Marcus R. Garvie, Department of Mathematics and Statistics, MacNaughton Building, University of Guelph, Guelph, ON N1G 2W1, Canada, Philip K. Maini, Centre for Mathematical Biology, Mathematical Institute, 24-29 St. Giles', University of Oxford, Oxford, OX1 3LB, England, and Catalin Trenchea* (trenchea@pitt.edu), 301 Thackeray Hall, Department of Mathematics, University of Pittsburgh, Pittsburgh, PA 15260. An efficient and robust numerical algorithm for estimating parameters in Turing systems.

We present a new algorithm for estimating parameters in reaction-diffusion systems that display pattern formation via the mechanism of diffusion-driven instability. A Modified Discrete Optimal Control Algorithm (MDOCA) is illustrated with the Schnakenberg and Gierer–Meinhardt reaction-diffusion systems using PDE constrained optimization techniques. The MDOCA algorithm is a modification of a standard variable step gradient algorithm that yields a huge saving in computational cost. The results of numerical experiments demonstrate that the algorithm accurately estimated key parameters associated with stationary target functions generated from the models themselves. Furthermore, the robustness of the algorithm was verified by performing experiments with target functions perturbed with various levels of additive noise. The MDOCA algorithm could have important applications in the mathematical modeling of realistic Turing systems when experimental data are available. (Received September 21, 2010)