Electromagnetic wave propagation in Particle-In-Cell codes

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Electromagnetic Waves: Outline

1 Numerical dispersion and Courant limit

- Dispersion and Courant limit in 1D
- Dispersion and Courant limit in 3D
- Spectral solvers and numerical dispersion

2 Open boundaries conditions

- Silver-Müller boundary conditions
- Perfectly Matched Layers

1D discrete propagation equation in vacuum

Reminder: 1D discrete Maxwell equations in vacuum

$$\frac{B_{y_{\ell+1/2}^{n+1/2}} - B_{y_{\ell+1/2}^{n+1/2}}}{\Delta t} = -\frac{E_{x_{\ell+1}^{n}} - E_{x_{\ell}^{n}}}{\Delta z} \quad (\text{from } \partial_t \boldsymbol{B} = -\boldsymbol{\nabla} \times \boldsymbol{E})$$
$$\frac{1}{c^2} \frac{E_{x_{\ell}^{n+1}} - E_{x_{\ell}^{n}}}{\Delta t} = -\frac{B_{y_{\ell+1/2}^{n+1/2}} - B_{y_{\ell-1/2}^{n+1/2}}}{\Delta z} \quad (\text{from } \frac{1}{c^2} \partial_t \boldsymbol{E} = \boldsymbol{\nabla} \times \boldsymbol{B})$$

These equations can be combined into a **propagation equation** for E_x :

$$\frac{1}{c^2} \frac{E_{x\ell}^{n+1} - E_{x\ell}^n}{\Delta t^2} - \frac{1}{c^2} \frac{E_{x\ell}^n - E_{x\ell}^{n-1}}{\Delta t^2} = -\frac{B_{y\ell+1/2}^{n+1/2} - B_{y\ell-1/2}^{n+1/2}}{\Delta z \Delta t} + \frac{B_{y\ell+1/2}^{n-1/2} - B_{y\ell-1/2}^{n-1/2}}{\Delta z \Delta t}$$
$$= -\frac{B_{y\ell+1/2}^{n+1/2} - B_{y\ell+1/2}^{n-1/2}}{\Delta z \Delta t} + \frac{B_{y\ell-1/2}^{n+1/2} - B_{y\ell-1/2}^{n-1/2}}{\Delta z \Delta t}$$
$$= -\frac{E_{x\ell+1}^n - E_{x\ell}^n}{\Delta z^2} - \frac{E_{x\ell}^n - E_{x\ell-1}^n}{\Delta z^2}$$

1D discrete propagation equation in vacuum

$$\frac{1}{c^2} \frac{E_x_{\ell}^{n+1} - 2E_x_{\ell}^n + E_x_{\ell}^{n-1}}{\Delta t^2} = \frac{E_x_{\ell+1}^n - 2E_x_{\ell}^n + E_x_{\ell-1}^n}{\Delta z^2} \quad i.e. \frac{1}{c^2} \partial_t^2 E_x|_{\ell}^n = \partial_z^2 E_x|_{\ell}^n$$

1D dispersion relation

1D discrete propagation equation in vacuum

$$\frac{1}{c^2} \frac{E_{x\ell}^{n+1} - 2E_{x\ell}^n + E_{x\ell}^{n-1}}{\Delta t^2} = \frac{E_{x\ell+1}^n - 2E_{x\ell}^n + E_{x\ell-1}^n}{\Delta z^2}$$

 \rightarrow Von Neumann analysis: assume the solutions of this equation are of the form $E_0 e^{ikz-i\omega t}$ (propagating wave), i.e.

$$E_{x\ell}^{\ n} = E_0 e^{ik \ \ell \Delta z - i\omega n \Delta t}$$

Replacing this ansatz into the discrete progagation equation yields

$$\frac{e^{ik\ell\Delta z}}{c^2} \frac{e^{-i\omega(n+1)\Delta t} - 2e^{-i\omega n\Delta t} + e^{-i\omega(n-1)\Delta t}}{\Delta t^2}}{c^2} = e^{-i\omega n\Delta t} \frac{e^{ik(\ell+1)\Delta z} - 2e^{ik\ell\Delta z} + e^{ik(\ell-1)\Delta z}}{\Delta z^2}}{c^2}$$
$$\frac{e^{ik\ell\Delta z - i\omega n\Delta t}}{c^2} \frac{e^{-i\omega\Delta t} - 2 + e^{i\omega\Delta t}}{\Delta t^2}}{c^2} = e^{ik\ell\Delta z - i\omega n\Delta t} \frac{e^{ik\Delta z} - 2 + e^{-ik\Delta z}}{\Delta z^2}}{c^2}$$
$$\frac{1}{c^2} \frac{(e^{-i\omega\Delta t/2} - e^{i\omega\Delta t/2})^2}{\Delta t^2}}{c^2} = \frac{(e^{ik\Delta z/2} - e^{-ik\Delta z/2})^2}{c^2}$$

1D dispersion relation

$$\frac{1}{c^2 \Delta t^2} \sin^2 \left(\frac{\omega \Delta t}{2}\right) = \frac{1}{\Delta z^2} \sin^2 \left(\frac{k \Delta z}{2}\right) \quad \text{(instead of } \omega^2 = c^2 k^2)$$

$c\Delta t \leq \Delta z \rightarrow \text{Numerical dispersion}$

For $c\Delta t \leq \Delta z$, the discrete dispersion relation

$$\frac{1}{c^2 \Delta t^2} \sin^2\left(\frac{\omega \Delta t}{2}\right) = \frac{1}{\Delta z^2} \sin^2\left(\frac{k \Delta z}{2}\right)$$

has real solutions ω , for any k:

$$\omega = \pm \frac{2}{\Delta t} \arcsin\left(\frac{c\Delta t}{\Delta z} \sin\left(\frac{k\Delta z}{2}\right)\right)$$

Thus, the phase velocity $v_{\phi} = \omega/k$ is:

$$v_{\phi} = \pm \frac{2}{k\Delta t} \arcsin\left(\frac{c\Delta t}{\Delta z}\sin\left(\frac{k\Delta z}{2}\right)\right)$$

Numerical dispersion

In a PIC code, the **electromagnetic waves** propagate (in vacuum) at a **velocity which depends on** k (and on Δt , Δz),

instead of propagating at the speed of light: $v_{\phi} = \pm c$

$c\Delta t \leq \Delta z \rightarrow \text{Numerical dispersion}$

$$v_{\phi} = \frac{2}{k\Delta t} \arcsin\left(\frac{c\Delta t}{\Delta z}\sin\left(\frac{k\Delta z}{2}\right)\right)$$



NB: $k = \pi/\Delta z$, $\lambda = 2\Delta z$: shortest wavelength supported by the grid.

The shorter the wavelength, the slower the propagation.



$c\Delta t > \Delta z \rightarrow \text{Courant limit}$

For $c\Delta t > \Delta z$, the discrete dispersion relation

$$\frac{1}{c^2 \Delta t^2} \sin^2 \left(\frac{\omega \Delta t}{2}\right) = \frac{1}{\Delta z^2} \sin^2 \left(\frac{k \Delta z}{2}\right)$$

has no real solutions ω , for k close to $\pi/\Delta z$. The solution ω is imaginary and the corresponding mode is unstable.

Courant limit (a.k.a. CFL limit)

Standard EM-PIC codes are **unstable** for $c\Delta t > \Delta z$ (in 1D).

- Thus, practical use of **electromagnetic PIC** codes is restricted to $\Delta t \leq \Delta z/c$.
- For a given spatial resolution Δz , this limits how fast a simulation can advance in time.
- Electrostatic PIC codes do not have this limitation \rightarrow Can be much faster than EM-PIC codes to simulate a system over a given period of time, by taking large timesteps Δt .

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Dispersion and Courant limit in 3D

Derivation of dispersion relation

Combine discrete Maxwell equation \rightarrow Discrete propagation equation \rightarrow Von Neumann analysis \rightarrow Numerical dispersion relation

Same process in 3D. The Von Neumann analysis assumes:

$$E = E_0 e^{ik_x x + ik_y y + ik_z z - i\omega t}$$

3D Numerical dispersion relation

$$\frac{\sin^2\left(\frac{\omega\Delta t}{2}\right)}{c^2\Delta t^2} = \frac{\sin^2\left(\frac{k_x\Delta x}{2}\right)}{\Delta x^2} + \frac{\sin^2\left(\frac{k_y\Delta y}{2}\right)}{\Delta y^2} + \frac{\sin^2\left(\frac{k_z\Delta z}{2}\right)}{\Delta z^2}$$

instead of the physical dispersion $\omega^2 = c^2(k_x^2 + k_y^2 + k_z^2)$

Courant limit (a.k.a CFL limit) in 3D

$$c\Delta t \le \frac{1}{\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}$$

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Numerical dispersion in 3D

3D Discrete dispersion relation

$$\frac{\sin^2\left(\frac{\omega\Delta t}{2}\right)}{c^2\Delta t^2} = \frac{\sin^2\left(\frac{k_x\Delta x}{2}\right)}{\Delta x^2} + \frac{\sin^2\left(\frac{k_y\Delta y}{2}\right)}{\Delta y^2} + \frac{\sin^2\left(\frac{k_z\Delta z}{2}\right)}{\Delta z^2}$$

Velocity depends on the wavelength and propagation direction.

Example: expanding electromagnetic wave





Even for $\Delta t = \Delta t_{CFL}$: waves are slower than c along the main axes.

Impact of numerical dispersion

Animation: laser-wakefield acceleration

- A short and intense **laser pulse**, followed by a relativistic **electron bunch**, enters a **plasma** (generated from a gas jet).
- The laser pulse generates a **wake** in the plasma, with **electric fields** that can **accelerate** the electron bunch.
- Simulation with the Yee scheme (and low resolution):
 - The laser is **artificially slow** (numerical dispersion)
 - Thus the electron bunch **catches up** with the laser very soon!

Standard Yee scheme (unphysical)



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Yee scheme

Finite-difference in space and time

e.g. continuous equation :
$$\frac{\partial B_z}{\partial t} = -\left(\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y}\right)$$
$$\rightarrow \text{ discrete equation : } B_z^{n+1/2} = B_z^{n-1/2} - \Delta t (\hat{\partial}_x E_y|^n - \hat{\partial}_y E_x|^n)$$
with $\hat{\partial}_x F|_{i,j,\ell}^n = \frac{F_{i+\frac{1}{2},j,\ell}^{n-F_{i-\frac{1}{2},j,\ell}^n}}{\Delta x}$

Physical



Simulated

- Anisotropic
- Waves propagate **slower** than *c*.

Pseudo-spectral solver

Fourier transform in space, finite-difference in time

e.g. continuous equation :
$$\frac{\partial B_z}{\partial t} = -\left(\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y}\right)$$

 \rightarrow Fourier space : $\frac{\partial \hat{B}_z}{\partial t} = -\left(ik_x\hat{\mathcal{E}}_y - ik_y\hat{\mathcal{E}}_x\right)$
 \rightarrow Finite difference in time : $\hat{\mathcal{B}}_z^{n+1/2} = \hat{\mathcal{B}}_z^{n-1/2} - \Delta t\left(ik_x\hat{\mathcal{E}}_y^n - ik_y\hat{\mathcal{E}}_x^n\right)$
 \rightarrow Use backwards FFT to obtain $B_z^{n+1/2}$ from $\hat{\mathcal{B}}_z^{n+1/2}$





- Isotropic
- Waves propagate **faster** than *c*.

Analytical pseudo-spectral solver (Haber et al., 1973)

Fourier transform in space, finite-difference in time

e.g. continuous equation :
$$\frac{\partial B_z}{\partial t} = -\left(\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y}\right)$$

$$\rightarrow$$
 Fourier space : $\frac{\partial \hat{\mathcal{B}}_z}{\partial t} = -\left(ik_x\hat{\mathcal{E}}_y - ik_y\hat{\mathcal{E}}_x\right)$

 \rightarrow Analytical integration of the coupled Maxwell equations in time:

$$\hat{\mathcal{B}}_z^{n+1} = \cos(kc\Delta t)\hat{\mathcal{B}}_z^n - \frac{\sin(kc\Delta t)}{kc}\left(ik_x\hat{\mathcal{E}}_y^n - ik_y\hat{\mathcal{E}}_x^n\right) \qquad k = \sqrt{k_x^2 + k_y^2 + k_z^2}$$

 \rightarrow Use backwards FFT to obtain B_z^{n+1} from $\hat{\mathcal{B}}_z^{n+1}$





• Isotropic

• Waves propagate **exactly** at *c*.

Dispersion and Courant limit: conclusions

- Electromagnetic solvers have a **maximum value** for the timestep Δt (Courant limit), which depends on the dimension (and the method of discretization)
- Below the Courant limit, waves may propagate at speeds that **artificially differ** from *c* (numerical dipersion). This can have a strong impact in some physical situations.
- Spectral solvers can mitigate (or even eliminate) numerical dispersion.

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Boundary conditions and EM-PIC

Reminder: 1D discrete Maxwell equations in vacuum



The grid is finite:

- For $\ell = 0$: $B_{y_{\ell-1/2}}^{n+1/2}$ is undefined.
- For $\ell = N$: $B_{y_{\ell+1/2}}^{n+1/2}$ is undefined.

 \rightarrow Assumptions are needed, for the value of $B_{y_{-1/2}}^{n+1/2}$ and $B_{y_{N+1/2}}^{n+1/2}$.

Boundary conditions and EM-PIC



Typical assumptions

- Periodic: $B_{y_{-1/2}}^{n+1/2} = B_{y_{N-1/2}}^{n+1/2}$ and $B_{y_{N+1/2}}^{n+1/2} = B_{y_{1/2}}^{n+1/2}$
- Dirichlet: $B_{y_{-1/2}}^{n+1/2} = 0$ and $B_{y_{N+1/2}}^{n+1/2} = 0$
- Neumann: $B_{y_{-1/2}}^{n+1/2} = B_{y_{1/2}}^{n+1/2}$ and $B_{y_{N+1/2}}^{n+1/2} = B_{y_{N-1/2}}^{n+1/2}$ (i.e. $\partial_z B_y|_0^{n+1/2} = 0$ and $\partial_z B_y|_N^{n+1/2} = 0$)

Boundary conditions and EM-PIC

Problem:

Dirichlet and Neumann boundary conditions **reflect** the EM waves. For many physical problems, we need the boundaries to **absorb** the waves.



This is because, physically, an **outgoing wave** does not satisfy $B_y(n\Delta z) = 0$ (Dirichlet) or $\partial_z B_y(n\Delta z) = 0$ (Neumann)

Silver-Müller absorbing boundary (right-hand side)



The value of $B_{y_{N+1/2}}^{n+1/2}$ should be chosen so as to be consistent with an outgoing wave.

Physically, for an outgoing wave propagating to the right (from Maxwell's equation):

$$B_y(z,t) = \frac{1}{c}E_x(z,t)$$

Numerically, we can express it as:

$$B_y|_N^{n+1/2} = \frac{1}{c} E_x|_N^{n+1/2}$$

Because of **staggering**:

$$\frac{B_{y_{N+1/2}}^{n+1/2} + B_{y_{N-1/2}}^{n+1/2}}{2} = \frac{1}{c} \frac{E_{x_N}^{n+1} + E_{x_N}^{n}}{2}$$

Silver-Müller absorbing boundary (right-hand side)



By combining the equations:

$$\frac{B_{y_{N+1/2}}^{n+1/2} + B_{y_{N-1/2}}^{n+1/2}}{2} = \frac{1}{c} \frac{E_{x_N}^{n+1} + E_{x_N}^{n}}{2} \quad \text{(right-propagating wave)}$$
$$\frac{E_{x_N}^{n+1} - E_{x_N}^{n}}{\Delta t} = -c^2 \frac{B_{y_{N+1/2}}^{n+1/2} - B_{y_{N-1/2}}^{n+1/2}}{\Delta z} \quad \text{(Maxwell equation)}$$

we obtain

Silver-Müller boundary condition (right-hand side)

$$E_{xN}^{n+1} = \left(1 - \frac{2c\Delta t}{c\Delta t + \Delta z}\right)E_{xN}^{n} + \frac{2c^2\Delta t}{c\Delta t + \Delta z}B_{yN-1/2}^{n+1/2}$$

See e.g. Bjorn Engquist (1977)

Silver-Müller absorbing boundary (right-hand side)

Silver-Müller boundary condition (right-hand side)

$$E_{xN}^{n+1} = \left(1 - \frac{2c\Delta t}{c\Delta t + \Delta z}\right) E_{xN}^{n} + \frac{2c^2\Delta t}{c\Delta t + \Delta z} B_{yN-1/2}^{n+1/2}$$

Animation: Silver-Müller boundary conditions



Silver-Müller absorbing boundary (left-hand side)



By combining the equations:

$$\frac{B_{y_{1/2}}^{n+1/2} + B_{y_{-1/2}}^{n+1/2}}{2} = -\frac{1}{c} \frac{E_{x_{0}}^{n+1} + E_{x_{0}}^{n}}{2} \quad \text{(left-propagating wave)}$$
$$\frac{E_{x_{0}}^{n+1} - E_{x_{0}}^{n}}{\Delta t} = -c^{2} \frac{B_{y_{1/2}}^{n+1/2} - B_{y_{-1/2}}^{n+1/2}}{\Delta z} \quad \text{(Maxwell equation)}$$

we obtain

Silver-Müller boundary condition (left-hand side)

$$E_{x0}^{n+1} = \left(1 - \frac{2c\Delta t}{c\Delta t + \Delta z}\right) E_{x0}^{n} - \frac{2c^2\Delta t}{c\Delta t + \Delta z} B_{y1/2}^{n+1/2}$$

Silver-Müller absorbing boundary in 3D

Maxwell equation:

$$\frac{E_{x_{i+\frac{1}{2},j,\ell}^{n+1}} - E_{x_{i+\frac{1}{2},j,\ell}^{n}}}{c^{2}\Delta t} = \frac{B_{z_{i+\frac{1}{2},j+\frac{1}{2},0}^{n+\frac{1}{2}}} - B_{z_{i+\frac{1}{2},j-\frac{1}{2},0}^{n+\frac{1}{2}}}{\Delta y} - \frac{B_{y_{i+\frac{1}{2},j,\ell+\frac{1}{2}}^{n+\frac{1}{2}}} - B_{y_{i+\frac{1}{2},j,\ell-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta z}$$

Silver-Müller boundary condition (left-hand side)

$$E_{x}_{i+\frac{1}{2},j,0}^{n+1} = \left(1 - \frac{2c\Delta t}{c\Delta t + \Delta z}\right) E_{x}_{i+\frac{1}{2},j,0}^{n} - \frac{2c^{2}\Delta t}{c\Delta t + \Delta z} B_{y}_{i+\frac{1}{2},j,\frac{1}{2}}^{n+\frac{1}{2}} + c^{2}\Delta t \frac{B_{z}_{i+\frac{1}{2},j+\frac{1}{2},0}^{n+\frac{1}{2}} - B_{z}_{i+\frac{1}{2},j-\frac{1}{2},0}^{n+\frac{1}{2}}}{\Delta y}$$

+ Similar equations for the right-hand side

+ Similar equations for B_x and E_y

Silver-Müller absorbing boundary in 3D

Limitation

In 3D, the Silver-Müller boundary conditions are only well-adapted for waves in **normal incidence**.

The reflection coefficient $R(\theta)$ quickly increases with the angle of incidence θ .



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Perfectly Matched Layers (in 2D)

Perfectly Matched Layers (Berenger, 1994)

Surround the simulation box by **additional layers of cells**, where the Maxwell equations are **modified** so as to **progressively damp** the waves.

In the bulk:

$$\partial_t E_x = c^2 \partial_y B_z$$
$$\partial_t E_y = -c^2 \partial_x B_z$$
$$\partial_t B_z = -\partial_x E_y + \partial_y E_x$$

In e.g. the right-hand layer:

 $\partial_t E_x = c^2 \partial_y B_z$ $\partial_t E_y = -c^2 \partial_x B_z - \frac{\sigma}{\epsilon_0} E_y$ $B_z = B_{zx} + B_{zy}$ $\partial_t B_{zx} = -\partial_x E_y - \frac{\sigma}{\epsilon_0} B_{zx}$ $\partial_t B_{zy} = \partial_y E_x$



Modified Maxwell equations:

- Artificial (unphysical) conductivity σ
- The B_z field is (artificially) split in two

Perfectly Matched Layers (in 2D)



Animation with propagating waves:

- Waves in normal incidence are **absorbed**.
- Waves in grazing incidence **propagate** as if they did not "feel" the boundary.

References

Perfectly Matched Layers: normal incidence

Explanation based on **continuous equations**

Transverse EM wave propagating along x

$$E_x = 0 \quad E_y \neq 0 \quad \to B_{zy} = 0 \quad B_z = B_{zx}$$

In the bulk:

$$\begin{array}{lll} \partial_t E_x &= c^2 \partial_y B_z \\ \partial_t E_y &= -c^2 \partial_x B_z \\ \partial_t B_z &= -\partial_x E_y + \partial_y E_x \end{array} \rightarrow \begin{array}{lll} \partial_t E_y &= -c^2 \partial_x B_z \\ \partial_t B_z &= -\partial_x E_y + \partial_y E_x \end{array}$$



In the right-hand layer:

$$\begin{array}{lll} \partial_t E_x &= c^2 \partial_y B_z \\ \partial_t E_y &= -c^2 \partial_x B_z - \frac{\sigma}{\epsilon_0} E_y \\ B_z &= B_{zx} + B_{zy} & \rightarrow \\ \partial_t B_{zx} &= -\partial_x E_y - \frac{\sigma}{\epsilon_0} B_{zx} \\ \partial_t B_{zy} &= \partial_y E_x \end{array} \rightarrow \begin{array}{lll} \partial_t E_y &= -c^2 \partial_x B_z - \frac{\sigma}{\epsilon_0} E_y \\ \partial_t B_z &= -\partial_x E_y - \frac{\sigma}{\epsilon_0} B_{zx} \end{array}$$

Perfectly Matched Layers: normal incidence

There is a solution (continuous in E_y and B_z) with **no reflected wave**.



x

0

References

Perfectly Matched Layers: grazing incidence

Transverse EM wave propagating along y

$$E_x \neq 0$$
 $E_y = 0$ $\rightarrow B_{zx} = 0$ $B_z = B_{zy}$

In the bulk:

$$\begin{array}{lll} \partial_t E_x &= c^2 \partial_y B_z \\ \partial_t E_y &= -c^2 \partial_x B_z \\ \partial_t B_z &= -\partial_x E_y + \partial_y E_x \end{array} \rightarrow \begin{array}{lll} \partial_t E_x &= c^2 \partial_y B_z \\ \partial_t B_z &= \partial_y E_x \end{array}$$





In the right-hand layer:

$$\begin{array}{lll} \partial_t E_x &= c^2 \partial_y B_z \\ \partial_t E_y &= -c^2 \partial_x B_z - \frac{\sigma}{\epsilon_0} E_y \\ B_z &= B_{zx} + B_{zy} & \rightarrow \\ \partial_t B_{zx} &= -\partial_x E_y - \frac{\sigma}{\epsilon_0} B_{zx} \\ \partial_t B_{zy} &= \partial_y E_x \end{array} \rightarrow \begin{array}{lll} \partial_t E_x &= c^2 \partial_y B_z \\ \partial_t B_z &= \partial_y E_x \end{array}$$

The propagation equations are **identical** in the bulk and the outer layer. A wave in **grazing indidence** does not "feel" the boundary.

Open boundary conditions: conclusion

- If no **special care** is taken at the boundary, it will **by default** produce a reflected wave.
- Silver-Müller boundary conditions:
 - Easy to implement
 - But only cancels reflection for waves at normal incidence

• Perfectly Matched Layers

- Need extra layers of cells, where the Maxwell equations are artificially modified.
- The anisotropic Maxwell equations lead to proper behavior for waves with any incidence angle.

References

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