Q-POP-FerroDyn

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Formulation for Q-POP-FerroDyn

The total free energy of the system is defined as

$$F = F_{Landau} + F_{gradient} + F_{electrostatic} + F_{elastic}, \tag{1}$$

where

$$F_{Landau} = \int (a_i P_i^2 + a_{ij} P_i^2 P_j^2 + a_{ijk} P_i^2 P_j^2 P_k^2) dx^3 \tag{2}$$

$$F_{gradient} = \int g_{ijkl} \frac{\partial P_i}{\partial x_j} \frac{\partial P_k}{\partial x_l} dx^3 \tag{3}$$

$$F_{electrostatic} = \int \Big(-\frac{1}{2} \kappa_0 \kappa_{ij}^b E_i E_j - E_i P_i \Big) dx^3 \tag{4}$$

$$F_{elastic} = \int \frac{1}{2} c_{ijkl} (\epsilon_{ij} - \epsilon_{ij}^0)(\epsilon_{kl} - \epsilon_{kl}^0) dx^3 \tag{5}$$

Dynamical equation for polarization $\mathbf{P}$(x, t):

$$\mu_{ij} \frac{\partial^2 P_j}{\partial t^2} + \gamma_{ij} \frac{\partial P_j}{\partial t} + \frac{\delta F}{\delta P_i} = 0, \tag{6}$$

where $\boldsymbol{\mu}$ and $\boldsymbol{\gamma}$ are mass and damping coefficients, respectively.

The driving force term in the dynamic equation for polarization is

$$\frac{\delta F}{\delta P_i} = \frac{\delta}{\delta P_j} (F_{Landau} + F_{gradient} + F_{electrostatic} + F_{elastic}) \tag{7}$$

$$= 2a_i P_i + 2a_{ij} P_i P_j^2 + 2a_{ijk} P_i P_j^2 P_k^2 + g_{ijkl} \frac{\partial^2 P_k}{\partial x_j \partial x_l} - E_i \tag{8}$$

Elastodynamics equation for mechanical displacement $\mathbf{u}$(x, t):

$$\rho \frac{\partial^2 u_i}{\partial t^2} = f_i^v + \frac{\partial}{\partial x_j} \Big(\sigma_{ij} + \beta \frac{\partial \sigma_{ij}}{\partial t} \Big), \tag{9}$$

where ρ, β, and f^v are the material mass density, the stiffness damping coefficient, and the external body force density, respectively.

The stress field $\boldsymbol{\sigma}(x, t)$ is defined as

$$\boldsymbol{\sigma}(\boldsymbol{x}, t) \equiv \sigma_{ij} = c_{ijkl} (\epsilon_{kl} - \epsilon_{kl}^0), \tag{10}$$

where $\boldsymbol{c}$ is the elastic stiffness tensor, $\boldsymbol{\epsilon}(\mathbf{x}, t)$ is the strain field given by $\boldsymbol{\epsilon} = [\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T]/2$, and $\boldsymbol{\epsilon}^0(\boldsymbol{x}, t) \equiv \epsilon_{ij}^0 = Q_{ijkl} P_k P_l$ is the eigenstrain field with an electrostrictive coefficient $\boldsymbol{Q}$.

Maxwell's Equations

Starting from Ampere's Law,

$$\begin{aligned}\nabla \times \boldsymbol{H} &= \boldsymbol{J} + \frac{\partial \boldsymbol{D}}{\partial t} \\ &= \boldsymbol{J} + \epsilon\frac{\partial \boldsymbol{E}}{\partial t} + \frac{\partial \boldsymbol{P}}{\partial t} \qquad (11)\end{aligned}$$

$$\begin{aligned}\implies \frac{\partial \boldsymbol{E}}{\partial t} &= \frac{1}{\epsilon}\Big(\nabla \times \boldsymbol{H} - \boldsymbol{J} - \frac{\partial \boldsymbol{P}}{\partial t}\Big) \\ &= \frac{1}{\epsilon_0\epsilon_r}\Big(\nabla \times \boldsymbol{H} - \boldsymbol{J}^f - \frac{\partial \boldsymbol{P}}{\partial t}\Big) \qquad (12)\end{aligned}$$

Faraday's law reads

$$\nabla \times \boldsymbol{E} = -\mu\Big(\frac{\partial \boldsymbol{M}}{\partial t} + \frac{\partial \boldsymbol{H}}{\partial t}\Big) \qquad (13)$$

$$\implies \frac{\partial \boldsymbol{H}}{\partial t} = -\frac{1}{\mu}(\nabla \times \boldsymbol{E}) - \frac{\partial \boldsymbol{M}}{\partial t} \qquad (14)$$

The Maxwell's equations are solved using the finite-difference time-domain method (FDTD), using a staggered Yee grid. The stencil used by the Yee grid is as follows:

$$\begin{aligned}&1:(i-1,j-1,k-1), 2:(i-1,j-1,k), 3:(i-1,j,k-1), 4:(i-1,j,k)\\ &5:(i,j-1,k-1), 6:(i,j-1,k), 7:(i,j,k-1), 8:(i,j,k)\end{aligned}$$

The permittivity and conductivity tensors are computed at each node by averaging over the stencil.

$$\begin{aligned}\epsilon_{ij} &= \frac{\sum_{n=1}^{8}\epsilon_{ij,n}}{8}\\ \sigma_{ij} &= \frac{\sum_{n=1}^{8}\sigma_{ij,n}}{8}\end{aligned}$$

Similarly, the source-terms representing various types of current are averaged over the same stencil.

A fourth-order explicit Runge-Kutta (RK4) method is used for time-marching.

For n = 1, 2, 3, 4, where each n represents the respective strides between two formal time-steps, an example of the update equation at node (i, j, k) is as follows:

$$\begin{aligned}\Delta E_x^{(t+\frac{n\Delta t}{4})}|_{i,j,k} = &\Bigg[\frac{\Delta t}{\epsilon_0}\Big(\frac{\epsilon_{yy}\epsilon_{zz} - \epsilon_{yz}\epsilon_{zy}}{||\epsilon||}\Big)\Bigg|_{i,j,k} \times \dots\\ &\Big(\frac{\partial H_z}{\partial y}\Big|_{i,j,k}^{(t+\frac{(n-1)\Delta t}{4})} - \frac{\partial H_y}{\partial z}\Big|_{i,j,k}^{(t+\frac{(n-1)\Delta t}{4})} - \Delta J_x^{(t+\frac{(n-1)\Delta t}{4})} - \sigma_{xi}E_{i,store}^{(t+\frac{(n-1)\Delta t}{4})} - \frac{\Delta P_x^{(t+\frac{n\Delta t}{4})}}{\Delta t}\Big)\Bigg]\\ &+\Bigg[\frac{\Delta t}{\epsilon_0}\Big(\frac{\epsilon_{xz}\epsilon_{zy} - \epsilon_{xy}\epsilon_{zz}}{||\epsilon||}\Big)\Bigg|_{i,j,k} \times \dots\\ &\Big(\frac{\partial H_x}{\partial z}\Big|_{i,j,k}^{(t+\frac{(n-1)\Delta t}{4})} - \frac{\partial H_z}{\partial x}\Big|_{i,j,k}^{(t+\frac{(n-1)\Delta t}{4})} - \Delta J_y^{(t+\frac{(n-1)\Delta t}{4})} - \sigma_{yi}E_{i,store}^{(t+\frac{(n-1)\Delta t}{4})} - \frac{\Delta P_y^{(t+\frac{n\Delta t}{4})}}{\Delta t}\Big)\Bigg]\\ &+\Bigg[\frac{\Delta t}{\epsilon_0}\Big(\frac{\epsilon_{xy}\epsilon_{yz} - \epsilon_{xz}\epsilon_{yy}}{||\epsilon||}\Big)\Bigg|_{i,j,k} \times \dots\\ &\Big(\frac{\partial H_y}{\partial x}\Big|_{i,j,k}^{(t+\frac{(n-1)\Delta t}{4})} - \frac{\partial H_x}{\partial y}\Big|_{i,j,k}^{(t+\frac{(n-1)\Delta t}{4})} - \Delta J_z^{(t+\frac{(n-1)\Delta t}{4})} - \sigma_{zi}E_{i,store}^{(t+\frac{(n-1)\Delta t}{4})} - \frac{\Delta P_z^{(t+\frac{n\Delta t}{4})}}{\Delta t}\Big)\Bigg] \qquad (15)\end{aligned}$$

where

$$\frac{\partial H_x}{\partial y}\Big|^{(t+\frac{(n-1)\Delta t}{4})} = \frac{H_x^{(t+\frac{(n-1)\Delta t}{4})}|_{i,j,k} - H_x^{(t+\frac{(n-1)\Delta t}{4})}|_{i-1,j,k}}{\Delta y}, \qquad (16)$$

$$\Delta J_i = \Delta J_{f,i} + \Delta J_{p,i} + \Delta J_{ISHE,i}, \tag{17}$$

$\Delta J_{f,i}$ is the change in the free charge current density.

$\Delta J_{p,i}$ is the change in the polarization current density (eddy current). Its evolution is governed by the Drude equation

$$\frac{\partial \boldsymbol{J}_p}{\partial t} + \frac{\boldsymbol{J}_p}{\tau} = \epsilon_0 \omega_p^2 \boldsymbol{E} \tag{18}$$

For n = 1, 2, 3, 4:

$$\begin{aligned}\Delta J_{p,i}^{(t+\frac{n\Delta t}{4})} &= \Delta J_{p,i,n1}^{(t+\frac{n\Delta t}{4})} + \Delta J_{p,i,n2}^{(t+\frac{n\Delta t}{4})} + \Delta J_{p,i,n3}^{(t+\frac{n\Delta t}{4})} \\ &= \epsilon_0 E_{i,cell}^t (\omega_{p,n1}\omega_{p,n1} comp_{n1} + \omega_{p,n2}\omega_{p,n2} comp_{n2} + \omega_{p,n3}\omega_{p,n3} comp_{n3}) - \dots \\ &\Delta t \Big(\frac{J_{p,i,n1}^{(t+\frac{(n-1)\Delta t}{4})}}{\tau_{e,n1}} + \frac{J_{p,i,n2}^{(t+\frac{(n-1)\Delta t}{4})}}{\tau_{e,n2}} + \frac{J_{p,i,n3}^{(t+\frac{(n-1)\Delta t}{4})}}{\tau_{e,n3}} \Big),\end{aligned} \tag{19}$$

where

$$J_{p,i,store}^{(t+\frac{(n-1)\Delta t}{4})} = \begin{cases} J_{p,i}^{(t)}, & n = 1 \\ J_{p,i}^{(t)} + 0.5 * \Delta J_{p,i}^{(t+\frac{(n-1)\Delta t}{4})}, & n = 2, 3 \\ J_{p,i}^{(t)} + \Delta J_{p,i}^{(t+\frac{3\Delta t}{4})}, & n = 4, \end{cases} \tag{20}$$

$\Delta J_{ISHE,i}$ is the change in the current density induced by the spin current via the inverse spin-Hall effect.

$$\Delta J_{ISHE,i} = \dots \tag{21}$$

$$E_{i,store}^{(t+\frac{(n-1)\Delta t}{4})} = \begin{cases} E_i^{(t)}, & n = 1 \\ E_i^{(t)} + 0.5 * \Delta E_i^{(t+\frac{(n-1)\Delta t}{4})}, & n = 2, 3 \\ E_i^{(t)} + \Delta E_i^{(t+\frac{3\Delta t}{4})}, & n = 4 \end{cases} \tag{22}$$

Finally, the polarization current is calculated by evolving the polarization dynamical equation using RK4 time-stepping.

$$\Delta H_x^{(t+\frac{n\Delta t}{4})}|_{i,j,k} = -\frac{\Delta t}{\mu_0}\Big(\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z}\Big) - \frac{\Delta M_{x,1} + \Delta M_{x,2}}{M_{\text{count}}} \tag{23}$$

$$E_x^{t+\Delta t} = E_x^t + \frac{\Delta E_x^{(t+\frac{\Delta t}{4})}}{6} + \frac{\Delta E_x^{(t+\frac{2\Delta t}{4})}}{3} + \frac{\Delta E_x^{(t+\frac{3\Delta t}{4})}}{3} + \frac{\Delta E_x^{(t+\frac{4\Delta t}{4})}}{6} \tag{24}$$

$$H_x^{t+\Delta t} = H_x^t + \frac{\Delta H_x^{(t+\frac{\Delta t}{4})}}{6} + \frac{\Delta H_x^{(t+\frac{2\Delta t}{4})}}{3} + \frac{\Delta H_x^{(t+\frac{3\Delta t}{4})}}{3} + \frac{\Delta H_x^{(t+\frac{4\Delta t}{4})}}{6} \tag{25}$$

PML Modification

The time-harmonic forms of the Maxwell's equations (11) and (13) are

$$\nabla \times \widehat{\boldsymbol{H}} = \widehat{\boldsymbol{J}} + i\omega\epsilon_0\epsilon_r\widehat{\boldsymbol{E}} + i\omega\widehat{\boldsymbol{P}} \tag{26}$$

$$\nabla \times \widehat{\boldsymbol{E}} = -i\omega\mu_0\mu_r(\widehat{\boldsymbol{M}} + \widehat{\boldsymbol{H}}) \tag{27}$$

where $\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{H}}, \widehat{\boldsymbol{J}}, \widehat{\boldsymbol{M}}, \text{and} \widehat{\boldsymbol{P}}$ are all in the frequency-domain.

A UPML constitutive tensor is now defined,

$$\bar{\bar{s}} = \begin{bmatrix} s_x^{-1} & 0 & 0 \\ 0 & s_x & 0 \\ 0 & 0 & s_x \end{bmatrix} \begin{bmatrix} s_y & 0 & 0 \\ 0 & s_y^{-1} & 0 \\ 0 & 0 & s_y \end{bmatrix} \begin{bmatrix} s_z & 0 & 0 \\ 0 & s_z & 0 \\ 0 & 0 & s_z^{-1} \end{bmatrix} \tag{28}$$

$$= \begin{bmatrix} s_x^{-1}s_y s_z & 0 & 0 \\ 0 & s_x s_y^{-1} s_z & 0 \\ 0 & 0 & s_x s_y s_z^{-1} \end{bmatrix} \tag{29}$$

where

$$s_x = \kappa_x + \frac{\sigma_x}{i\omega\epsilon}; \quad s_y = \kappa_y + \frac{\sigma_y}{i\omega\epsilon}; \quad s_z = \kappa_z + \frac{\sigma_z}{i\omega\epsilon} \tag{30}$$

κ and σ are all one-dimensional functions that are equal to unity and zero respectively in the physical non-PML region, ensuring that the PML constitutive tensor and PML auxilliary equations are active only in the PML.

There are no sources of current, polarization and magnetization densities within the PML, consequently reducing the time-harmonic equations to simply

$$\nabla \times \widehat{\boldsymbol{H}} = i\omega\bar{\bar{s}}\epsilon_0\epsilon_r\widehat{\boldsymbol{E}} \tag{31}$$

$$\nabla \times \widehat{\boldsymbol{E}} = -i\omega\bar{\bar{s}}\mu_0\mu_r\widehat{H} \tag{32}$$

To decouple the frequency-dependent terms and thereby avoid a convolution between the material tensors and the EM-fields in the time-domain, new constitutive relationships are defined as follows:

$$\widehat{\boldsymbol{D_x}} = \epsilon_0\epsilon_r\frac{s_z}{s_x}\widehat{\boldsymbol{E_x}} \tag{33}$$

$$\widehat{\boldsymbol{B_x}} = \epsilon_0\epsilon_r\frac{s_z}{s_x}\widehat{\boldsymbol{H_x}} \tag{34}$$

$$\tag{35}$$

Following an inverse Fourier transform, the time-domain differential equations are now

$$\begin{bmatrix} \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \\ \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \\ \frac{\mathrm{d}H_y}{\mathrm{d}x} - \frac{\partial H_x}{\partial y} \end{bmatrix} = \frac{\partial}{\partial t}\begin{bmatrix} \kappa_y & 0 & 0 \\ 0 & \kappa_z & 0 \\ 0 & 0 & \kappa_x \end{bmatrix}\begin{bmatrix} D_x \\ D_y \\ D_z \end{bmatrix} + \frac{1}{\epsilon_0}\begin{bmatrix} \sigma_y & 0 & 0 \\ 0 & \sigma_z & 0 \\ 0 & 0 & \sigma_x \end{bmatrix}\begin{bmatrix} D_x \\ D_y \\ D_z \end{bmatrix} \tag{36}$$

Taking for instance the update equation for D_x,

$$\frac{\partial D_x}{\partial t} = \frac{\left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}\right)}{\kappa_x} - \frac{\sigma_x D_x}{\kappa_x\epsilon_0} \tag{37}$$

A similar RK4 treatment as earlier yields

$$\Delta D_x^{(t+\frac{n\Delta t}{4})}|_{i,j,k} = \frac{\Delta t}{\kappa_y}\left(\frac{\partial H_z}{\partial y}\bigg|_{i,j,k}^{(t+\frac{(n-1)\Delta t}{4})} - \frac{\partial H_y}{\partial z}\bigg|_{i,j,k}^{(t+\frac{(n-1)\Delta t}{4})}\right) - \frac{\sigma_y\Delta t}{\kappa_y\epsilon_0}D_{x,store}^{(t+\frac{(n-1)\Delta t}{4})}$$

$$D_x^{t+\Delta t} = D_x^t + \frac{\Delta D_x^{(t+\frac{\Delta t}{4})}}{6} + \frac{\Delta D_x^{(t+\frac{2\Delta t}{4})}}{3} + \frac{\Delta D_x^{(t+\frac{3\Delta t}{4})}}{3} + \frac{\Delta D_x^{(t+\frac{4\Delta t}{4})}}{6} \tag{38}$$

Multiplying (33) by $i\omega$ and performing an inverse Fourier transform returns the new value of the electric field.

$$\frac{\partial}{\partial t}\begin{bmatrix}\kappa_x & 0 & 0\\ 0 & \kappa_y & 0\\ 0 & 0 & \kappa_z\end{bmatrix}\begin{bmatrix}D_x\\ D_y\\ D_z\end{bmatrix}+\frac{1}{\epsilon_0}\begin{bmatrix}\sigma_x & 0 & 0\\ 0 & \sigma_y & 0\\ 0 & 0 & \sigma_z\end{bmatrix}\begin{bmatrix}D_x\\ D_y\\ D_z\end{bmatrix}=\frac{\partial}{\partial t}\begin{bmatrix}\epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz}\\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz}\\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz}\end{bmatrix}\begin{bmatrix}\kappa_z & 0 & 0\\ 0 & \kappa_x & 0\\ 0 & 0 & \kappa_y\end{bmatrix}\begin{bmatrix}E_x\\ E_y\\ E_z\end{bmatrix}+\dots \tag{39}$$

$$\frac{1}{\epsilon_0}\begin{bmatrix}\epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz}\\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz}\\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz}\end{bmatrix}\begin{bmatrix}\sigma_z & 0 & 0\\ 0 & \sigma_x & 0\\ 0 & 0 & \sigma_y\end{bmatrix}\begin{bmatrix}E_x\\ E_y\\ E_z\end{bmatrix} \tag{40}$$

The update equation for E is then

$$\Delta E_x^{(t+\frac{n\Delta t}{4})}|_{i,j,k} = \frac{\Delta t}{\kappa_z}\times\left(\frac{\epsilon_{yy}\epsilon_{zz}-\epsilon_{yz}\epsilon_{zy}}{||\epsilon||}\right)\Bigg|_{i,j,k}\times\dots$$

$$\left(\frac{\kappa_x\Delta D_x^{(t+\frac{n\Delta t}{4})}|_{i,j,k}}{\Delta t}+\frac{\sigma_x D_{x,store}^{(t+\frac{(n-1)\Delta t}{4})}}{\epsilon_0}\right)-\frac{\Delta t}{\kappa_z}\frac{\sigma_z E_{x,store}^{(t+\frac{(n-1)\Delta t}{4})}}{\epsilon_0} \tag{41}$$