Erin M. Kiley: Statement of Research

Since 2006, my research has been in the general realm of creating and refining mathematical models of microwave heating, which necessarily involves solving both the electromagnetic problem (Maxwell's Equations within a cavity) and the thermal problem (the heat equation on a domain with multiple boundaries). That year, I completed the first [1] among many projects in this scope, including a year-long study of resolution of integral equations for electromagnetics, an M.Sc. project that developed a method for modeling microwave cavities with perforated walls [3], a report on techniques for estimating material properties for input to these models [4], and the production of computer models of an existing state-of-the-art system for microwave processing of nanomaterials, giving that system's users (engineers and materials scientists) a tool that facilitated their investigations of microwave sintering, a subject that remains of interest to our general research group and that became the main topic of my Ph.D. research.

Sintering is a manufacturing technique that subjects particulate materials to temperatures and pressures that induce the microstructural changes necessary for evolution of the material properties (e.g., stiffness, strength). Sintering of ceramics has been done in kilns relying on only convection for thousands of years, but for micro- and nanopowders, using microwaves as the heat source has shown many potential advantages, including faster processing, finer microstructure or otherwise improved material properties of the resulting new materials, and—in well designed systems—the potential for vast energy savings. Despite these promising results, the technique remains underutilized in industry, due mostly to the difficulty of controlling the process and the resulting problems with reproducibility of experiments.

A number of innovative microwave manufacturers, including SAIREM SAS and Püschner GmbH & Co., have successfully incorporated computer models into their design process, replacing expensive and time-consuming cut-and-try experimentation and broadening the scope of their investigations into the possibilities of microwave processing. My most recent research has therefore focused on creating and using mathematical models of microwave sintering and computer simulations that employ these models, with the strong belief that if such computational tools are used judiciously in the design of systems for microwave sintering, they could help rectify the challenges that have prevented microwaves from fulfilling their potential as a green and efficient way of conducting sintering as an industrial manufacturing process, in production of new materials with unique physical properties.

Existing techniques for modeling certain limited aspects of microwave sintering have yet to be synthesized into a comprehensive model of the different complex physical phenomena that occur simultaneously during the process, on varying spatial and temporal scales. This multiphysics, multiscale nature of microwave sintering warrants especially careful mathematical treatment, and my research has been an interdisciplinary effort focused on development of the first fully mathematically consistent computer models of microwave sintering intended for use by experimentalists and design engineers.

My first attempts toward this goal involved the coupling of two separate pieces of modeling software to represent a macroscopic (component-sized) spatial scale; these efforts [5] were undertaken jointly with the Laboratory for Materials Science and Processing (SIMaP) at the Grenoble Institute of Technology (INP), and they revealed the necessity of finer characterization of the constitutive equations and their evolution during the course of sintering through the creation of an in-house, ground-up model whose general operation is outlined in Figure 1. Each of the purple (rounded) blocks in the flow chart represents a method of solving the indicated physical problem; of course, multiple such methods exist for each problem, and each has its particular strengths. For the electromagnetic problem, I have implemented solvers based on integral equation methods and analytical approximation techniques, in addition to numerical methods based on the Finite Difference Time Domain (FDTD) method and the Finite Element Method (FEM); for the heat equation, I have implemented solvers based on both Finite Difference Methods and FEM. The mechanical solver is conceptually different from either of the other two, as mechanical deformation at the particle level influences changes at the component scale, and so in addition to my current model, which employs an approximation based on the evolution of average relative density in the sample, I am currently developing a phenomenological model using density kinetics to represent microscale changes. The other blocks in the chart represent a particular type of coupling between the physical phenomena by which solution of the constitutive equations is conditioned by changes of the material properties, including complex permittivity and permeability ε, μ; specific heat capacity c; thermal conductivity κ; and particle packing density D and average grain radius R.

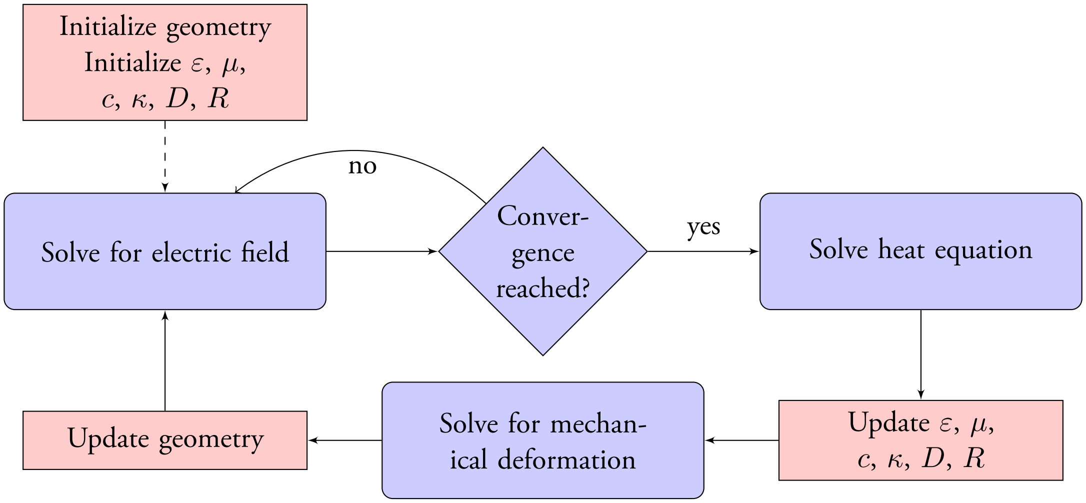

Figure 1: Numerical algorithm simulating microwave sintering.

I am currently in the middle of one semester in residence at SIMaP/INP conducting a comparison of simulated and experimental results. Future development of the model will be conducted in view of these results, but already includes plans for further refinement of the densification model and phenomenological density kinetics that underly it, and possible inclusion of simulated nonthermal effects of microwaves on the sintering process, which have not been incorporated into any coupled solvers.

I have greatly enjoyed my research, which since 2006 has been conducted at Worcester Polytechnic Institute (WPI) under the guidance of Prof. Vadim V. Yakovlev, in the mathematics department of Penza State University (Russia) under a Fulbright fellowship in 2008 [2], at the Swiss Federal Laboratories for Materials Science and Technology (EMPA) in Thun, CH under a ThinkSwiss Fellowship given by the swissnex division of the Embassy of Switzerland in 2008 and 2009, and most currently, at SIMaP/INP under the Chateaubriand Fellowship given by the French Embassy.

After my defense in May, I intend to continue improving my model of microwave sintering by adding solvers for a greater number of micromechanical phenomena; by exploring the possibility of mathematical homogenization for the physical problem; and by hastening the computational solution of the electromagnetic model. These developments are expected to further my current goal of creating the most accurate and mathematically consistent computer simulations of microwave sintering for use by design engineers working on reproducibility of trials for industrial applications.

References

[1] D.A. Feldman, E.M. Kiley, S.L. Weekes, V.V. Yakovlev, "Modelling of temperature fields in 1D and 2D heating scenarios with pulsing microwave energy," 9^{th} *Computer Modelling and Microwave Power Engineering Seminar, Valencia, Spain*, 2007.

[2] Yu.G. Smirnov, "Application of GRID-technology for the solution of the nonlinear volume singular integral equation for determining the effective dielectric permeability of nanomaterials," *Trans. of the Univ. of the Volga Reg.: Phys.-Math. Sci.*, 3:39–54, 2008.

[3] E.M. Kiley, V.V. Yakovlev, "Modeling of Microwave Ovens with Perforated Metal Walls," *IEEE MTT-S Int. Microw. Symp. Dig.*, 2011.

[4] E.M. Kiley, V.V. Yakovlev, S. Vaucher, K. Ishizaki, "Applicability study of classical and contemporary models for effective complex permittivity of metal powders," *J. Microw. Pow. & Electromagn. Energy*, 46(1):26–38, 2012.

[5] S. Bogachev, D. Bouvard, E.M. Kiley, V.V. Yakovlev, "An iterative routine for macroscopic modeling of electromagnetic, thermal, and mechanical phenomena in microwave sintering," in *Microw. &RF Power Appl.*, Junwu Tao, Ed., Cépaduès Éditions, 2011.