel F Marcia (Electrical and Computer Engineering)
Piotr E Marszalek (Mechanical Engineering and Materials Science)
Daniel W McShea (Biology)
Thomas C Mehen (Physics)
James Nolen (Mathematics)
Mohamed A. Noor (Biology)
Richard G Palmer (Physics)
Ronald E Parr (Computer Science)
Arlie O Petters (Mathematics / Physics)
M. Ronen Plesser (Physics / Mathematics)
Amilcare M Porporato (Civil and Environmental Engineering)
Mark D Rausher (Biology)
Michael C Reed (Mathematics)
John H. Reif (Computer Science)
Scott C Schmidler (Statistical Science)

Roxanne Springer (Physics)
Xiaobai Sun (Computer Science)
Stacy Tantum (Electrical and Computer Engineering)
Kishor S Trivedi (Electrical and Computer Engineering)
Marcy K Uyenoyama (Biology)
Mike West (Statistical Science)
William Wilson (Biology)