Introduction

Our program is a phase-field modeling code for calculating the microstructure evolution of ferroelectrics that allows complex electromechanical boundary conditions. We uses Boundary Elements and Dirichlet-to-Neumann map to enable accurate and efficient calculation of stray electric fields outside the specimen. The code is currently written in C/C++ and integrates with PetSc to solve large scale linear equations.

Program Description

Our program can be downloaded at: http://matforge.org/redmine/projects/real-space-ferro/files Inside the folder "C_Domian_Under_Point_Charge", there are 15 files.

- "Main.c" basically updates the microstructure evolution of ferroelectrics.
- "FEM.h" and "BEM.h" calculate both the elastic and electrostatic energy which is needed to update polarization in every time step. For more detailed description, please refer to the comments inside the code.
- Data file "G, H, K, K_x, K_y, K1, K2, KV" store the information of global matrices which is needed in every time step of the evolution.
- Data file "Mesh.1.ele" and "Mesh.1.nodes" store the mesh information while "Info_Mesh" records the total number of nodes and elements.
- At last, "makefile" is included to compile the code.

FEM Mesh and Calculation Time

Our program of calculating the domain microstructure of ferroelectrics usually takes 30,000 evolutional time steps to converge. The total CPU hours with respect to the number of degree of freedom is listed in the table below.

Degrees of freedom	Total CPU hours
5299	12 hours
8324	26 hours
16384	72 hours

One advantage of Finite Element method is to increase the density of mesh in the region of interest, while using coarse mesh elsewhere. Typically, we use 8324 degrees of freedom for most of our calculations.