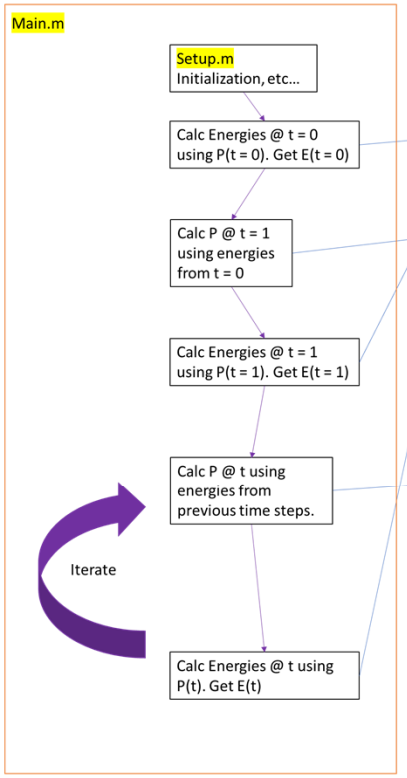

CalcEnergies.m

TimeStep_1stOrd.m
First order means the time method was first order. We are only using P(t) and E(t) to calculate P(t + dt)

TimeStep_2ndOrd.m
Second order means the time method was second order. We are using P(t), P(t – dt), E(t), and E(t – dt) to calculate P(t + dt)

Calc Elastic Energy $f_{el} = C_{ijkl}\left(\varepsilon_{ij} - \varepsilon_{ij}^{0}\right)\left(\varepsilon_{kl} - \varepsilon_{kl}^{0}\right)$ CalcElasticEnergy.m

Solve $C_{ijkl}u_{k,lj} = C_{ijkl}$ with boundary conditions

$u = displacement\ field$

$\varepsilon^{0} = eigenstrain, function\ of\ \vec{P}$

$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right) = strain$

See https://www.sciencedirect.com/science/article/pii/S1359645401003603, Summary Chapters 2-5

Computationally Expensive

The tensor equation $C_{ijkl}u_{k,lj} = C_{ijkl}$ is solved by performing a 2D (x,y) FFT This 2D FFT creates a 1D ODE for each (kx,ky) (x → kx, y → ky from the 2D FFT) point. This requires iterating through (kx,ky) and solving an ODE at each (kx,ky).

Calc Electric Energy $f_{elec} = -\frac{1}{2}E_i^d P_i$ CalcElecEnergy.m

Solve $\kappa_{ij}\phi_{,ji} = \frac{1}{\varepsilon_0}P_{i,i}$ with boundary conditions

$k = relative\ permittivity$

$\phi = electric\ potential$

$E_i^d = \phi_{,i}$

See http://www.mmm.psu.edu/SC2005ActaMater.pdf , Summary Chapter 6

Computationally Expensive

Similar 2D FFT method used to solve the tensor equation. Less computationally expensive than CalcElasticEnergy b/c easier to apply boundary conditions.

Calc Landau Energy. Plug into the polynomial equation.

Solve $\frac{\partial P_2}{\partial \tau} = -W_2\left(\vec{P}\right) + G_{11}P_{2,22}$ with boundary conditions.

W_2 represents all the energies.

$G_{11}P_{2,22}$ is the gradient energy, which accounts for the energy associated with the spatial variation of P.

Time Discretization: $P_2(\tau + \Delta\tau) - \Delta\tau G_{11}P_{2,22}(\tau + \Delta\tau) = -\Delta\tau W_2\left(\overrightarrow{P_2(\tau)}\right) + P_2(\tau)$

Long-Qing Chen's key step was to **consider the gradient term implicitly**.

Gradient is calculated with respect to the future time step $P_{2,22}(\tau + \Delta\tau)$ rather than the current time step τ

3D FFT: $\mathcal{F}_{3D}\left\{P_2(\tau + \Delta\tau) - \Delta\tau G_{11}P_{2,22}(\tau + \Delta\tau) = -\Delta\tau W_2\left(\overrightarrow{P_2(\tau)}\right) + P_2(\tau)\right\}$

$\widehat{P_2}(\tau + \Delta\tau) + \Delta\tau G_{11}\xi_2^2 P_2(\tau + \Delta\tau) = -\Delta\tau\widehat{W_2} + \widehat{P_2}(\tau)$

$\widehat{P_2}(\tau + \Delta\tau) = \frac{-\Delta\tau\widehat{W_2} + \widehat{P_2}(\tau)}{1 + \Delta\tau\left(G_{11}\xi_2^2\right)}$

ξ is the FFT axis. The hat notation means the FFT'ed function.

See https://www.sciencedirect.com/science/article/pii/S001046559700115X, Summary Chapter 7

NOTATION: comma in subscript indicates partial derivative

$$E_i^d = \phi_{,i} = \frac{\partial}{\partial x_i}\phi$$

NOTATION: repeated subscripts indicates summation

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} = \sum_{k,l} C_{ijkl}\varepsilon_{kl}$$