Computational Photonics

# Finite-Difference Time-Domain

# Boundary conditions

- most efficient boundary conditions are the PML
- more precise: material property, not an actual boundary
- published by Berenger in 1994 with reflections about 3000 times less than with 2$^{nd}$ order Mur boundary
- basic idea: constructing a media which absorbs light and at whose interfaces with the region of interest no reflections taking place

  ⇒ impedance matching of the medium with the surrounding

- impedance of a medium with electric and magnetic conductivity

$$\eta = \sqrt{\frac{\tilde{\mu}}{\tilde{\epsilon}}} = \sqrt{\frac{\mu' - \imath\mu''}{\epsilon' - \imath\epsilon''}}$$

$$\epsilon'' = \frac{\sigma_e}{\omega}$$ (electrical conductivity)

$$\mu'' = \frac{\sigma_m}{\omega}$$ (magnetic conductivity)

# Boundary conditions

- let the loss-less region being region 1, characterised by $\epsilon$ and $\mu$

$\Longrightarrow$ impedance: $\eta = \sqrt{\dfrac{\mu}{\epsilon}}$

- if the condition $\dfrac{\sigma_e}{\epsilon} = \dfrac{\sigma_m}{\mu}$ holds, the impedances are equal $\eta_l = \eta$

- plane waves propagating in each of the regions are characterised by their propagation constants, given as (by choosing $\epsilon = \epsilon'$ and $\mu = \mu'$)

$$k = \omega\sqrt{\epsilon\mu} \qquad k = \omega\sqrt{\epsilon\mu}\sqrt{\left(1 - i\frac{\sigma_e}{\omega\epsilon}\right)\left(1 - i\frac{\sigma_m}{\omega\mu}\right)}$$

- phase velocity given by $k = \omega\sqrt{\epsilon\mu} + i\eta\sigma_e$

the same as in free space but light is additionally absorbed

# Boundary conditions

- reflections coefficients of the interface are given generally by

$$R_\perp = \frac{E^r_\perp}{E^i_\perp} = \frac{\eta_2 \cos\theta_i - \eta_1 \cos\theta_t}{\eta_2 \cos\theta_i + \eta_1 \cos\theta_t} \qquad R_{||} = \frac{E^r_{||}}{E^i_{||}} = \frac{\eta_2 \cos\theta_t - \eta_1 \cos\theta_i}{\eta_2 \cos\theta_t + \eta_1 \cos\theta_i}$$

(with $n_1 \sin\theta_i = n_2 \sin\theta_t$ )

⇨ reflection is 0, only if the angle of incidence = the angle of transmittance

⇨ holds for interface between 2 media sustaining modes with same phase velocity

- following derivation exemplarily for 2D FDTD in TE polarisation

$$\epsilon \frac{\partial E_x}{\partial t} + \sigma_e E_x = \frac{\partial H_z}{\partial y}$$

$$\epsilon \frac{\partial E_y}{\partial t} + \sigma_e E_y = -\frac{\partial H_z}{\partial x}$$

$$\mu \frac{\partial H_z}{\partial t} + \sigma_m H_z = -\left(\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y}\right)$$

⇨ absorb light only in one direction, fields shall propagate parallel to surface

# Boundary conditions

- Berenger's idea: splitting the H field into a x and y component
  (x-derivative of the E field drives the $H_{zx}$ component and vice versa)

$$H_z = H_{zx} + H_{zy}$$

- introduction of an anisotropy of all properties

$$\mu \frac{\partial H_{zx}}{\partial t} + \sigma_{mx} H_{zx} = -\frac{\partial E_y}{\partial x} \qquad \epsilon \frac{\partial E_x}{\partial t} + \sigma_{ey} E_x = \frac{\partial (H_{zx} + H_{zy})}{\partial y}$$

$$\mu \frac{\partial H_{zy}}{\partial t} + \sigma_{my} H_{zy} = \frac{\partial E_x}{\partial y} \qquad \epsilon \frac{\partial E_y}{\partial t} + \sigma_{ex} E_y = -\frac{\partial (H_{zx} + H_{zy})}{\partial x}$$

⇨ can be shown, that the impedance of the Berenger medium equals the impedance of the free space, regardless of the angle of propagation

# Boundary conditions

- problem that denies a sudden change in the material properties: electric and magnetic field are evaluated at different spatial positions (staggered grid)
- asymmetric absorption
- choosing appropriate absorption profile for $\sigma_{ex}$ and $\sigma_{mx}$
- polynomial scaling $$\sigma_{ex} = \left(\frac{x}{d}\right)^m \sigma_{emax}$$

practical considerations

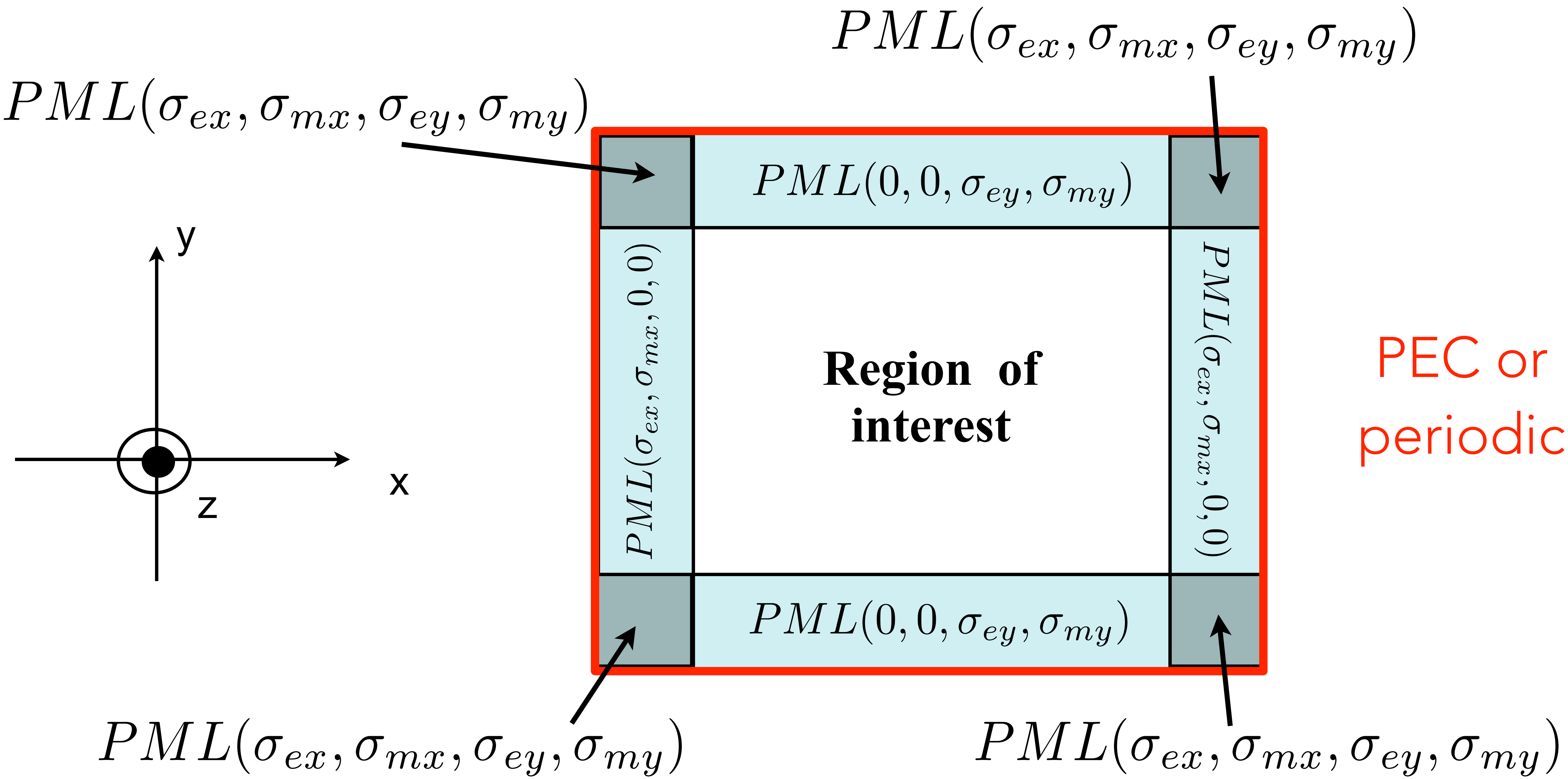
$$2 << m << 6$$

$$d = 10\Delta x$$

$\Longrightarrow$ $R = 10^{-16}$

# Boundary conditions

- important: waves propagating along the y-axis are not absorbed in the x-boundary



# Boundary conditions

- splitting the field in the boundaries

- adding the electrical and magnetic conductivity to the equations as material parameters

- only the components normal to the boundary are absorbed, adjusting the proper absorption profile for each component

  - electric and magnetic fields are evaluated a half discretisation step apart, hence the absorption profile is evaluated likewise at different spatial coordinates

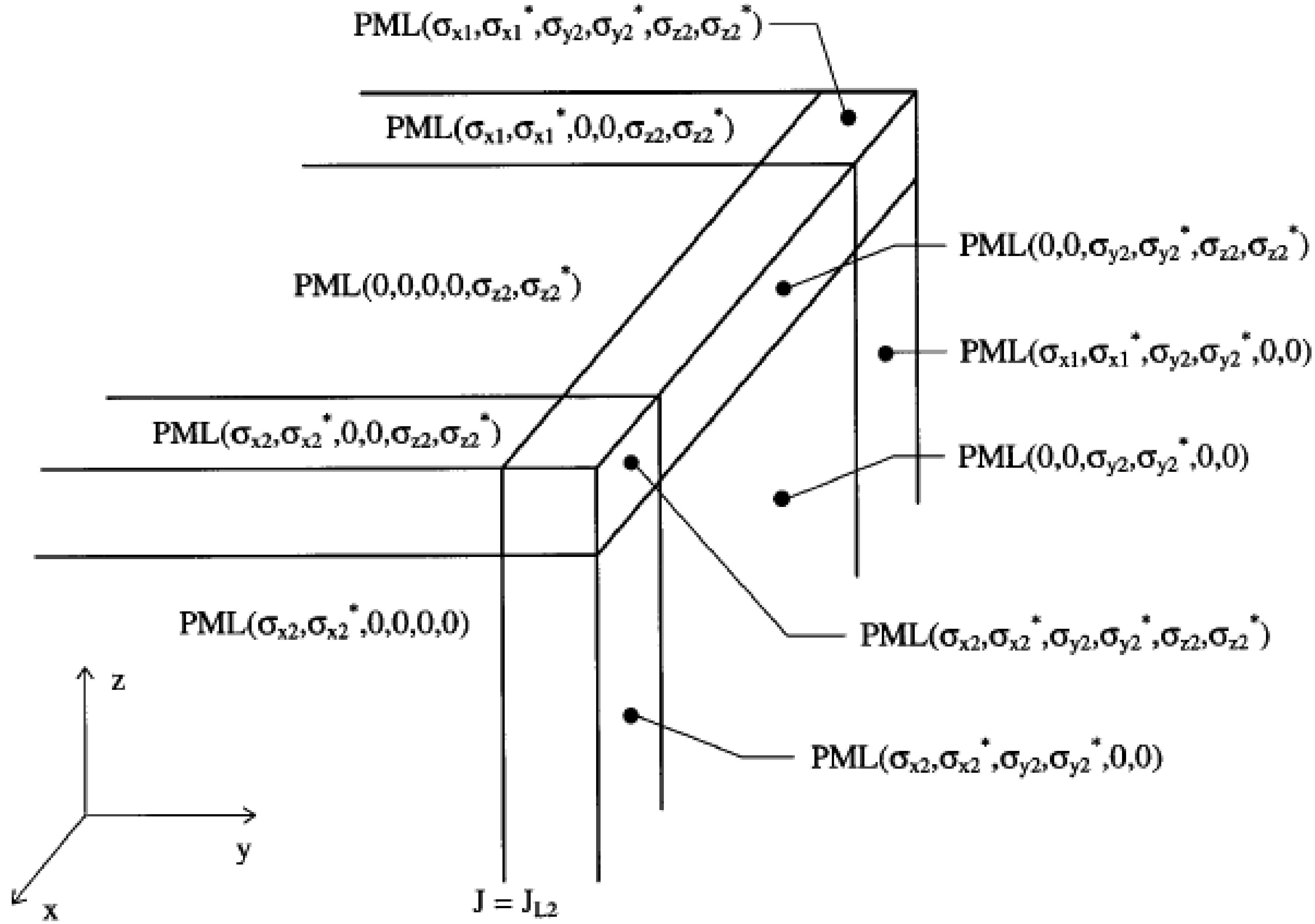
**J.P. Berenger, Journal of Computational Physics, Vol. 114, 185 (2D)**

# Boundary conditions

⟹ extensions for TM polarisation and 3D are straight forward

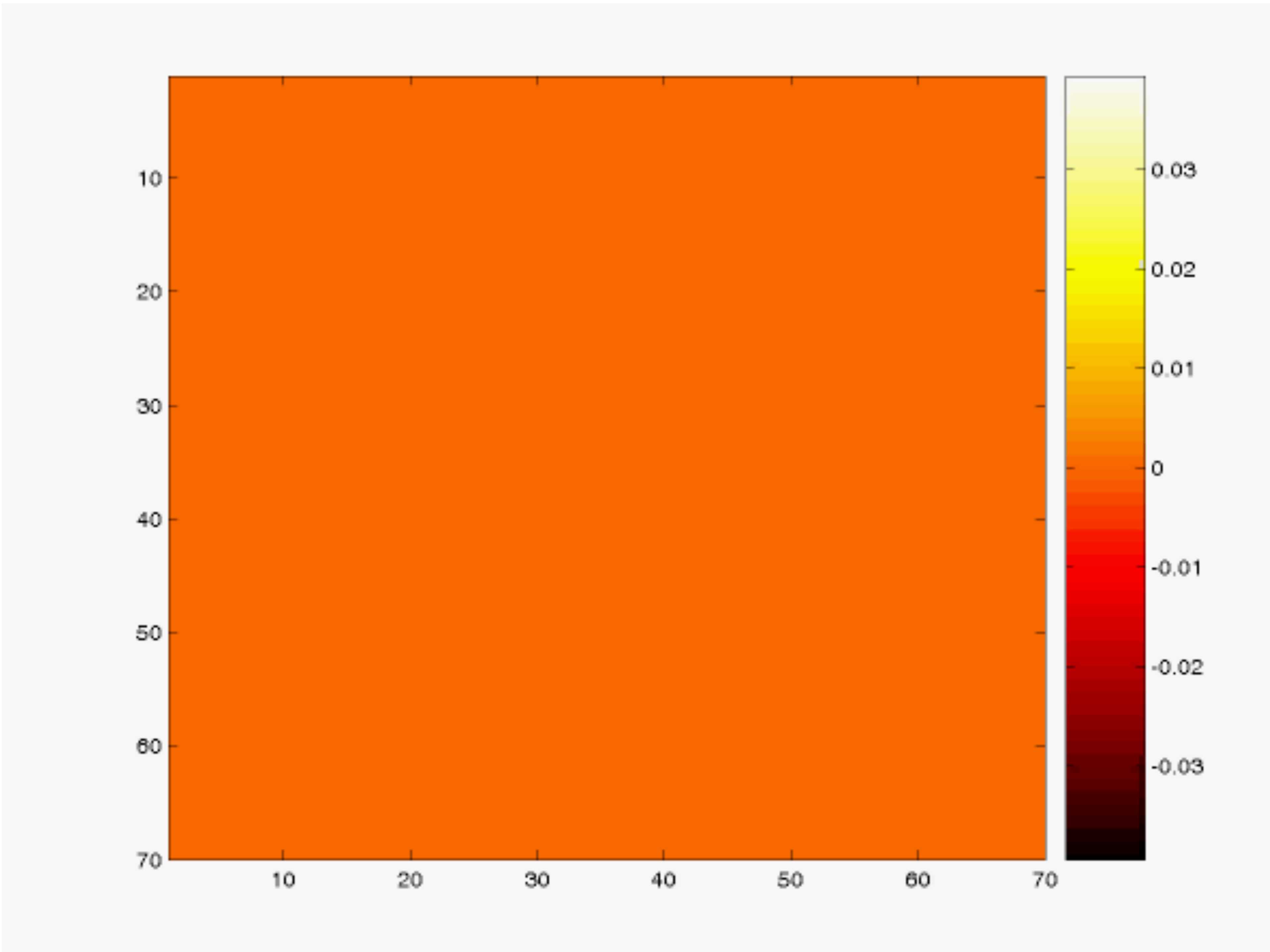
$$
\begin{aligned}
\left(\epsilon\frac{\partial}{\partial t}+\sigma_{ey}\right)E_{xy} &= \frac{\partial}{\partial y}(H_{zx}+H_{zy}) & \left(\epsilon\frac{\partial}{\partial t}+\sigma_{my}\right)H_{xy} &= -\frac{\partial}{\partial y}(E_{zx}+E_{zy})\\
\left(\epsilon\frac{\partial}{\partial t}+\sigma_{ez}\right)E_{xz} &= -\frac{\partial}{\partial z}(H_{yx}+H_{yz}) & \left(\epsilon\frac{\partial}{\partial t}+\sigma_{mz}\right)H_{xz} &= \frac{\partial}{\partial z}(E_{yx}+E_{yz})\\
\left(\epsilon\frac{\partial}{\partial t}+\sigma_{ex}\right)E_{yx} &= -\frac{\partial}{\partial x}(H_{zx}+H_{zy}) & \left(\epsilon\frac{\partial}{\partial t}+\sigma_{mx}\right)H_{yx} &= \frac{\partial}{\partial x}(E_{zx}+E_{zy})\\
\left(\epsilon\frac{\partial}{\partial t}+\sigma_{ez}\right)E_{yz} &= \frac{\partial}{\partial z}(H_{xy}+H_{xz}) & \left(\epsilon\frac{\partial}{\partial t}+\sigma_{mz}\right)H_{yz} &= -\frac{\partial}{\partial z}(E_{xy}+E_{xz})\\
\left(\epsilon\frac{\partial}{\partial t}+\sigma_{ex}\right)E_{zx} &= \frac{\partial}{\partial x}(H_{yx}+H_{yz}) & \left(\epsilon\frac{\partial}{\partial t}+\sigma_{mx}\right)H_{zx} &= -\frac{\partial}{\partial x}(E_{yx}+E_{yz})\\
\left(\epsilon\frac{\partial}{\partial t}+\sigma_{ey}\right)E_{zy} &= -\frac{\partial}{\partial y}(H_{xy}+H_{xz}) & \left(\epsilon\frac{\partial}{\partial t}+\sigma_{my}\right)H_{zy} &= \frac{\partial}{\partial y}(E_{xy}+E_{xz})
\end{aligned}
$$

# Boundary conditions



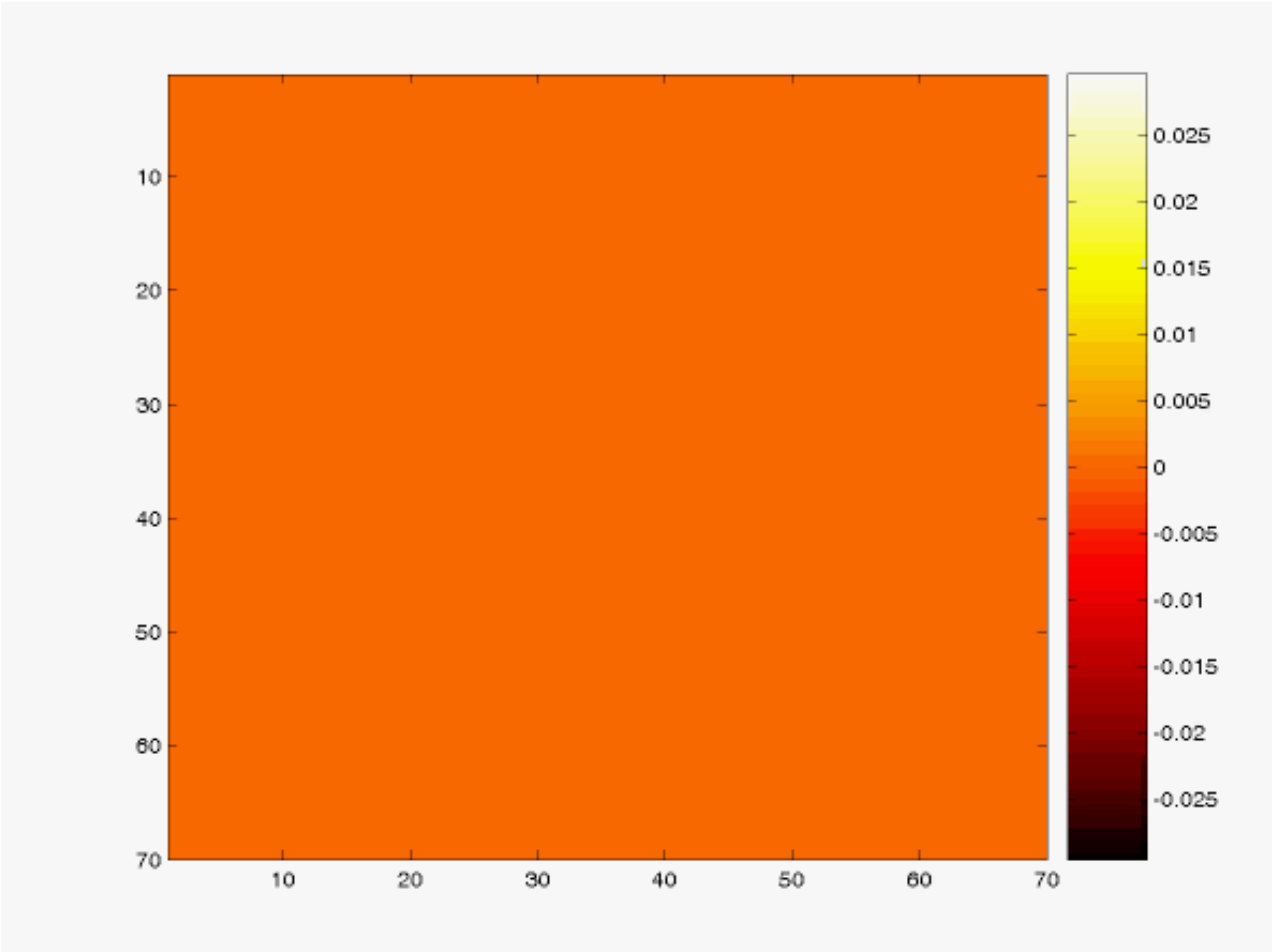

J.P. Berenger, Journal of Computational Physics, Vol. 127, 363 (3D)

# Boundary conditions



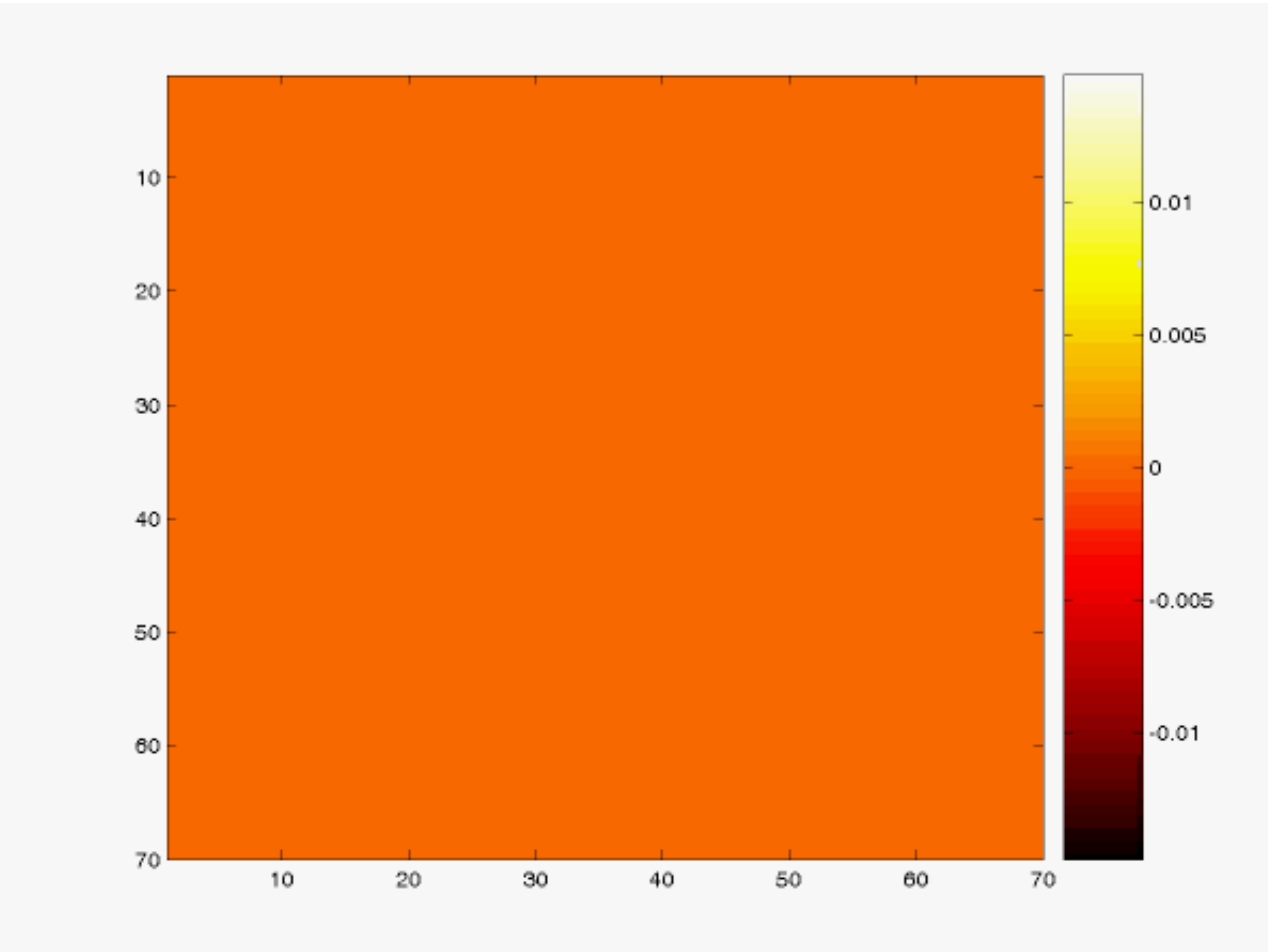

perfectly conducting boundary

# Boundary conditions




2nd order
Mur
boundary

# Boundary conditions




PML layers with

$$m = 3$$
$$d = 16\Delta x$$

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