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Principal Investigator: Westdickenberg, Maria G.   **Award ID:** 0706026
Organization: Georgia Tech Research Corp
Submitted By:
Westdickenberg, Maria - Principal Investigator
Title:
Slow Motion, Rare Events, and Sharp Bounds in High-Dimensional Systems

Project Participants

Senior Personnel
> **Name:** Westdickenberg, Maria
> **Worked for more than 160 Hours:** Yes
> **Contribution to Project:**

Post-doc

Graduate Student

Undergraduate Student

Technician, Programmer

Other Participant

Research Experience for Undergraduates

Organizational Partners

Other Collaborators or Contacts

Lia Bronsard, McMaster University, Canada

Natalie Grunewald, University of Bonn, Germany

Felix Otto, University of Bonn, Germany

Eric Vanden-Eijnden, Courant Institute, New York University

Cedric Villani, UMPA, Ecole Normale Superieure de Lyon, France

Xiaodong Yan, University of Connecticut

Sung Ha Kang, Georgia Institute of Technology (Image Processing)

Riccardo March, Istituto per le Applicazioni del Calcolo 'Mauro Picone' of C.N.R. (Image Processing)

Hendrik Weber (Warwick)

Mitch Luskin (U Minnesota)

Luca Mugnai (MPI, Leipzig)

Georg Menz (MPI, Leipzig)

Matthias Roeger (TU Dortmund)

Richard Fujimoto (lead PI on institutional IGERT proposal, not approved)

Yewande Olubummo (contact at Spelman College)

Luca Dieci (lead PI on departmental S-STEM proposal, approved)

John McCuan (co-teacher of undergrad Calc Var course and future co-author of corresponding textbook, coPI on S-STEM)

Ulrica Wilson (contact at Spelman College and coPI on S-STEM)

Activities and Findings

Research and Education Activities:

Research activities: In the portion of our work related to Dynamic Metastability, we have completed the final draft of our paper Slow Motion of Gradient Flows and have started working on application of the method to the one dimensional Cahn-Hilliard equation. We discussed this extension with Lia Bronsard when she visited to give an Applied and Computational Mathematics Seminar. We also discussed our Slow Motion framework with Dejan Slepcev and Andrea Bertozzi to see whether it may be applicable for a nonlocal swarming model that they have been studying. We are continuing to work on the Energy-Energy-Dissipation inequality for the Cahn Hilliard equation.

We have established the EED inequality for the 1-d Cahn Hilliard equation and observed that a weak norm (related to the H^{-1} norm, but weaker) suffices to put this EED into practice for the gradient flow framework. However we observed that the necessary bootstrapping step does not work. There is a mismatch of scales in the Cahn Hilliard equation, so that the weak control of the EED inequality does not rule out layer collapse on the timescale necessary for the initial excess energy to dissipate. This roadblock led to new questions about ways to exploit the additional convexity in the problem, i.e., the order one convexity transverse to the slow manifold. We have now completed a new (sharp) estimate on initial energy decay and intend to submit this as a separate paper. With this result in hand, we are also in line to complete the original project for Cahn Hilliard.

In the portion of our work related to Rare Events and Action Minimization, we completed and published the work on the 1-d Allen Cahn Action Functional with no assumption on multiplicity of interfaces. We also wrote and published a summary of the formal work related to rare events in large spatial systems.

We visited Eric Vanden-Eijnden to discuss about the use of numerical methods to further study the problem of nucleation in the presence of shear. We decided to begin with a simpler but not unrelated numerical investigation, using the String Method for metastable systems (connected to the previous section). This numerical investigation is now largely complete for the Allen Cahn equation. We will probably study one additional PDE example before submitting.

In the portion of our work related to Logarithmic Sobolev Inequalities, we finished our work on the two-scale approach to LSI and the hydrodynamic limit (with Grunewald, Otto, and Villani). We visited Petr Plechac (UTK) and Natalie Grunewald (visiting at UCLA this year) to discuss application to the analysis of a numerical algorithm. In a visit to Bonn in summers 2007 and 2009 we discussed with Georg Menz, a PhD student of Felix Otto who is working on the extension of our previous results to handle the case of weak interaction terms in the Hamiltonian for the canonical distribution. (Deniz Dizdar, the student mentioned in our grant application, finished his Diploma Thesis and decided to switch
to Economics for his PhD degree.)
We were planning to work together with Cedric Villani and a student of his, Max Fathi, on the convergence of entropy. However Fathi was particularly independent and completed the project on his own as his PhD thesis. This aspect of the project is now complete.

In the portion of our work on the Nusselt Number, we have continued to discuss with Felix Otto and Xiaodong Yan. We have made some progress in understanding the problem; for instance, we have proved that if the background profile decays like $1/z^3$ at infinity and is stable, then it must be identically zero. However $1/z$ is expected to be the 'critical' behavior at infinity, so there remains a gap. Felix Otto and a PhD student, Christian Seis, have just completed a new work in this area. It required additional information (maximal regularity). They have shown an upper bound that reduces the power on the log. They expect to also show that one *cannot* remove the logarithmic dependence with the pure background method.

Image Processing is an applied area in which nonlinear PDE and variational methods play an important role. We have been discussing with Sung Ha Kang and Riccardo March about a project to include numerical investigations and discrete Gamma convergence. Together with Sung Ha Kang we supervised four REU students in summer, 2009. During the academic year, together with Sung Ha Kang, we read a series of papers related to the new project. Together with SHK and Riccardo March, we defined the model we plan to study first and are starting work on it. Sung Ha Kang has conducted numerical experiments on four related 'true length' models. We are preparing a paper that examines the results.

In a new effort with Hendrik Weber (postdoc in Warwick) and Felix Otto, we have studied the invariant measure of the one dimensional stochastic Allen Cahn equation on large systems. The idea here is that transition layers between 1 and -1 are exponentially unlikely because of energetic effects in the measure. However when the system is large, there is an ENTROPIC effect: Namely, transition layers can appear at any point in the large system, making them more likely. The competition between energy and entropy is intriguing. Weber studied the problem in his thesis, but was only able to go up to (weakly) algebraically large systems. Combining 'soft' probabilistic methods like reflections and decomposition of measures with detailed information about the energy landscape, we are able to go up to exponential system sizes. We recover all the results that one would hope for. This work is not yet complete, but we have made significant progress and expect to finish soon.

Workshops, seminars, and research visits:
(1) AMS Sectional conference, Special Session on Variational Problems in Condensed Matter, I: Sharp Interface Limits in the Study of Rare Events

(2) Research Horizons Seminar (graduate student seminar at GA Tech): Rare Events and Action Minimization

(3) Workshop at the Hausdorff Institute for Mathematics (Bonn, Germany) on Particle systems, nonlinear diffusions, and equilibration: Invited lecture on Two Recent Results on the Logarithmic Sobolev Inequality

(4) Visit Xiaodong Yan (UConn) and gave PDE seminar: Slow Motion of Gradient Flows

(5) SIAM Conference on Analysis of PDE. Minisymposium 'Energy Based Approaches to Nonlinear PDEs' (org Slepcev, Fonseca, Leoni): Nusselt Number Scaling in Thermal Convection. Minisymposium 'Current Trends in the Calc of Variations' (org Serfaty, Kohn): Slow Motion of Gradient Flows

(6) Visit Felix Otto in Bonn

(7) Math Colloquium and WISELI speaker at Madison: Noise driven rare events and action minimization

(8) Visit Natalie Grunewald (UCLA)

(9) Visit Eric Vanden-Eijnden (NYU)

(10) Visit Lia Bronsard (McMaster) and give Applied Math Seminar.

(11) May-June 2008: One month visiting position in Toulouse to discuss Logarithmic Sobolev Inequalities

(12) June/July 2009: Research visit in Bonn, Germany.

(13) December 2009: SIAM PDE conference.
(14) Workshop at Banff (spring, 2010)
(15) Workshop at CMU (fall, 2009)
(16) Workshop at Oberwolfach (summer, 2010)
(17) Visit Felix Otto in Leipzig (summer, 2010 and December, 2010)
(18) PDE Seminar at IU (spring, 2010)

(19) BU/Brown PDE Seminar (Oct, 2010)
(20) Research visit with Felix Otto and Mitch Luskin in Minnesota (April, 2011)
(21) Math Phys Seminar at Georgia Tech (May, 2011)
(22) ICIAM: two minisymposium talks (July, 2011)

Other education activities:
(1) Host four REU students from Agnes Scott College, Spelman College, and Emory University (summer, 2009)
(2) Organized and taught a graduate class in applied mathematics (fall, 2009)
(3) Co-taught an Honors Course (undergrad) on the Calculus of Variations (fall, 2010). Planning to write a Springer textbook on the material together with my co-teacher, John McCuan.
(4) Guest lecture at Georgia Tech: Some problems in applied analysis (undergraduate level)
(5) Research Horizons Seminar at Georgia Tech: Towards a rigorous upper bound for a scaling problem in thermal convection (graduate level)

Findings:

Dynamic Metastability: Final version of Slow Motion of Gradient Flows has appeared in J. Differential Equations. Abstract sufficient conditions for so-called dynamic metastability are presented. An application to the 1-d Allen Cahn equation is demonstrated, illustrating an energy method that produces sharp bounds.

Action Minimization: Issue of multiplicity in the 1-d Allen Cahn Action Functional is resolved. Final version has appeared in IUMJ.

Project on 'Rare events in stochastic partial differential equations on large spatial domains' has appeared in Journal of Statistical Physics.

LSI: Two-scale work on LSI and the hydrodynamic limit is completed and accepted to Ann. Henri Poincare. Here we develop abstract sufficient conditions for LSI and convergence to the hydrodynamic limit. Moreover, our method for the hydrodynamic limit produces error estimates for the convergence.

Energy-energy-dissipation inequality for the 1-d Cahn Hilliard equation, involving the solution u and an associated state v in a weak norm compatible with the gradient flow structure.

Optimal energy decay rate for a kink in the Cahn Hilliard equation on R with order one H^{-1} perturbation.

Large deviation type bounds for the invariant measure of the stochastic Allen Cahn equation on exponentially large systems.

Training and Development:

The project has helped to develop the research skills of the PI. In addition, we've invited many seminar guests and have had interesting discussions related to the grant material. We've also continued to visit other universities, give seminar talks, and open discussions related to the research topics. Students have expressed interest in some of the problems. Four REU students worked on projects this summer (2009). Note in particular that two were from Agnes Scott College (women's college) and one was from Spelman (historically black women's college). In December, 2009 we co-organized a Minisymposium at SIAM PDE and invited a number of young people (PhD students and postdocs) to speak. We gave a series of lectures (short course) in Leipzig in June, 2010.

A student from our graduate course used his class project to write an applied mathematics paper in the area of aerospace. We supported him to present this paper at a national conference in Feb, 2011. I am attaching a summary from the student, Jarret Lafleur.

Outreach Activities:

(1) Hosted Robert V. Kohn as Stelson Lecturer (distinguished lecture series) at Georgia Tech. The Stelson Lectures include two lectures: a broad talk intended for a general audience (alumni, students, people from other departments) and a specialized research talk intended for experts. Both were well attended.
(2) Gave a presentation on graduate school and careers in mathematics at Spelman College.
(3) Met with Gordon Moore of Georgia Tech's Office of Minority Education and Development to discuss issues related to the recruiting of graduate students from minority groups.
(4) Visited 'Research Day' at Spelman College to see poster presentations by undergraduate math majors and discuss with them about graduate school in mathematics.

(5) Developed interdisciplinary mailing list for the Applied & Computational Mathematics Seminar to try to draw scientists from other departments to the seminars.

(6) As part of the Colloquium/WISELI vist to Madison, we had lunch with a dozen female graduate students there, which was an opportunity to discuss graduate school and careers in mathematics.

(7) Attend AWM luncheon with Georgia Benkart at Emory University.

(8) Faculty participant at the Women's Resource Center Graduate Women's Lunch (Georgia Tech). Answering questions from female grad students (from Mechanical and Bio-Medical Engineering) re finishing the thesis, applying for jobs, work-life balance, etc.

(9) Invited panelist at the AWM Job Panel Luncheon at Emory University (April, 2009), Department of Math and Computer Science.

(10) Outreach to Agnes Scott College and Spelman College

(11) Although not specifically related to my current grant, I have become involved in outreach activities related to recruiting and retaining graduate students who are women or minorities.

(12) Visit Excursion in Math for undergraduate math majors at Emory University (Saturday workshop)

(13) Co-organize the Applied and Computational Math Seminar and continue to run the interdisciplinary mailing list

(14) SIAM PDE Conference: Co-organize Minisymposium on Interface Problems and Variational Methods in Image Processing (3 sections)

(15) Co-organize events for women graduate students at Tech, including a Panel Discussion for women in the Sciences with speakers from Chemistry and Emory Mathematics (AWM group)

(16) Hosted various seminar speakers.

(17) EDGE speaker (summer program for women about to enter graduate school in Mathematics)

(18) Outreach talk to Alumni from the School of Mathematics

(19) Co-PI on S-STEM grant (approved)

(20) Participant in institutional IGERT grant (not approved, but learned a lot about colleagues and the process)

(21) Submitted a proposal for Math+X Chair through the Simons Foundation. It was not successful, but it was a useful exercise for us in Mathematics and for our communication with Mechanical Engineering.

(22) Faculty mentor to the Women's Group in Mathematics, which is now officially a student chapter of the AWM.

(23) Guest Lecture in GT 1000, an outreach seminar for freshmen

(24) Member of the AWM Travel Grants committee (2010/2011)

(25) Talks at liberal arts colleges (Agnes Scott, St Olaf, Bryn Mawr, Hampshire).

(26) Co-organizer of women's workshop in connection with upcoming MSRI workshop

(27) Attend networking events like MathFest (2010) and the Joint Meetings (2011)

Journal Publications

Otto, F; Reznikoff, MG, "Slow motion of gradient flows", JOURNAL OF DIFFERENTIAL EQUATIONS, p. 372, vol. 237, (2007). Published, 10.1016/j.jde.2007.03.00

Otto, F; Reznikoff, MG, "A new criterion for the logarithmic Sobolev inequality and two applications", JOURNAL OF FUNCTIONAL ANALYSIS, p. 121, vol. 243, (2007). Published, 10.1016/j.jfa.2006.10.00

Vanden-Eijnden, E; Westdickenberg, MG, "Rare events in stochastic partial differential equations on large spatial domains", JOURNAL OF STATISTICAL PHYSICS, p. 1023, vol. 131, (2008). Published, 10.1007/s10955-008-9537-

Westdickenberg, MG, "Rare events, action minimization, and sharp interface limits", SINGULARITIES IN PDE AND THE CALCULUS OF VARIATIONS, p. 217, vol. 44, (2008). Published,

Westdickenberg, MG; Tonegawa, Y, "Higher multiplicity in the one-dimensional Allen-Cahn action functional", INDIANA UNIVERSITY MATHEMATICS JOURNAL, p. 2935, vol. 56, (2007). Published,

N. Grunewald, F. Otto, C. Villani, and M.G. Westdickenberg, "A two-scale approach to logarithmic Sobolev inequalities and the hydrodynamic limit", Annales de l'Institut Henri Poincar?? (B) Probabilit??s et Statistiques, p. 302, vol. 45, (2009). Published,

Books or Other One-time Publications

Maria G. Westdickenberg, "Rare events, action minimization, and sharp interface limits", (2008). Book, Published

Web/Internet Site

Other Specific Products

Contributions

Contributions within Discipline:

The work on the Allen-Cahn functional represents progress on a new, time-dependent Calculus of Variations problem. In addition, it resolves the issue of higher multiplicity interfaces, an issue which is often confounding in sharp-interface limits.

The work on Logarithmic Sobolev Inequalities develops a new sufficient condition for a measure to satisfy an LSI, a condition which does not require convexity of the Hamiltonian. Moreover, the bound produced in the theorem is shown to be sharp for a certain class of Gaussian measures. The work on the 'two-scale approach' takes the idea of coarse-graining from physics and uses it to develop a quantitative and mathematically rigorous result for LSI and convergence to the hydrodynamic limit. New sufficient conditions for LSI and the hydrodynamic limit are established. They allow for a simpler and more intuitive proof of some existing results, and include new, quantitative error estimates. They also led to the continuation about entropy convergence that was carried out by Max Fathi (PhD student of Cedric Villani), and the contributions to LSI by Georg Menz (PhD student of Felix Otto) and Menz & Otto.

The work on Slow Motion of Gradient Flows develops sufficient conditions on an infinite dimensional energy landscape in order for the associated gradient flow to demonstrate so-called dynamic metastability. This is a new kind of energy method, one which is shown to produce sharp bounds for the 1-d Allen Cahn equation. The ongoing work to apply the method to the 1-d Cahn Hilliard equation would give a mathematical proof of numerically observed dynamic behavior. The real break-through is the development of sufficient conditions that do not require a maximum principle; Cahn Hilliard is the first example on which to exploit this. The work on Cahn Hilliard led us to develop a new technique for energy dissipation in the case of 'approximate convexity.' This extends a result of Brezis on energy decay for gradient flows of a convex functional.

The work on rare events in large spatial systems introduces a methodology to attack rare events in stochastically perturbed partial differential equations in the setting where the system size is so large (exponentially large in the inverse noise strength) that standard techniques cannot be applied.

The work on the invariant measure of the stochastic Allen Cahn equation in the case of exponentially large system size is new and optimal in terms of scaling. It is interesting in terms of method, as well, as it combines truly probabilistic and truly energetic/PDE arguments at its core.

The numerical application of the String Method to metastable problems gives a new method for computing trajectories in slow systems.

The image processing project with Sung Ha Kang and Riccardo March will give a variational method that finds the 'true length' for curves, unlike the traditional methods. This is important in some applications.

Contributions to Other Disciplines:

Contributions to Human Resource Development:

The goal of the outreach to Spelman and Agnes Scott Colleges is to create bridges between these colleges and the GA Institute of Technology that may lead to involvement of women from those institutions in REUs or graduate school at GA Tech. Although no concrete results have yet manifested, we did receive interest (emails, personal contact) from students wanting to find out more about opportunities at GA Tech. This is an ongoing endeavor.

We enrolled four students (two from Agnes Scott, one from Spelman, and one from Emory) for a summer REU (2009) on mathematical approaches to image processing. The students gained valuable experience in research, presentation, and writing up of mathematical results. Furthermore, we hope to continue to develop links among the institutions which may be valuable for attracting graduate students and

developing other mutually beneficial programs. We have supported the development of a women's group for graduate students, which can also play a supportive role and help address the issue of the 'leaky pipeline.' It is now officially a student chapter of the AWM. We also arranged for Chan Jin from Agnes Scott College to network with Dan Margalit (GT) and use Tech computing resources to pursue a project of hers in algebra. We helped line up a student from Wesleyan College for an internship with Dan Goldman in GT, Physics. I am not sure whether the student has followed through on the internship (there were some questions that arose), but it is important that students (and in particular, women, minorities, and domestic students) from smaller colleges have the opportunity to meet and work with faculty from larger institutions, as this experience may encourage them to pursue a higher degree in mathematics or science. I found out about the student from Wesleyan College through a faculty there (Ha Nguyen) whom I originally met when she was co-president of the AWM student group at Emory University. And so I see firsthand how networking activities like women's groups and trans-generational meetings can generate multiple, long-term benefits.

Contributions to Resources for Research and Education:

Contributions Beyond Science and Engineering:

Conference Proceedings

Categories for which nothing is reported:

Organizational Partners

Any Web/Internet Site

Any Product

Contributions: To Any Other Disciplines

Contributions: To Any Resources for Research and Education

Contributions: To Any Beyond Science and Engineering

Any Conference

From February 13-17, 2011, I attended the 21st AAS/AIAA Space Flight Mechanics Meeting in New Orleans, Louisiana, to present paper AAS 11-173, "Extension of a Simple Mathematical Model for Orbital Debris Proliferation and Mitigation". Based on a capstone project in Dr. Maria Westdickenberg's Fall 2009 Industrial Math (MATH 6514) class, this paper extends a previously proposed analytic orbital debris proliferation model consisting of two coupled differential equations. Analyzed in the paper are both the transient and equilibrium behavior of the extended model, leading to conclusions on the likely effectiveness of potential debris mitigation measures.

This conference provided me with several valuable opportunities. It allowed me to publicly contribute an analysis technique toward the current problem facing the space industry of dealing with the proliferation of debris in Earth orbit, and the paper on the topic will be available via the American Astronautical Society's *Advances in the Astronautical Sciences* series of published proceedings. One professor who attended my presentation suggested that I also submit the work for publication in a peer-reviewed aerospace journal such as the *Journal of Spacecraft and Rockets* or *Acta Astronautica*. This conference also provided me the opportunity to gain feedback from orbital debris experts and other aerospace professionals. Among the conversations that followed my presentation were with Mr. Jer Chyi Liou, a well-known analyst in the NASA Orbital Debris Program Office, and Dr. David Finkleman, former Director of Studies and Analysis for the North American Aerospace Defense Command (NORAD) and U.S. Space Command. I also had the opportunity to meet Mr. Donald Kessler, the conference's keynote speaker for whom the "Kessler Syndrome" of orbital debris collisional cascading is named. More generally, I was able to use my time at the conference to attend sessions and better understand the state of the art in astronautics as well as the application of mathematical modeling techniques in the astronautical community. Finally, as an added bonus, I was able to organize a successful visit for 19 of the conference attendees to the nearby NASA Michoud Assembly Facility, the site where the Space Shuttle's External Tank and the Saturn V rocket's first stage were once manufactured.

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