THE GRADUATE SCHOOL
of
**THE UNIVERSITY OF COLORADO
AT BOULDER**

DISSERTATION DEFENSE
of

Lieutenant Colonel Dustin D. Keck

FOR THE DEGREE

DOCTOR OF PHILOSOPHY

Date/Time: May 21, 2014 from 1:00 pm.

Bldg./Rm: ECCR, 257 - Newton Lab

Examining Committee Members:
David Bortz, Vanja Dukic, Keith Julien, Juan Restrepo, and John Younger

OUTLINE OF STUDIES

Major Field: Applied Mathematics

BIOGRAPHICAL NOTES

Dustin was born in Sharon, Pennsylvania. At North Carolina State University in 1997, he received a BS in aerospace engineering and earned a commission as a second lieutenant in the Air Force. He flew C-17s until 2007, after which he earned an MS in applied mathematics at the University of Colorado Colorado Springs. He followed that degree with three years as a math teacher and flight instructor at the United States Air Force Academy. He has spent the last three years at CU-Boulder studying and researching in the math biology group in the Department of Applied Mathematics. In his free time, Dustin tries to take advantage of the boundless outdoor activities that Colorado has to offer.

THESIS

Complete title of thesis:
Aggregation Dynamics: Numerical Approximations, Inverse Problems, and Generalized Sensitivity

Faculty Advisor David Bortz

ABSTRACT

In this dissertation, we investigate several important mathematical and computational issues that arise when using the Smoluchowski coagulation equation as a model for bacterial aggregation. In particular, we study the accuracy and robustness of numerical simulations and their impact upon related inverse problems. We also study how generalized sensitivity enhances experimental design optimization with an ultimate goal of comparing with experimental data.

First, we study the impact of discretization strategy on the accuracy of solution moment. We perform this investigation in anticipation of comparing with different distributions moments reported by specific experimental devices. For multiplicative aggregation kernels, finite volume methods are superior to finite element methods both in accuracy and computational effort. Conversely, for slowly aggregating systems the finite element approach can produce as little error as the finite volume approach and achieves more accuracy approximating the zeroth moment (at a substantially reduced computational cost).

A better understanding of bacterial aggregation dynamics could also lead to improvements in the treatment of bacterially mediated, life-threatening human illnesses. Therefore, to reach towards our ultimate goal, we examine the inverse problem of estimating the aggregation rate from experimental data. In this study, we develop a methodology for a software implementation of parameter fitting when solving inverse problems involving the Smoluchowski coagulation equation. Additionally, we make the novel extension of generalized sensitivity functions (GSFs) for ordinary differential equations to GSFs for partial differential equations. We analyze the GSFs in the context of size-structured population models, and specifically analyze the Smoluchowski coagulation equation in order to determine the most relevant time and volume domains for three distinct aggregation kernels. Finally, we provide evidence that parameter estimation for the Smoluchowski coagulation equation does not require post-gelation data.