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Ferret: an open-source code for simulating thermodynamical evolution and phase transformations in complex materials systems at mesoscale SERGE NAKHMANSON, JOHN MANGERI, KRISHNA PITIKE, LUKASZ KUNA, University of Connecticut, ANDREA JOKISAARI, Northwestern University, S. PAMIR ALPAY, University of Connecticut, OLLE HEINONEN, Argonne National Laboratory — Ferret is an open-source real-space finite-element-method (FEM) based code for simulating behavior of materials systems with coupled physical properties at mesoscale. It is built on MOOSE, Multiphysics Object Oriented Simulation Environment, and is being developed by the UConn-ANL collaboration. Here we provide an overview of computational approach utilized by the code, as well as its technical features and the associated software within our computational tool chain. We also highlight a variety of code application examples that are being pursued in collaboration with a number of different experimental groups. These applications include (a) evaluations of size- and microstructure-dependent elastic and optical properties of core-shell nanoparticles, including Zn/ZnO and ZnO/TiO_2 core/shell material combinations; (b) modeling of the influence of shape, size and elastic distortions of monolithic ZnO and Zn/ZnO core/shell nanowires on their optical properties; (c) studies of the properties and domain-wall dynamics in perovskite-ferroelectric films, nanowires and nanoridges, and (d) investigation of topological phases and size effects in ferroelectric nanoparticles embedded in a dielectic matrix.

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