PMLs in PySIT

Russell J. Hewett

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1 Purpose

This document is meant to function as documentation for the PML implementation within PySIT. It expands upon the existing derivations of PML for 2D and 3D problems given in [4], using a slightly different formuliation, and fills in some small details so there is a reference for how the PML in PySIT came about. It also develops a PML for 1D problems, based on the 2D and 3D developments that is not present in [4].

2 Definitions

This document considers the constant-density acoustic wave equation (CDAWE) (or the wave equation in second-order form) (or the scalar wave equation),

$$m(\boldsymbol{x})\frac{\partial^2}{\partial t^2}u(\boldsymbol{x},t) - \Delta u(\boldsymbol{x},t) = f((x),t), \tag{1}$$

and its corresponding Helmholtz equation,

$$m(\boldsymbol{x})(-\omega^2)\hat{u}(\boldsymbol{x},\omega) - \Delta\hat{u}(\boldsymbol{x},t) = \hat{f}(\boldsymbol{x},\omega). \tag{2}$$

Assume that m is intelligently extended to the PML region and that f is zero in the PML region.

There is no theory in this document, see [4], [3], or [1] for details. This document merely give the derivations of the PMLs used in PySIT.

While [4] defines the Helmholtz equation above in terms of the Laplace transform and its damping parameter s, we will stick with the more conventional Fourier transform / frequency-domain specification. In keeping with the usual (to me) definition of the (forward) Fourier transform[1],

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} f(t)e^{-i\omega t}\mathrm{d}t, \tag{3}$$

we relate the Laplace transform,

$$\bar{f}(s) = \int_{-\infty}^{\infty} f(t)e^{-st}\mathrm{d}t, \tag{4}$$

used in [4] to define the Helmholtz problem, to the Fourier transform by $s = i\omega$ (in a fast-and-loose sense). This results in the complex coordinate stretching

$$\begin{aligned}\frac{\partial}{\partial\tilde{x}_j} &= \frac{1}{1+\frac{1}{s}\sigma_j(\boldsymbol{x})}\frac{\partial}{\partial x_j}\\ &= \frac{1}{1-\frac{i}{\omega}\sigma_j(\boldsymbol{x})}\frac{\partial}{\partial x_j},\end{aligned} \tag{5}$$

[1]For convenience, I neglect the normalization when writing the Fourier transform in terms of angular frequency. In PySIT, all Fourier transforms are done in terms of frequency (Hz) so there is no normalization necessary.

where $\sigma_j(\boldsymbol{x})$ is the PML profile function and the subscript j corresponds to the problem dimension[2]. Additionally, we assume that $\sigma_j(\boldsymbol{x}) = 0$ away from the PML. Our notation for the coordinate stretching differs from the standard notation,

$$\frac{\partial}{\partial \tilde{x}_j} = \frac{1}{1 + \frac{i}{\omega}\sigma_j(\boldsymbol{x})} \frac{\partial}{\partial x_j}, \tag{6}$$

which is likely due to the different convention for the definition of the Fourier transform used in acoustics [2].

For convenience, and following [4], let

$$\gamma_j(\boldsymbol{x}) = 1 - \frac{i}{\omega}\sigma_j(\boldsymbol{x}). \tag{7}$$

3 PML for 1D Problems

3.1 Derivations

(Note: This derivation is not present in [4].)

In the frequency domain (dropping the function arguments for convenience), the Helmholtz-PML problem is

$$m(-\omega^2)\hat{u} - \frac{\partial}{\partial \tilde{x}_z}\frac{\partial}{\partial \tilde{x}_z}\hat{u} = \hat{f}, \tag{8}$$

or equivalently,

$$m(-\omega^2)\hat{u} - \frac{1}{\gamma_z}\frac{\partial}{\partial x_z}\frac{1}{\gamma_z}\frac{\partial}{\partial x_z}\hat{u} = \hat{f}. \tag{9}$$

Pre-multiplying by γ_z yields,

$$\gamma_z m(-\omega^2)\hat{u} - \frac{\partial}{\partial x_z}\frac{1}{\gamma_z}\frac{\partial}{\partial x_z}\hat{u} = \gamma_z\hat{f}. \tag{10}$$

We consider each term of (10) individually.

3.1.1 Time Derivatives of u

$$\begin{aligned} \gamma_z m(-\omega^2)\hat{u} &= -m\omega^2(1 - \frac{i}{\omega}\sigma_z)\hat{u} \\ &= -m\omega^2\hat{u} + mi\omega\sigma_z\hat{u} \end{aligned} \tag{11}$$

3.1.2 Spatial Derivatives of u

First, observe that

$$\frac{1}{\gamma_z} = \frac{1}{1 - \frac{i}{\omega}\sigma_z} = \frac{\omega^2}{\omega^2 - i\omega\sigma_z} = \frac{\omega^2 - i\omega\sigma_z + i\omega\sigma_z}{\omega^2 - i\omega\sigma_z} = 1 + \frac{i\omega\sigma_z}{\omega^2 - i\omega\sigma_z}. \tag{12}$$

Then,

$$\begin{aligned} \frac{\partial}{\partial x_z}\frac{1}{\gamma_z}\frac{\partial}{\partial x_z}\hat{u} &= \frac{\partial}{\partial x_z}\left(1 + \frac{i\omega\sigma_z}{\omega^2 - i\omega\sigma_z}\right)\frac{\partial}{\partial x_z}\hat{u} \\ &= \frac{\partial^2}{\partial {x_z}^2}\hat{u} + \frac{\partial}{\partial x_z}\left(\frac{i\omega\sigma_z}{\omega^2 - i\omega\sigma_z}\right)\frac{\partial}{\partial x_z}\hat{u}, \\ &= \frac{\partial^2}{\partial {x_z}^2}\hat{u} + \frac{\partial}{\partial x_z}\hat{\phi}^z, \end{aligned} \tag{13}$$

[2]In keeping with PySIT convention, this means that for 1D problems $j = z$, for 2D problems $j = \{x, z\}$ and for 3D problems, $j = \{x, y, z\}$.

where

$$\hat{\phi}^z = \frac{i\omega\sigma_z}{\omega^2 - i\omega\sigma_z}\frac{\partial}{\partial x_z}\hat{u}. \tag{14}$$

Then,

$$\begin{aligned}
\frac{\omega^2 - i\omega\sigma_z}{i\omega}\hat{\phi}^z &= \sigma_z\frac{\partial}{\partial x_z}\hat{u}, \\
\frac{\omega}{i}\hat{\phi}^z - \sigma_z\hat{\phi}^z &= \sigma_z\frac{\partial}{\partial x_z}\hat{u}, \\
-i\omega\hat{\phi}^z &= \sigma_z\hat{\phi}^z + \sigma_z\frac{\partial}{\partial x_z}\hat{u}. \qquad (15)
\end{aligned}$$

3.1.3 The Right-hand Side

Trivially, we have

$$\gamma_z\hat{f} = (1 - \frac{i}{\omega}\sigma_z)\hat{f} = \hat{f}, \tag{16}$$

because $\hat{f}$ is zero in the PML region and σ_z is zero away from the PML.

3.2 Helmholtz with PML

Assembling everything yields a system, equivalent to (10),

$$-\omega^2 m\hat{u} + i\omega m\sigma_z\hat{u} - \frac{\partial^2}{\partial {x_z}^2}\hat{u} - \frac{\partial}{\partial x_z}\hat{\phi}^z = \hat{f} \tag{17}$$

$$i\omega\hat{\phi}^z + \sigma_z\hat{\phi}^z + \sigma_z\frac{\partial}{\partial x_z}\hat{u} = 0. \tag{18}$$

In a more convenient notation, this reduces to the Helmholtz equation,

$$(-\omega^2\boldsymbol{M} + i\omega\boldsymbol{C} + \boldsymbol{K})\hat{\boldsymbol{u}} = \hat{\boldsymbol{f}}, \tag{19}$$

for

$$\begin{aligned}
&\hat{\boldsymbol{u}} = \begin{bmatrix} \hat{u} \\ \hat{\phi}^z \end{bmatrix}, && \hat{\boldsymbol{f}} = \begin{bmatrix} \hat{f} \\ 0 \end{bmatrix}, && \\
&\boldsymbol{M} = \begin{bmatrix} m & 0 \\ 0 & 0 \end{bmatrix}, && \boldsymbol{C} = \begin{bmatrix} m\sigma_z & 0 \\ 0 & 1 \end{bmatrix}, && \boldsymbol{K} = \begin{bmatrix} -\Delta & -\partial_z \\ \sigma_z\partial_z & \sigma_z \end{bmatrix}. \qquad (20)
\end{aligned}$$

Here, we have introduced the notation $\partial_j = \frac{\partial}{\partial x_j}$ for simplicity.

3.3 Wave Equation with PML

Equations 17 and 18 can be transformed into an equivalent time-domain wave equation via the inverse Fourier transform, yielding the system,

$$m\partial_t^2 u + m\sigma_z\partial_t u = \Delta u + \partial_z\phi^z + f \tag{21}$$

$$\partial_t\phi^z = -\sigma_z\phi^z - \sigma_z\partial_z u. \tag{22}$$

This system can be transformed into a matrix formulation that is dependent on the discretization, e.g., second- or fourth-order finite differences in time, and the method used to solve it, e.g., an explicit or implicit method. I will fill this in as time permits (and the implementation happens).

4 PML for 2D Problems

4.1 Derivations

(Note: This derivation *is* present in [4].)

In the frequency domain (dropping the function arguments for convenience), the Helmholtz-PML problem is

$$m(-\omega^2)\hat{u} - \frac{\partial}{\partial \tilde{x}_x}\frac{\partial}{\partial \tilde{x}_x}\hat{u} - \frac{\partial}{\partial \tilde{x}_z}\frac{\partial}{\partial \tilde{x}_z}\hat{u} = \hat{f}, \tag{23}$$

or equivalently,

$$m(-\omega^2)\hat{u} - \frac{1}{\gamma_x}\frac{\partial}{\partial x_x}\frac{1}{\gamma_x}\frac{\partial}{\partial x_x}\hat{u} - \frac{1}{\gamma_z}\frac{\partial}{\partial x_z}\frac{1}{\gamma_z}\frac{\partial}{\partial x_z}\hat{u} = \hat{f}. \tag{24}$$

Pre-multiplying by $\gamma_x\gamma_z$ yields,

$$\gamma_x\gamma_z m(-\omega^2)\hat{u} - \frac{\partial}{\partial x_x}\frac{\gamma_z}{\gamma_x}\frac{\partial}{\partial x_x}\hat{u} - \frac{\partial}{\partial x_z}\frac{\gamma_x}{\gamma_z}\frac{\partial}{\partial x_z}\hat{u} = \gamma_x\gamma_z\hat{f}. \tag{25}$$

We consider each term of (25) individually.

4.1.1 Time Derivatives of u

First, observe that

$$\gamma_x\gamma_z = \left(1 - \frac{i}{\omega}\sigma_x\right)\left(1 - \frac{i}{\omega}\sigma_z\right) = 1 - \frac{i}{\omega}(\sigma_x + \sigma_z) + \frac{i^2}{\omega^2}\sigma_x\sigma_z. \tag{26}$$

Then,

$$\begin{aligned}\gamma_x\gamma_z m(-\omega^2)\hat{u} &= -m\omega^2(1 - \frac{i}{\omega}(\sigma_x + \sigma_z) + \frac{i^2}{\omega^2}\sigma_x\sigma_z)\hat{u} \\ &= -m\omega^2\hat{u} + mi\omega(\sigma_x + \sigma_z)\hat{u} + m\sigma_x\sigma_y\hat{u}. \end{aligned} \tag{27}$$

4.1.2 Spatial Derivatives of u

First, observe that

$$\frac{\gamma_z}{\gamma_x} = \frac{1 - \frac{i}{\omega}\sigma_z}{1 - \frac{i}{\omega}\sigma_x} = \frac{\omega^2 - i\omega\sigma_z}{\omega^2 - i\omega\sigma_x} = \frac{\omega^2 - i\omega\sigma_z + i\omega\sigma_x - i\omega\sigma_x}{\omega^2 - i\omega\sigma_x} = 1 - \frac{i\omega(\sigma_z - \sigma_x)}{\omega^2 - i\omega\sigma_x}. \tag{28}$$

Similarly,

$$\frac{\gamma_x}{\gamma_z} = 1 - \frac{i\omega(\sigma_x - \sigma_z)}{\omega^2 - i\omega\sigma_z}. \tag{29}$$

Then,

$$\begin{aligned}\frac{\partial}{\partial x_x}\frac{\gamma_z}{\gamma_x}\frac{\partial}{\partial x_x}\hat{u} &= \frac{\partial}{\partial x_x}\left(1 - \frac{i\omega(\sigma_z - \sigma_x)}{\omega^2 - i\omega\sigma_x}\right)\frac{\partial}{\partial x_x}\hat{u} \\ &= \frac{\partial^2}{\partial {x_x}^2}\hat{u} + \frac{\partial}{\partial x_x}\left(-\frac{i\omega(\sigma_z - \sigma_x)}{\omega^2 - i\omega\sigma_x}\right)\frac{\partial}{\partial x_x}\hat{u}, \\ &= \frac{\partial^2}{\partial {x_x}^2}\hat{u} + \frac{\partial}{\partial x_x}\hat{\phi}^x, \end{aligned} \tag{30}$$

where

$$\hat{\phi}^x = -\frac{i\omega(\sigma_z - \sigma_x)}{\omega^2 - i\omega\sigma_x}\frac{\partial}{\partial x_x}\hat{u}. \tag{31}$$

Then,

$$\begin{aligned}
\frac{\omega^2 - i\omega\sigma_x}{i\omega}\hat{\phi}^x &= -(\sigma_z - \sigma_x)\frac{\partial}{\partial x_x}\hat{u}, \\
\frac{\omega}{i}\hat{\phi}^x - \sigma_x\hat{\phi}^x &= -(\sigma_z - \sigma_x)\frac{\partial}{\partial x_x}\hat{u}, \\
-i\omega\hat{\phi}^x &= \sigma_x\hat{\phi}^x - (\sigma_z - \sigma_x)\frac{\partial}{\partial x_x}\hat{u}.
\end{aligned} \tag{32}$$

Similarly we have that,

$$\frac{\partial}{\partial x_z}\frac{\gamma_x}{\gamma_z}\frac{\partial}{\partial x_z}\hat{u} = \frac{\partial^2}{\partial {x_z}^2}\hat{u} + \frac{\partial}{\partial x_z}\hat{\phi}^z \tag{33}$$

with $\hat{\phi}^z$ defined as in (31) and

$$-i\omega\hat{\phi}^z = \sigma_z\hat{\phi}^z - (\sigma_x - \sigma_z)\frac{\partial}{\partial x_z}\hat{u}. \tag{34}$$

4.1.3 The Right-hand Side

Trivially, we have

$$\gamma_x\gamma_z\hat{f} = (1 - \frac{i}{\omega}\sigma_x - \frac{i}{\omega}\sigma_z + \frac{i^2}{\omega^2}\sigma_x\sigma_z)\hat{f} = \hat{f}, \tag{35}$$

because $\hat{f}$ is zero in the PML region and σ_x and σ_z are zero away from the PML.

4.2 Helmholtz with PML

Assembling everything yields a system, equivalent to (25),

$$-m\omega^2\hat{u} + mi\omega(\sigma_x + \sigma_z)\hat{u} + m\sigma_x\sigma_z\hat{u} - \Delta\hat{u} - \frac{\partial}{\partial x_x}\hat{\phi}^x - \frac{\partial}{\partial x_z}\hat{\phi}^z = \hat{f} \tag{36}$$

$$i\omega\hat{\phi}^x + \sigma_x\hat{\phi}^x - (\sigma_z - \sigma_x)\frac{\partial}{\partial x_x}\hat{u} = 0 \tag{37}$$

$$i\omega\hat{\phi}^z + \sigma_z\hat{\phi}^z - (\sigma_x - \sigma_z)\frac{\partial}{\partial x_z}\hat{u} = 0. \tag{38}$$

In a more convenient notation, this reduces to the Helmholtz equation,

$$(-\omega^2\boldsymbol{M} + i\omega\boldsymbol{C} + \boldsymbol{K})\hat{\boldsymbol{u}} = \hat{\boldsymbol{f}}, \tag{39}$$

for

$$\hat{\boldsymbol{u}} = \begin{bmatrix} \hat{u} \\ \hat{\phi}^x \\ \hat{\phi}^z \end{bmatrix}, \qquad \hat{\boldsymbol{f}} = \begin{bmatrix} \hat{f} \\ 0 \\ 0 \end{bmatrix},$$

$$\boldsymbol{M} = \begin{bmatrix} m & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \boldsymbol{C} = \begin{bmatrix} m(\sigma_x + \sigma_z) & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \boldsymbol{K} = \begin{bmatrix} m\sigma_x\sigma_z - \Delta & -\partial_x & -\partial_z \\ -(\sigma_z - \sigma_x)\partial_x & \sigma_x & 0 \\ -(\sigma_x - \sigma_z)\partial_z & 0 & \sigma_z \end{bmatrix}. \tag{40}$$

Here, we have introduced the notation $\partial_j = \frac{\partial}{\partial x_j}$ for simplicity.

4.3 Wave Equation with PML

Equations 36-38 can be transformed into an equivalent time-domain wave equation via the inverse Fourier transform, yielding the system,

$$m\partial_t^2 u + m(\sigma_x + \sigma_z)\partial_t u + m\sigma_x\sigma_z u = \Delta u + \partial_x\phi^x + \partial_z\phi^z + f \tag{41}$$
$$\partial_t\phi^x = -\sigma_x\phi^x + (\sigma_z - \sigma_x)\partial_x u \tag{42}$$
$$\partial_t\phi^z = -\sigma_z\phi^z + (\sigma_x - \sigma_z)\partial_z u. \tag{43}$$

This system can be transformed into a matrix formulation that is dependent on the discretization, e.g., second- or fourth-order finite differences in time, and the method used to solve it, e.g., an explicit or implicit method. I will fill this in as time permits (and the implementation happens).

5 PML for 3D Problems

5.1 Derivations

(Note: This derivation *is* present in [4].)

In the frequency domain (dropping the function arguments for convenience), the Helmholtz-PML problem is

$$m(-\omega^2)\hat{u} - \frac{\partial}{\partial\tilde{x}_x}\frac{\partial}{\partial\tilde{x}_x}\hat{u} - \frac{\partial}{\partial\tilde{x}_y}\frac{\partial}{\partial\tilde{x}_y}\hat{u} - \frac{\partial}{\partial\tilde{x}_z}\frac{\partial}{\partial\tilde{x}_z}\hat{u} = \hat{f}, \tag{44}$$

or equivalently,

$$m(-\omega^2)\hat{u} - \frac{1}{\gamma_x}\frac{\partial}{\partial x_x}\frac{1}{\gamma_x}\frac{\partial}{\partial x_x}\hat{u} - \frac{1}{\gamma_y}\frac{\partial}{\partial x_y}\frac{1}{\gamma_y}\frac{\partial}{\partial x_y}\hat{u} - \frac{1}{\gamma_z}\frac{\partial}{\partial x_z}\frac{1}{\gamma_z}\frac{\partial}{\partial x_z}\hat{u} = \hat{f}. \tag{45}$$

Pre-multiplying by $\gamma_x\gamma_y\gamma_z$ yields,

$$\gamma_x\gamma_y\gamma_z m(-\omega^2)\hat{u} - \frac{\partial}{\partial x_x}\frac{\gamma_y\gamma_z}{\gamma_x}\frac{\partial}{\partial x_x}\hat{u} - \frac{\partial}{\partial x_y}\frac{\gamma_x\gamma_z}{\gamma_y}\frac{\partial}{\partial x_y}\hat{u} - \frac{\partial}{\partial x_z}\frac{\gamma_x\gamma_y}{\gamma_z}\frac{\partial}{\partial x_z}\hat{u} = \gamma_x\gamma_y\gamma_z\hat{f}. \tag{46}$$

We consider each term of (46) individually.

5.1.1 Time Derivatives of u

First, observe that

$$\begin{aligned}\gamma_x\gamma_y\gamma_z &= \left(1 - \frac{i}{\omega}\sigma_x\right)\left(1 - \frac{i}{\omega}\sigma_y\right)\left(1 - \frac{i}{\omega}\sigma_z\right) \\ &= 1 - \frac{i}{\omega}(\sigma_x + \sigma_y + \sigma_z) + \frac{i^2}{\omega^2}(\sigma_x\sigma_y + \sigma_x\sigma_z + \sigma_y\sigma_z) - \frac{i^3}{\omega^3}\sigma_x\sigma_y\sigma_z. \end{aligned} \tag{47}$$

Then,

$$\begin{aligned}\gamma_x\gamma_y\gamma_z m(-\omega^2)\hat{u} &= -m\omega^2(1 - \frac{i}{\omega}(\sigma_x + \sigma_y + \sigma_z) + \frac{i^2}{\omega^2}(\sigma_x\sigma_y + \sigma_x\sigma_z + \sigma_y\sigma_z) - \frac{i^3}{\omega^3}\sigma_x\sigma_y\sigma_z)\hat{u} \\ &= -m\omega^2(1 - \frac{i}{\omega}(\sigma_x + \sigma_y + \sigma_z) + \frac{i^2}{\omega^2}(\sigma_x\sigma_y + \sigma_x\sigma_z + \sigma_y\sigma_z) - \frac{i^3}{\omega^3}\sigma_x\sigma_y\sigma_z)\hat{u} \\ &= -m\omega^2\hat{u} + mi\omega(\sigma_x + \sigma_y + \sigma_z)\hat{u} + m(\sigma_x\sigma_y + \sigma_x\sigma_z + \sigma_y\sigma_z)\hat{u} - m\frac{i}{\omega}(\sigma_x\sigma_y\sigma_z)\hat{u} \\ &= -m\omega^2\hat{u} + mi\omega(\sigma_x + \sigma_y + \sigma_z)\hat{u} + m(\sigma_x\sigma_y + \sigma_x\sigma_z + \sigma_y\sigma_z)\hat{u} + m(\sigma_x\sigma_y\sigma_z)\hat{\psi}, \end{aligned} \tag{48}$$

where,

$$\hat{u} = i\omega\hat{\psi}. \tag{49}$$

5.1.2 Spatial Derivatives of u

First, observe that

$$\begin{aligned}
\frac{\gamma_y\gamma_z}{\gamma_x} = \frac{\left(1-\frac{i}{\omega}\sigma_y\right)\left(1-\frac{i}{\omega}\sigma_z\right)}{1-\frac{i}{\omega}\sigma_x} &= \frac{\omega^2 - i\omega(\sigma_y+\sigma_z) - \sigma_y\sigma_z}{\omega^2 - i\omega\sigma_x} \\
&= \frac{\omega^2 - i\omega(\sigma_y+\sigma_z) - \sigma_y\sigma_z + i\omega\sigma_x - i\omega\sigma_x}{\omega^2 - i\omega\sigma_x} \\
&= 1 - \frac{i\omega(\sigma_y+\sigma_z-\sigma_x) - \sigma_y\sigma_z}{\omega^2 - i\omega\sigma_x}. \qquad (50)
\end{aligned}$$

Similarly,

$$\frac{\gamma_x\gamma_z}{\gamma_y} = 1 - \frac{i\omega(\sigma_x+\sigma_z-\sigma_y) - \sigma_x\sigma_z}{\omega^2 - i\omega\sigma_y}, \qquad (51)$$

$$\frac{\gamma_x\gamma_y}{\gamma_z} = 1 - \frac{i\omega(\sigma_x+\sigma_y-\sigma_z) - \sigma_x\sigma_y}{\omega^2 - i\omega\sigma_z}. \qquad (52)$$

Then,

$$\begin{aligned}
\frac{\partial}{\partial x_x}\frac{\gamma_y\gamma_z}{\gamma_x}\frac{\partial}{\partial x_x}\hat{u} &= \frac{\partial}{\partial x_x}\left(1 - \frac{i\omega(\sigma_y+\sigma_z-\sigma_x) - \sigma_y\sigma_z}{\omega^2 - i\omega\sigma_x}\right)\frac{\partial}{\partial x_x}\hat{u} \\
&= \frac{\partial^2}{\partial {x_x}^2}\hat{u} + \frac{\partial}{\partial x_x}\left(-\frac{i\omega(\sigma_y+\sigma_z-\sigma_x) - \sigma_y\sigma_z}{\omega^2 - i\omega\sigma_x}\right)\frac{\partial}{\partial x_x}\hat{u}, \\
&= \frac{\partial^2}{\partial {x_x}^2}\hat{u} + \frac{\partial}{\partial x_x}\hat{\phi}^x, \qquad (53)
\end{aligned}$$

where

$$\hat{\phi}^x = -\frac{i\omega(\sigma_y+\sigma_z-\sigma_x) - \sigma_y\sigma_z}{\omega^2 - i\omega\sigma_x}\frac{\partial}{\partial x_x}\hat{u}. \qquad (54)$$

Then,

$$\begin{aligned}
\frac{\omega^2 - i\omega\sigma_x}{i\omega}\hat{\phi}^x &= -(\sigma_y+\sigma_z-\sigma_x)\frac{\partial}{\partial x_x}\hat{u} - \frac{1}{i\omega}(\sigma_y\sigma_z)\frac{\partial}{\partial x_x}\hat{u}, \\
\frac{\omega}{i}\hat{\phi}^x - \sigma_x\hat{\phi}^x &= -(\sigma_y+\sigma_z-\sigma_x)\frac{\partial}{\partial x_x}\hat{u} - \sigma_y\sigma_z\frac{\partial}{\partial x_x}\hat{\psi}, \\
-i\omega\hat{\phi}^x &= \sigma_x\hat{\phi}^x - (\sigma_y+\sigma_z-\sigma_x)\frac{\partial}{\partial x_x}\hat{u} - \sigma_y\sigma_z\frac{\partial}{\partial x_x}\hat{\psi}, \qquad (55)
\end{aligned}$$

where we made use of (49) in the last term. Similarly we have that,

$$\frac{\partial}{\partial x_z}\frac{\gamma_x\gamma_z}{\gamma_y}\frac{\partial}{\partial x_y}\hat{u} = \frac{\partial^2}{\partial {x_y}^2}\hat{u} + \frac{\partial}{\partial x_y}\hat{\phi}^y, \qquad (56)$$

$$\frac{\partial}{\partial x_z}\frac{\gamma_x\gamma_y}{\gamma_z}\frac{\partial}{\partial x_z}\hat{u} = \frac{\partial^2}{\partial {x_z}^2}\hat{u} + \frac{\partial}{\partial x_z}\hat{\phi}^z, \qquad (57)$$

with $\hat{\phi}^y$ and $\hat{\phi}^z$ defined as in (54) and

$$-i\omega\hat{\phi}^y = \sigma_y\hat{\phi}^y - (\sigma_x+\sigma_z-\sigma_y)\frac{\partial}{\partial x_y}\hat{u} - \sigma_x\sigma_z\frac{\partial}{\partial x_y}\hat{\psi}, \qquad (58)$$

$$-i\omega\hat{\phi}^z = \sigma_z\hat{\phi}^z - (\sigma_x+\sigma_y-\sigma_z)\frac{\partial}{\partial x_z}\hat{u} - \sigma_x\sigma_y\frac{\partial}{\partial x_z}\hat{\psi}. \qquad (59)$$

5.1.3 The Right-hand Side

Trivially, we have

$$\gamma_x \gamma_y \gamma_z \hat{f} = (1 - \frac{i}{\omega}\sigma_x)(1 - \frac{i}{\omega}\sigma_y)(1 - \frac{i}{\omega}\sigma_z) = \hat{f}, \tag{60}$$

because $\hat{f}$ is zero in the PML region and σ_x, σ_y, and σ_z are zero away from the PML.

5.2 Helmholtz with PML

Assembling everything yields a system, equivalent to (46),

$$\begin{aligned} -m\omega^2 \hat{u} + mi\omega(\sigma_x + \sigma_y + \sigma_z)\hat{u} + m(\sigma_x\sigma_y + \sigma_x\sigma_z + \sigma_y\sigma_z)\hat{u} + m(\sigma_x\sigma_y\sigma_z)\hat{\psi} & \\ -\Delta\hat{u} - \frac{\partial}{\partial x_x}\hat{\phi}^x - \frac{\partial}{\partial x_y}\hat{\phi}^y - \frac{\partial}{\partial x_z}\hat{\phi}^z = \hat{f} & \quad (61) \\ i\omega\hat{\psi} - \hat{u} = 0 & \quad (62) \\ i\omega\hat{\phi}^x + \sigma_x\hat{\phi}^x - (\sigma_y + \sigma_z - \sigma_x)\frac{\partial}{\partial x_x}\hat{u} - \sigma_y\sigma_z\frac{\partial}{\partial x_x}\hat{\psi} = 0 & \quad (63) \\ i\omega\hat{\phi}^y + \sigma_y\hat{\phi}^y - (\sigma_x + \sigma_z - \sigma_y)\frac{\partial}{\partial x_y}\hat{u} - \sigma_x\sigma_z\frac{\partial}{\partial x_y}\hat{\psi} = 0 & \quad (64) \\ i\omega\hat{\phi}^z + \sigma_z\hat{\phi}^z - (\sigma_x + \sigma_y - \sigma_z)\frac{\partial}{\partial x_z}\hat{u} - \sigma_x\sigma_y\frac{\partial}{\partial x_z}\hat{\psi} = 0. & \quad (65) \end{aligned}$$

In a more convenient notation, this reduces to the Helmholtz equation,

$$(-\omega^2\boldsymbol{M} + i\omega\boldsymbol{C} + \boldsymbol{K})\hat{\boldsymbol{u}} = \hat{\boldsymbol{f}}, \tag{66}$$

for

$$\hat{\boldsymbol{u}} = \begin{bmatrix} \hat{u} \\ \hat{\psi} \\ \hat{\phi}^x \\ \hat{\phi}^y \\ \hat{\phi}^z \end{bmatrix}, \qquad \hat{\boldsymbol{f}} = \begin{bmatrix} \hat{f} \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix},$$

$$\boldsymbol{M} = \begin{bmatrix} m & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \qquad \boldsymbol{C} = \begin{bmatrix} m(\sigma_x + \sigma_y + \sigma_z) & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$\boldsymbol{K} = \begin{bmatrix} m(\sigma_x\sigma_y + \sigma_x\sigma_z + \sigma_y\sigma_z) - \Delta & m\sigma_x\sigma_y\sigma_z & -\partial_x & -\partial_y & -\partial_z \\ -1 & 0 & 0 & 0 & 0 \\ -(\sigma_y + \sigma_z - \sigma_x)\partial_x & -\sigma_y\sigma_z\partial_x & \sigma_x & 0 & 0 \\ -(\sigma_x + \sigma_z - \sigma_y)\partial_y & -\sigma_x\sigma_z\partial_y & 0 & \sigma_y & 0 \\ -(\sigma_x + \sigma_y - \sigma_z)\partial_z & -\sigma_x\sigma_y\partial_z & 0 & 0 & \sigma_z \end{bmatrix}. \tag{67}$$

Here, we have introduced the notation $\partial_j = \frac{\partial}{\partial x_j}$ for simplicity.

5.3 Wave Equation with PML

Equations 61-65 can be transformed into an equivalent time-domain wave equation via the inverse Fourier transform, yielding the system that appears in [4],

$$\begin{aligned} m\partial_t^2 u + m(\sigma_x + \sigma_y + \sigma_z)\partial_t u + m(\sigma_x\sigma_y + &\sigma_x\sigma_z + \sigma_y\sigma_z)u \\ &= \Delta u + \partial_x\phi^x + \partial_y\phi^y + \partial_z\phi^z - m\sigma_x\sigma_y\sigma_z\psi + f \quad (68) \\ \partial_t\psi &= u \quad (69) \\ \partial_t\phi^x &= -\sigma_x\phi^x + (\sigma_y + \sigma_z - \sigma_x)\frac{\partial}{\partial x_x}u + \sigma_y\sigma_z\frac{\partial}{\partial x_x}\psi \quad (70) \\ \partial_t\phi^y &= -\sigma_y\phi^y + (\sigma_x + \sigma_z - \sigma_y)\frac{\partial}{\partial x_y}u + \sigma_x\sigma_z\frac{\partial}{\partial x_y}\psi \quad (71) \\ \partial_t\phi^z &= -\sigma_z\phi^z + (\sigma_x + \sigma_y - \sigma_z)\frac{\partial}{\partial x_z}u + \sigma_x\sigma_y\frac{\partial}{\partial x_z}\psi. \quad (72) \end{aligned}$$

This system can be transformed into a matrix formulation that is dependent on the discretization, e.g., second- or fourth-order finite differences in time, and the method used to solve it, e.g., an explicit or implicit method. I will fill this in as time permits (and the implementation happens).

References

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