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Analysis of Nonlinear Effects in Ferroelectric Materials Using Phase Field Simulations in Open Source Finite Elements Software

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Ferroelectric materials are currently a topic of intense research in electronics, due to their extremely high permittivity and possible use in new transistor technologies. On a fundamental level, ferroelectric materials are the electric counterpart of ferromagnetic materials, where permanent electric dipole moments in the crystal structure may be aligned and create a very strong bulk material polarization. This presents important challenges in electromagnetic modelling and simulation, due to the nonlinear nature of such processes. The nonlinearity can be quantified in a phase field simulation based on the combination of Maxwell's equations with a Landau-Ginzburg equation for the temporal evolution of the polarization P at each spatial location:

$$\frac{\partial P}{\partial t} = \kappa \nabla^2 P - \alpha P - \beta P^3 - \gamma P^5 + \sigma E \tag{1}$$

where the right hand side is a nonlinear function of the polarization P and the electric field E. This is a phase field simulation, where it is assumed the domain of interest is large enough to treat the material as a continuum, and use the polarization P as a variable of state. Equation (1) together with Maxwell's equations can be discretized using the open source finite elements software FEniCSx, see `https://fenicsproject.org/`. The result is a set of ordinary differential equations in time for the degrees of freedom representing the spatial discretization, which can be solved with standard ODE solvers. The programming language is python, and the weak formulation of the PDE:s can be written almost verbatim in the Unified Form Language (UFL), enabling simulation of many different PDE-based material models in addition to the ferroelectrics under study in this paper. As an example, a UFL formulation of a central time discretization of (1) (after rewriting it in weak form by multiplying with a test function Q and integrating over space) could be

```
P_mid = (P + P0)/2
L = (1/dt)*(inner(P, Q)*dx - inner(P0, Q)*dx) + inner(kappa*grad(P_mid), grad(Q))*dx \
+ inner(alpha*P_mid + beta*P_mid**3 + gamma*P_mid**5, Q)*dx - inner(sigma*E, Q)*dx
```

where `P` is the polarization at time t_{n+1}, `P0` is the polarization at time t_n, and `Q` is a test function. The resulting functional `L` can later be input to a general Newton solver that solves for `P` given values for `P0` and `E`, offering a straight-forward numerical solution to the nonlinear PDE.

The model enables the study of nonlinear effects, such as the switching dynamics of a ferroelectric cell subjected to a time varying electric field, often resulting in hysteresis effects. This is of great interest in electronics, where the switching of a ferroelectric gate affects the behavior of transistors. With a fixed frequency excitation, the solution can be expressed as a sum of harmonics due to the polynomial character of the right hand side in (1). In the presentation, I provide examples of how ferroelectric materials can be simulated, and how nonlinear effects such as hysteresis and generation of harmonics affect affect the solution of Maxwell's equations.