

# Mathematical Tools for Discontinuous Dynamical Systems

by

Matthew Ryan Billingsley

Submitted to the Department of Chemical Engineering  
on August 31, 2022, in partial fulfillment of the  
requirements for the degree of  
Doctor of Philosophy in Chemical Engineering

## Abstract

Nonsmooth equations and discontinuous dynamical systems can be used to model systems in a variety of applications, including modeling of certain physical systems and optimization problems. However, theoretical results are somewhat limited for these classes of problems, restricting their use in practical applications. In order to develop the necessary theory, existing theoretical results for other nonsmooth systems can be extended to these important classes of problems.

In this thesis, theoretical results and software implementations are developed for certain classes of nonsmooth and discontinuous systems. A method for evaluating lexicographical directional derivatives of functional programs is developed, extending existing methods to programs containing conditional branches and loops. A software implementation of the theoretical results is also developed. Next, well-posedness and sensitivity results are established for a class of discontinuous ordinary differential equations, which are derived from overarching differential-algebraic equations using directional differentiation. Next, a new nonsmooth formulation of Hamiltonian dynamics for Hamiltonian systems with nonsmooth potential energy is developed, using lexicographic differentiation to derive a system of discontinuous differential equations, and theoretical results are developed. Using this nonsmooth formulation of Hamiltonian dynamics, a new Hamiltonian Monte Carlo method is developed for systems with nonsmooth target probability densities. A software implementation of this method has been developed in Julia.

Thesis Supervisor: Paul I. Barton

Title: Lamot du Pont Professor of Chemical Engineering