Quantum Lattice Algorithm for Electromagnetic Pulse Propagation in a 2D Scalar Dielectric Medium

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- work supported by the Department of Energy

Motivation :

- QIS for plasma physics?

-- can we devise a unitary time evolution algorithm for Maxwell eqs.?

$$\Psi\left(t+\Delta t\right) = U_1.U_2.U_3..... U_{..} \Psi\left(t\right)$$

- since the 1930's connections were sought between Maxwell – Dirac.

- can these 3D QLA Maxwell codes be more efficient than classical codes on current classical supercomputers -- parallelization , memory ?

e.g., 3D QLA for spinor BECs :

no saturation to over 786,432 cores (*Mira*)

- quantum lattice algorithm (QLA) for the Maxwell equations

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \quad , \quad \mu_0 \varepsilon \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B}$$

$$\nabla \bullet \left(\varepsilon \mathbf{E} \right) = 0 \quad , \quad \nabla \bullet \mathbf{B} = 0$$

$$\Rightarrow (Khan\ \ 2005)\ \ Riemann - Silberstein - Weber \quad \mathbf{F}^{\pm} = \sqrt{\varepsilon}\,\mathbf{E} \pm i \frac{\mathbf{B}}{\sqrt{\mu_0}}$$

polarization vectors

- 8-spinor representation of the full inhomogeneous Maxwell Eqs. (Khan)

Let $\Psi^{\pm} = \begin{pmatrix} -F_x^{\pm} \pm iF_y^{\pm} \\ F_z^{\pm} \\ F_z^{\pm} \\ F_x^{\pm} \pm iF_y^{\pm} \end{pmatrix}$, $\mathbf{M} = \vec{\sigma} \times I_2$, $\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}$, $\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$

$$\rightarrow \quad \frac{\partial}{\partial t} \begin{pmatrix} \Psi^{+} \\ \Psi^{-} \end{pmatrix} = i \frac{1}{\left(\mu_0 \varepsilon \right)^{1/2}} \begin{pmatrix} i\left(\mathbf{M} \cdot \nabla - \vec{\Sigma} \cdot \frac{\nabla \varepsilon}{2\varepsilon} \right) & -M_z \vec{\Sigma} \cdot \frac{\nabla \varepsilon}{2\varepsilon} \alpha_y \\ -M_z \vec{\Sigma}^{*} \cdot \frac{\nabla \varepsilon}{2\varepsilon} \alpha_y & i\left(\mathbf{M}^{*} \cdot \nabla - \vec{\Sigma}^{*} \cdot \frac{\nabla \varepsilon}{2\varepsilon} \right) \end{pmatrix} \begin{pmatrix} \Psi^{+} \\ \Psi^{-} \end{pmatrix}$$

$$\frac{\partial \Psi}{\partial t} = i\, H\, \Psi \quad \rightarrow \quad \Psi\left(t + \Delta t \right) = e^{i H \Delta t}\ \Psi\left(t \right)$$

Special Case : *Homogeneous medium* ➔ $\varepsilon = const.$ ➔ Ψ^+ *and* Ψ^- *uncoupled polarizations*

$$\Psi^+ = \begin{pmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{pmatrix}$$

with

$$\frac{\partial}{\partial t}\begin{pmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{pmatrix} = -\frac{\partial}{\partial x}\begin{pmatrix} q_2 \\ q_3 \\ q_0 \\ q_1 \end{pmatrix} + i\frac{\partial}{\partial y}\begin{pmatrix} q_2 \\ q_3 \\ -q_0 \\ -q_1 \end{pmatrix} - \frac{\partial}{\partial z}\begin{pmatrix} q_0 \\ q_1 \\ -q_2 \\ -q_3 \end{pmatrix}$$

==========

Dirac equation for a free particle : 4-spinor eq.

$$\frac{\partial \psi}{\partial t} = c\sum_{j=1}^{3} a \otimes \sigma_j \frac{\partial \psi}{\partial x_j} + ib \otimes I_2 m\psi$$

For massless particle

$$\frac{\partial}{\partial t}\begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = \frac{\partial}{\partial x}\begin{pmatrix} \psi_3 \\ \psi_2 \\ \psi_1 \\ \psi_0 \end{pmatrix} + i\frac{\partial}{\partial y}\begin{pmatrix} -\psi_3 \\ \psi_2 \\ -\psi_1 \\ \psi_0 \end{pmatrix} + \frac{\partial}{\partial z}\begin{pmatrix} \psi_2 \\ -\psi_3 \\ \psi_0 \\ -\psi_1 \end{pmatrix}.$$

Yepez – 4-qubit QLA for 1D-Dirac (2005)

UNITARY ALGORITHM
- quantum computer

1D INHOMOGENEOUS MEDIUM, refractive index n(x)

$$\frac{\partial}{\partial t}\begin{pmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{pmatrix} = -\frac{1}{n(x)}\frac{\partial}{\partial x}\begin{pmatrix} q_2 \\ q_3 \\ q_0 \\ q_1 \end{pmatrix} - \frac{n'(x)}{2n^2(x)}\begin{pmatrix} q_1+q_6 \\ q_0-q_7 \\ q_3-q_4 \\ q_2+q_5 \end{pmatrix}$$

$$\frac{\partial}{\partial t}\begin{pmatrix} q_4 \\ q_5 \\ q_6 \\ q_7 \end{pmatrix} = -\frac{1}{n(x)}\frac{\partial}{\partial x}\begin{pmatrix} q_6 \\ q_7 \\ q_4 \\ q_5 \end{pmatrix} - \frac{n'(x)}{2n^2(x)}\begin{pmatrix} q_5+q_2 \\ q_4-q_3 \\ q_7-q_0 \\ q_6+q_1 \end{pmatrix}$$

QLA : collide-stream potential operators

Unitary operators

One or more Hermitian operators

1D QLA-x or y : 8 qubits/lattice node

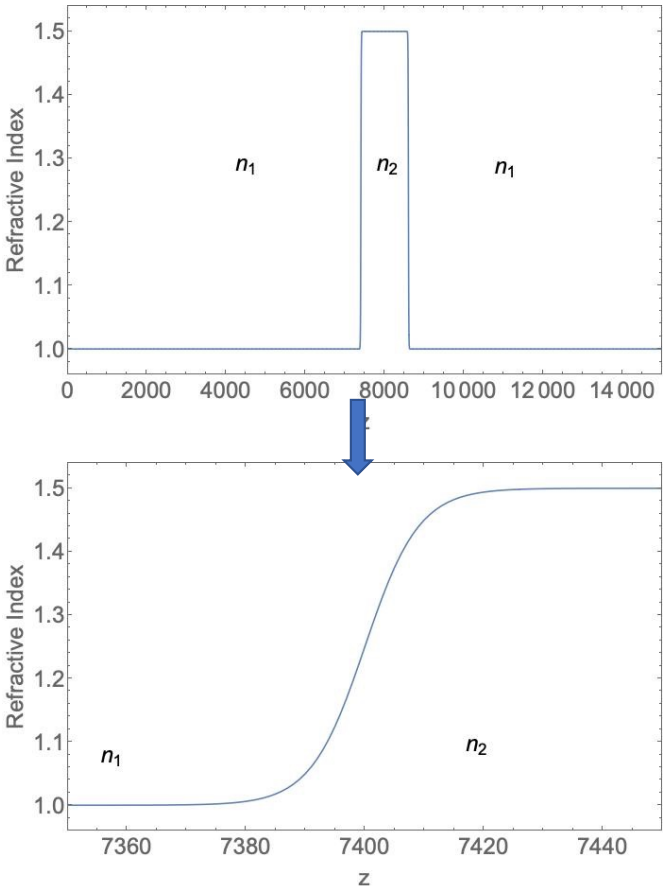
z– direction : 16 qubits/lattice node

QLA : INTERLEAVED SEQUENCE OF NON-COMMUTING COLLIDE-STREAM OPERATORS

- COLLISION OPERATORS LOCALLY ENTANGLE THE QUBITS AT EACH LATTICE SITE ,

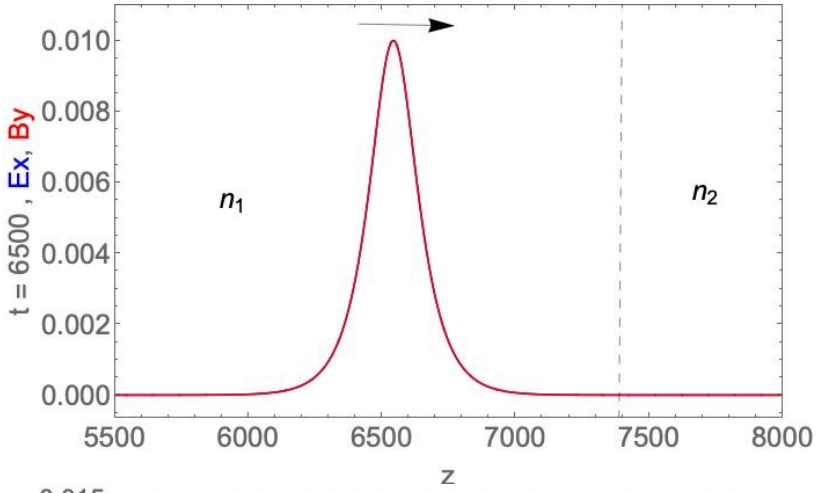
- STREAM OPERATORS MOVE THIS ENTANGLEMENT THROUGHOUT THE LATTICE.

Some 1D QLA simulations (z-inhomo.) : hyperbolic secant pulse

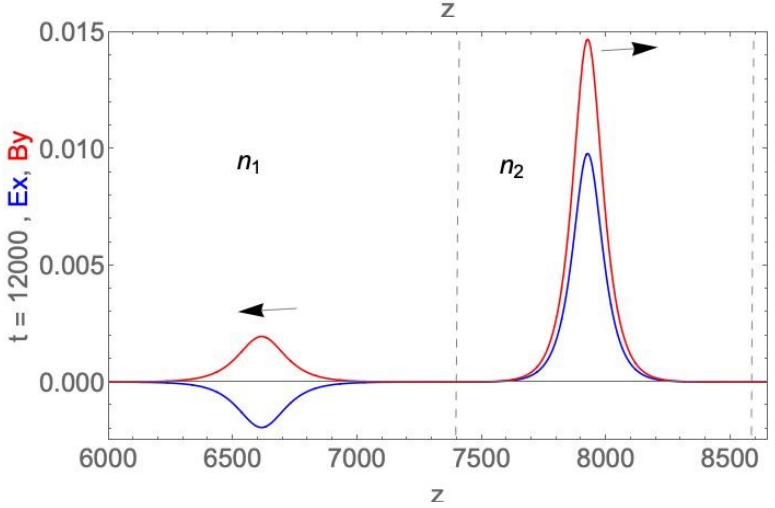


boundary layer : 40 units
Pulse width : 800 units

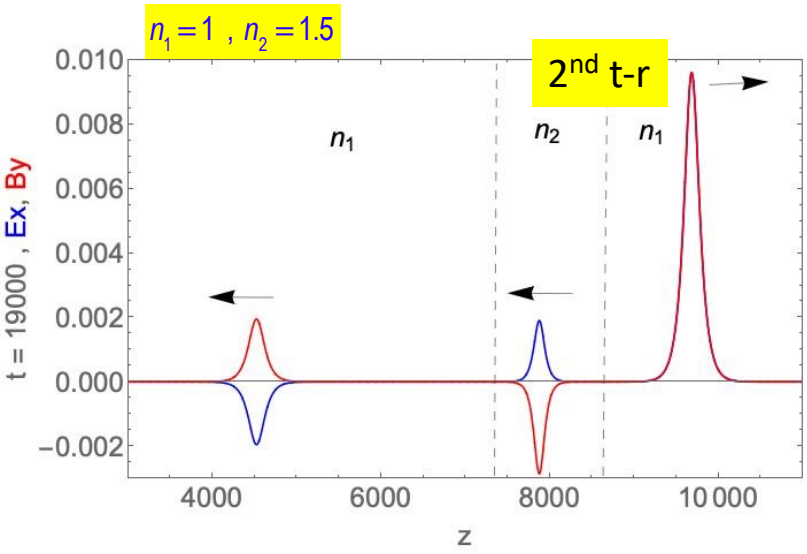
No boundary conditions at interface : initial value problem

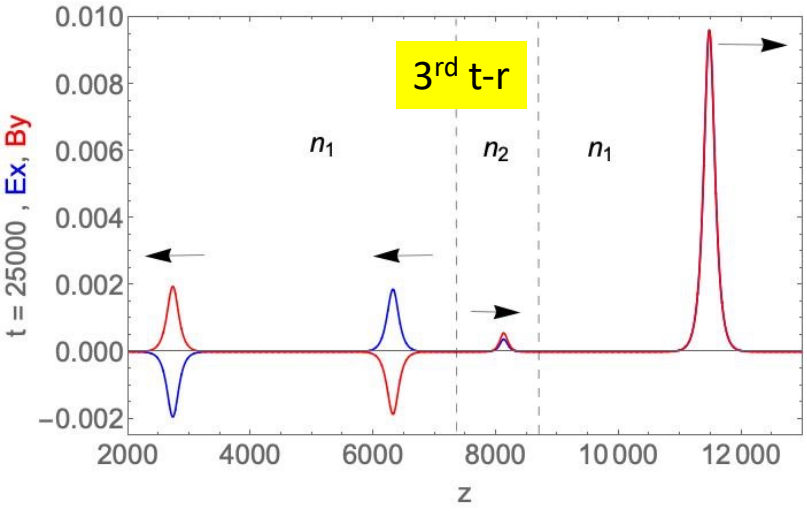


$n_1 = 1$, $n_2 = 1.5$



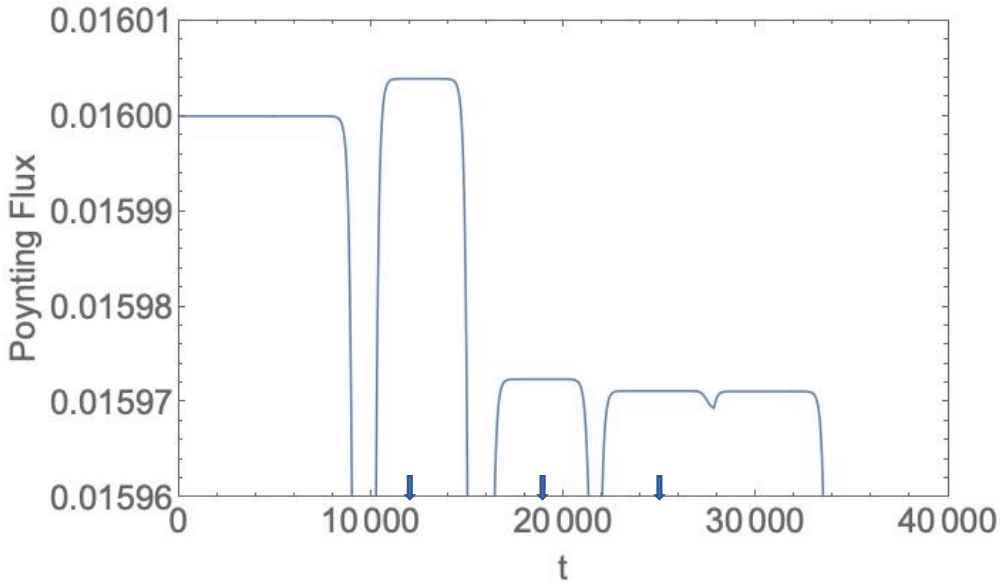
1st transmission
- reflection from leading edge of dielectric





Instantaneous Poynting Flux

$$S(t) = \int_0^L \mathbf{E}(z,t) \times \mathbf{B}(z,t) \cdot \hat{\mathbf{n}}\, dz$$

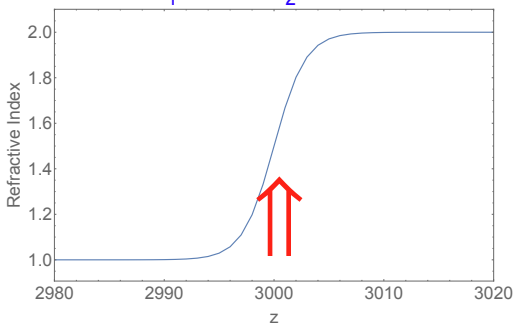


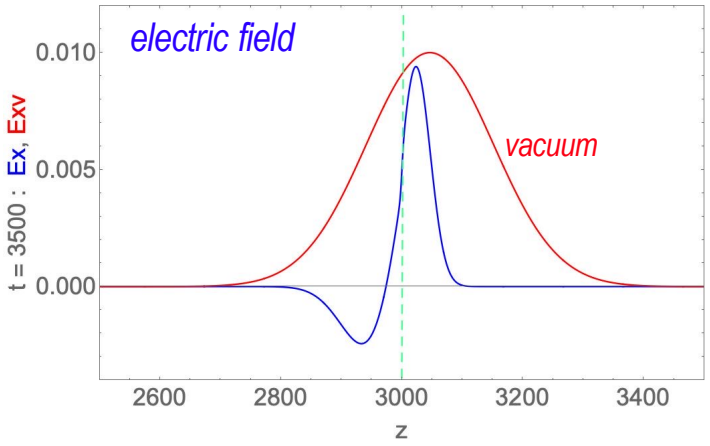
Excellent energy conservation in the quasi-asymptotic states

- dips in S(t) occur in time intervals when the pulse straddles both refractive media, and the outward normal is not that easily determined.

Determination of Poynting Flux at times when the pulse straddles the two dielectrics

$n_1 = 1$, $n_2 = 2.0$





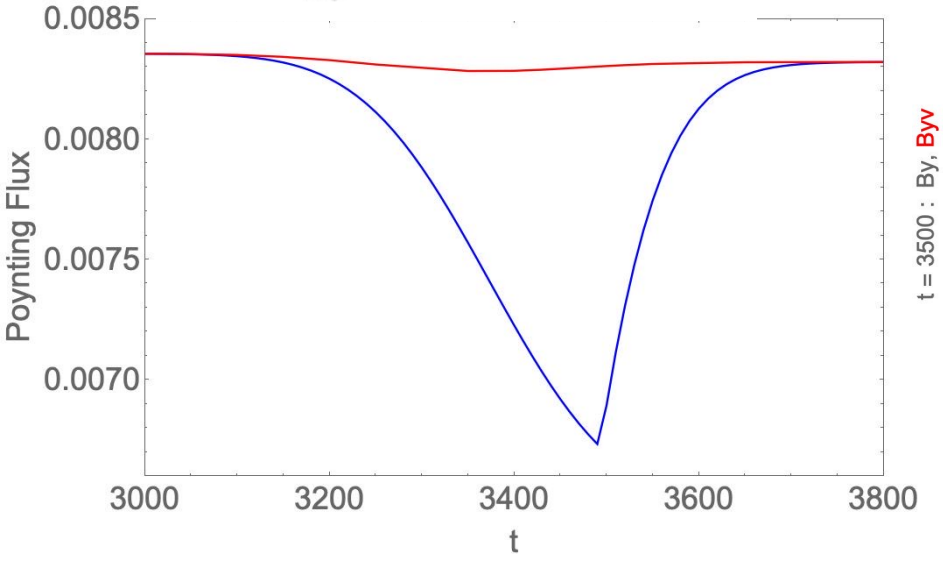
t = 3500

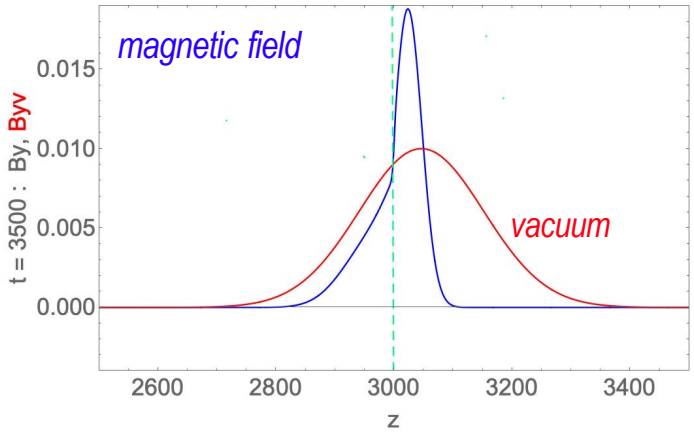
Choose pivot
Point z = 3000

$$S(t) = \int_0^L \mathbf{E}(z,t) \times \mathbf{B}(z,t) \cdot \hat{\mathbf{n}}\, dz$$

$$Ex\,|_{QLA} = Exv + Ex\,|_{refl}$$

$$Exv \;\; in + \hat{z} \;, \;\; Ex\,|_{refl} \;\; in - \hat{z}$$





SUMMARY of 1D QLA SIMULATIONS

- all the standard Fresnel jump conditions of a PLANE wave at a dielectric discontinuity are verified by QLA simulations
  - 180º phase change in Ex when one moves from low-to-high n(z)…
  - 180º phase change in By when one moves from high-to-low n(z)…

EXCEPT the ratio of transmitted to incident Electric field amplitude.

$$E_r = \frac{n_1 - n_2}{n_1 + n_2} E_0,$$

$$E_t = \frac{2n_1}{n_1 + n_2} \sqrt{\frac{n_2}{n_1}} E_0.$$

⇑

All QLA simulations show this result :
- pulses: Gaussian, exponential , sech ….
- for different choices of n_1, n_2
- for different perturbation parameters ε

A theory for Gaussian pulses has been developed that vindicates these results
- Ram, Vahala, Vahala and Soe : arXiv 2108.06880 (2021), AIP *Advances* (2021)

THEORY for this extra factor for Gaussian pulses

Refractive index discontinuity at z = 0

Consider an incident Gaussian pulse $$\mathbf{E}_I(z,t) = \frac{E_0}{\pi^{1/4}\sqrt{\sigma}}\, e^{-(z-v_1 t+z_0)^2/(2\sigma^2)}\,\hat{\mathbf{x}}, \quad \text{for } z<0,$$

Normalization $$\int_{-\infty}^{\infty} dz \left|\mathbf{E}_I(z,t)\right|^2 = E_0^2$$ with σ the width of pulse

Reflected and transmitted fields:

$$\mathbf{E}_R(z,t) = \frac{E_r}{\pi^{1/4}\sqrt{\sigma_1}}\, e^{-(z+z_1+v_1 t)^2/(2\sigma_1^2)}\,\hat{\mathbf{x}} \quad \text{for } z<0,$$

$$\mathbf{E}_T(z,t) = \frac{E_t}{\pi^{1/4}\sqrt{\sigma_2}}\, e^{-(z-z_2-v_2 t)^2/(2\sigma_2^2)}\,\hat{\mathbf{x}} \quad \text{for } z>0,$$

Decompose these pulses into their plane wave representations $$\mathbf{E}_I(z,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, E_0 \frac{\sqrt{2\pi\sigma}}{\pi^{1/4}} \exp\left[-\frac{\sigma^2 k^2}{2}\right] e^{ik(z+z_0-vt)}$$

⇑

Integrand is the plane wave repr.

Similarly for the plane wave representations of the reflected and transmitted pulses.

Fresnel jump conditions at z = 0 :

$$\frac{E_r}{\pi^{1/4}}\sqrt{2\pi\sigma_1}\,e^{-\sigma_1^2k_1^2/2}\,e^{ik_1z_1} = \frac{n_1-n_2}{n_1+n_2}\frac{E_0}{\pi^{1/4}}\sqrt{2\pi\sigma}\,e^{-\sigma^2k^2/2}e^{ikz_0},$$

$$\frac{E_t}{\pi^{1/4}}\sqrt{2\pi\sigma_2}\,e^{-\sigma_2^2k_2^2/2}\,e^{-ik_2z_2} = \frac{2n_1}{n_1+n_2}\frac{E_0}{\pi^{1/4}}\sqrt{2\pi\sigma}\,e^{-\sigma^2k^2/2}\,e^{ikz_0}.$$

Can show : *reflected* $\sigma_1=\sigma$, *transmitted* $\sigma_2=\frac{n_1}{n_2}\sigma$

$$\frac{E_r}{E_0}=\frac{n_1-n_2}{n_1+n_2}$$

$$\frac{E_t}{E_0}=\frac{2n_1}{n_1+n_2}\sqrt{\frac{n_2}{n_1}}=\frac{2\sqrt{n_1.n_2}}{n_1+n_2}$$

symmetric in $n_1 \rightleftarrows n_2$ ==> $\frac{E_t}{E_0}$ *independent of pulse direction*

1D-QLA and THEORY

$$E_r = \frac{n_1 - n_2}{n_1 + n_2} E_0,$$

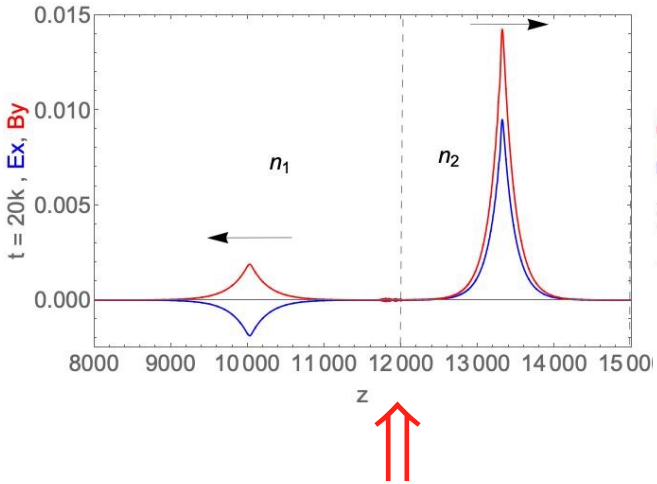
$$E_t = \frac{2n_1}{n_1 + n_2} \sqrt{\frac{n_2}{n_1}} E_0.$$

THEORY: 0.9798 indep. of pulse direction

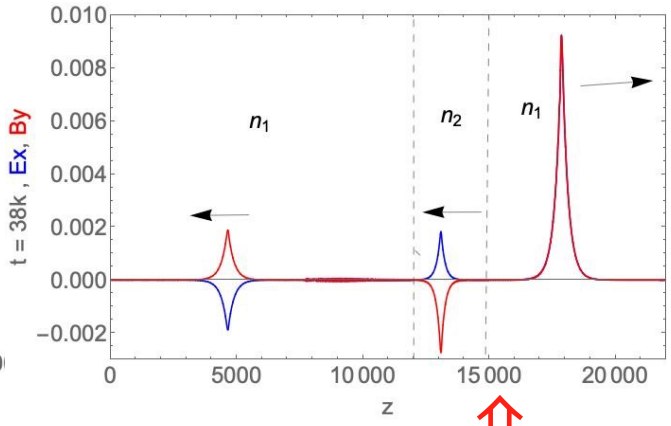
E_t/E_0	Gaussian	Exp	sech
1st	0.9800	0.9677	0.9799
2nd	0.9807	0.9724	0.9807
3rd	0.9806	0.9788	0.9806

E_r/E_0	Theory	Exp	sech
1st	- 0.2	- 0.192	- 0.195
2nd	0.2	0.192	0.194
3rd	0.2	0.196	0.195

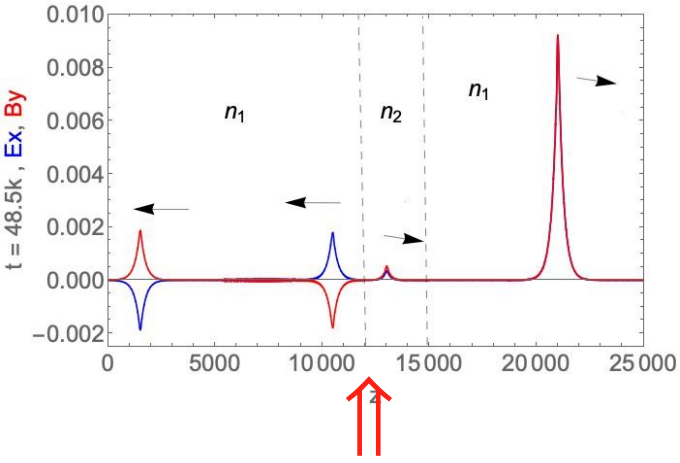
$n_1 = 1$, $n_2 = 1.5$ (exponential pulse)



1st



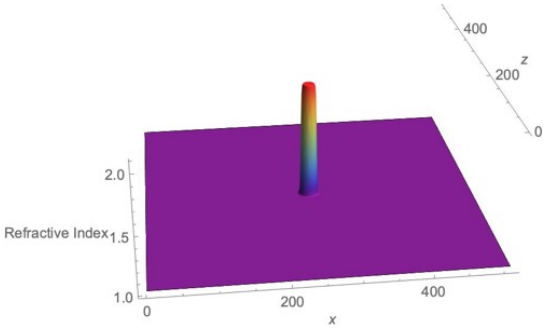
2nd



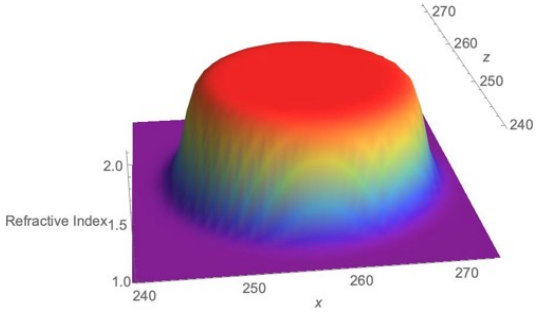
3rd

2D QLA : tensor product of x-z 1D propagations

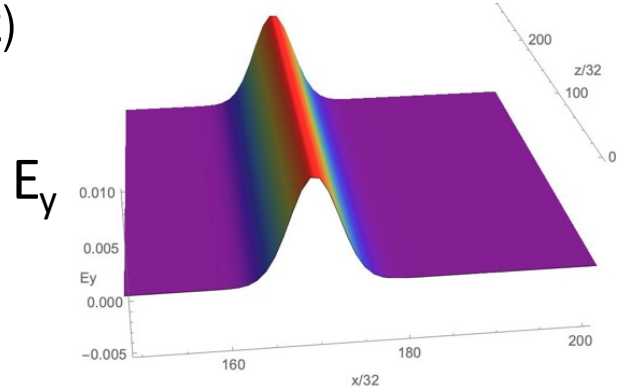
1D pulse propagating in x-direction : only initial non-zero fields: Ey(x,t) , Bz(x,t)
- interacts with a localized 2D dielectric, with n=n(x,z)



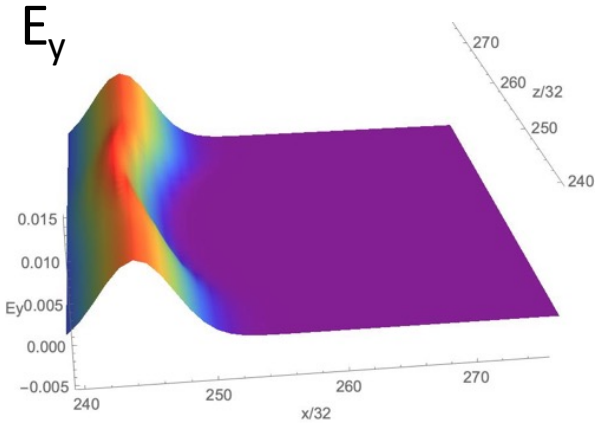
Dielectric cylinder (256,256)



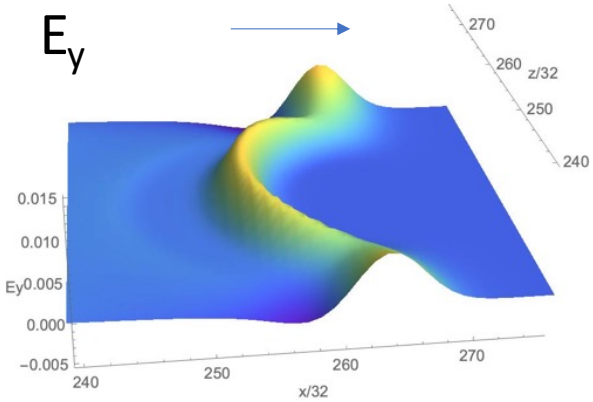
Blow-up of 2D dielectric n(x,z)



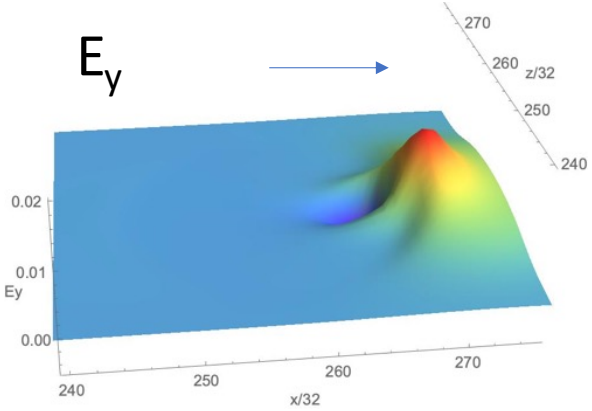
t = 8k : 1D pulse in x-direction



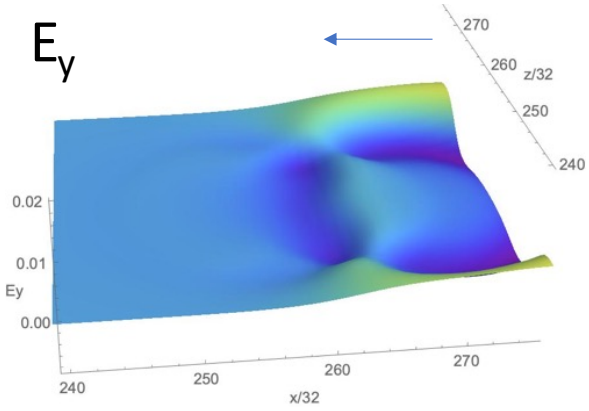
t =16k : 1st interaction with dielectric



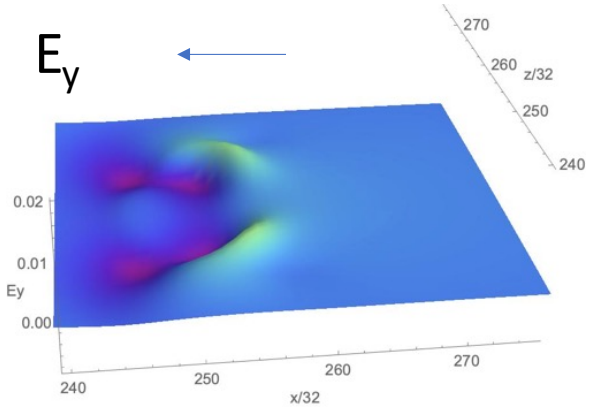
t = 18k, weak reflection from , strong transmission into dielectric



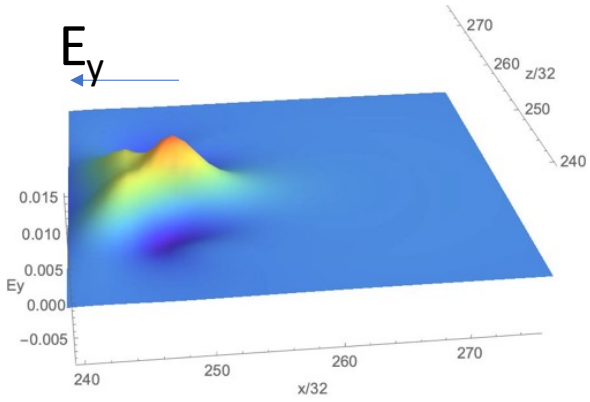
t = 21k : impact of that part of the pulse with back of dielectric



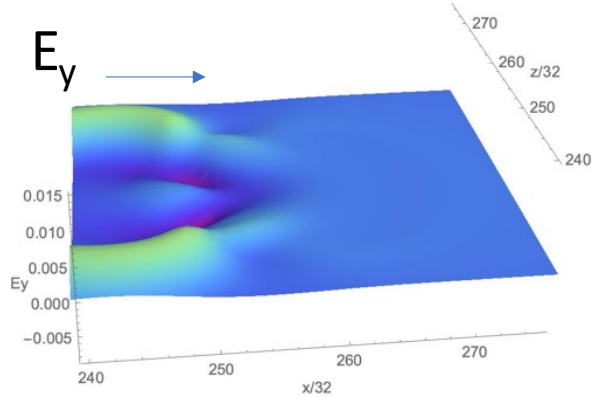
t = 23k : reflected part of pulse in dielectric



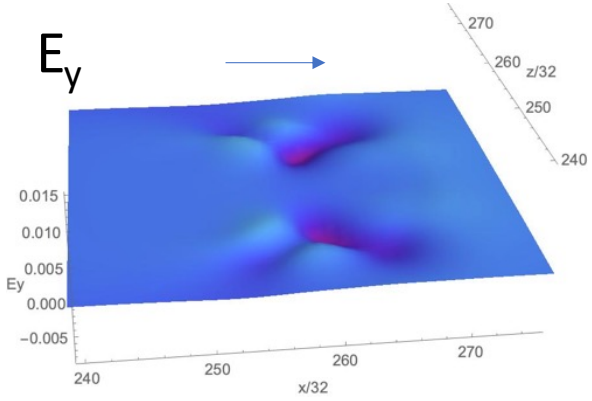
t = 25k : reflected part of pulse in dielectric



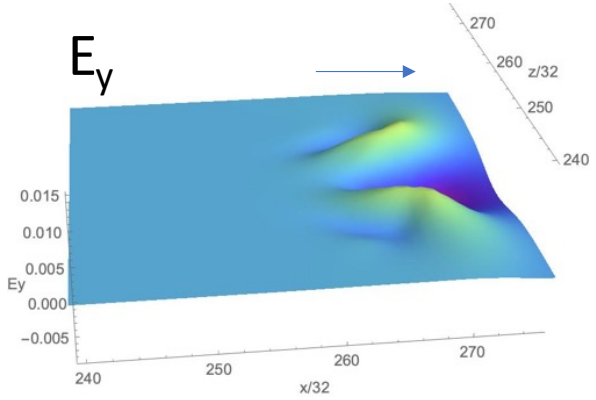
t – 27k : pulse about to hit the leading edge of dielectric



t = 29k : 2nd reflection of pulse from the leading dielectric edge

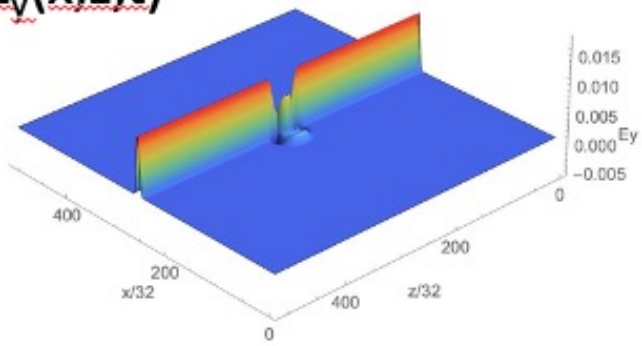


t = 31k : propagating towards the back end of dielectric

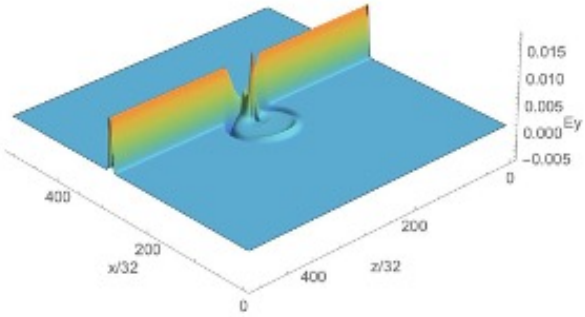


t = 33k : pulse about to collide with the back end of dielectric

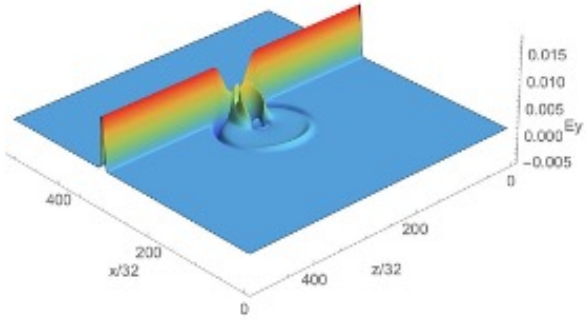
$E_y(x,z,t)$



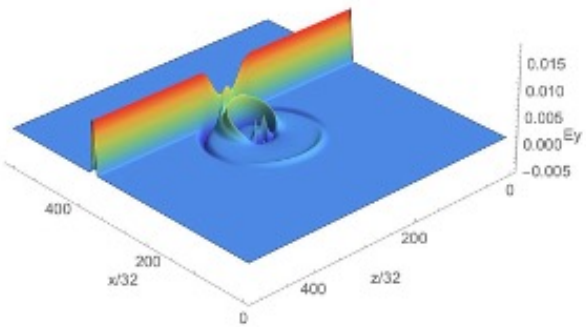
t = 18k



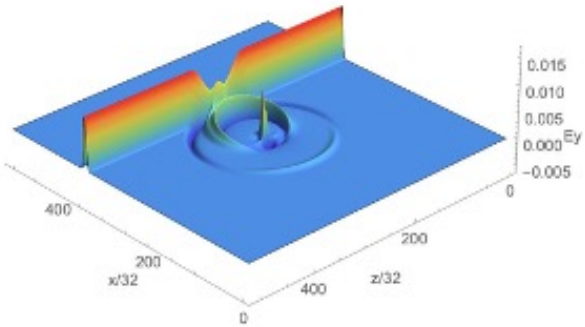
t = 21 k



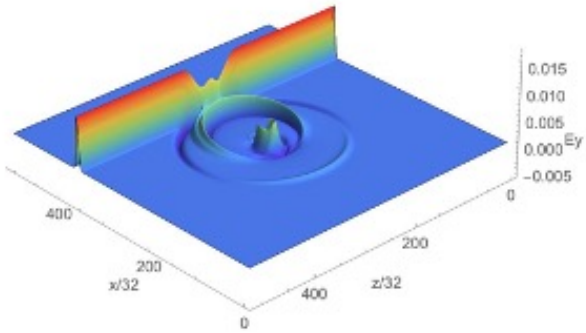
t= 23k



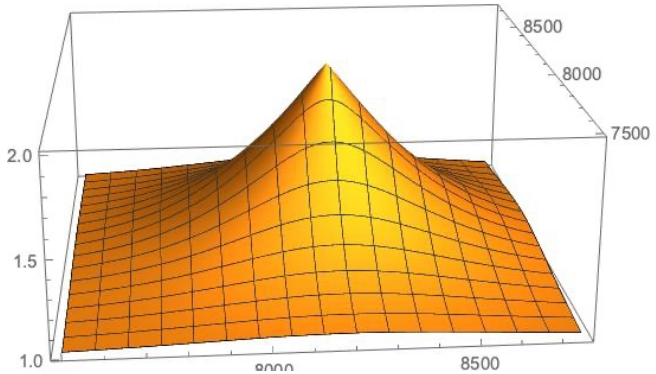
t = 25k

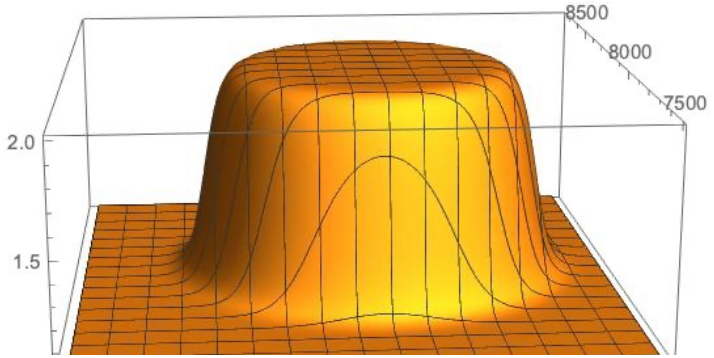


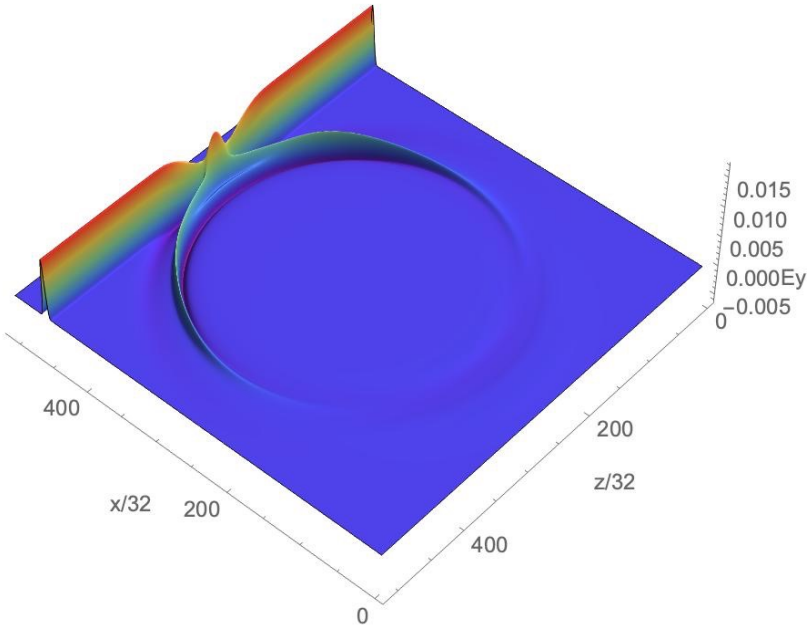
t = 27k

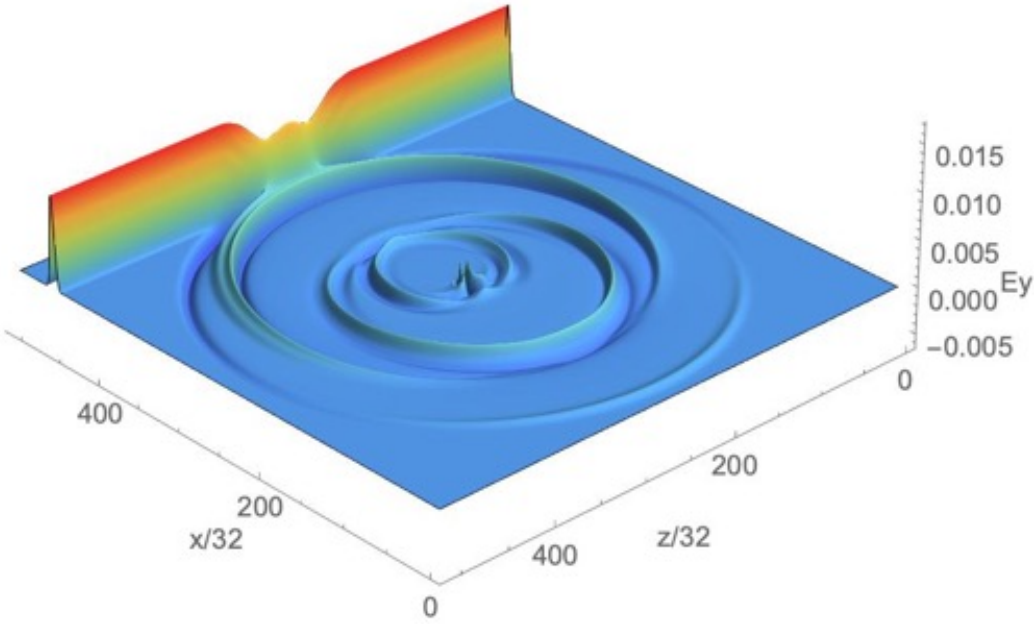


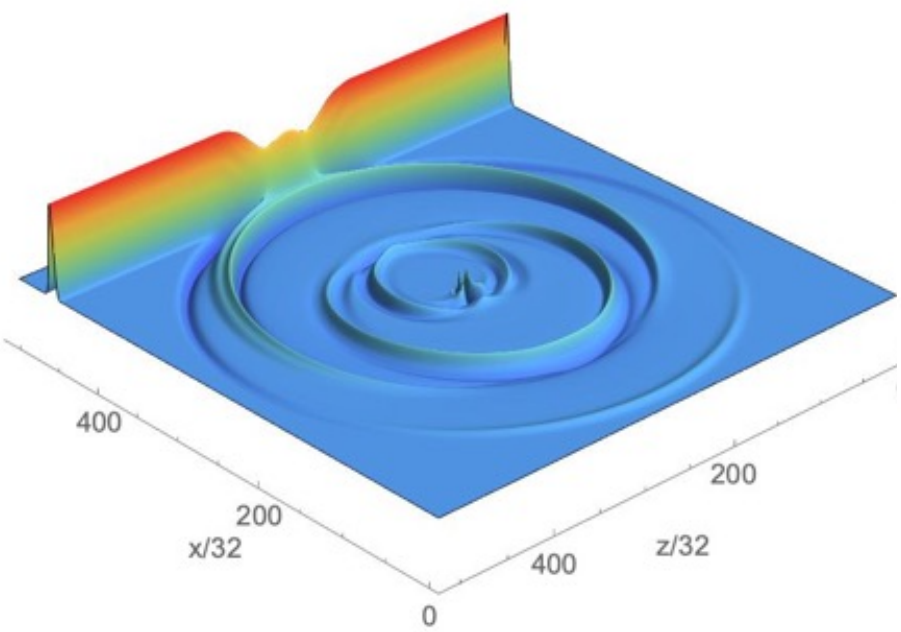
EFFECT of DIELECTRIC GEOMETRY on the RESULTANT Ey-FIELD

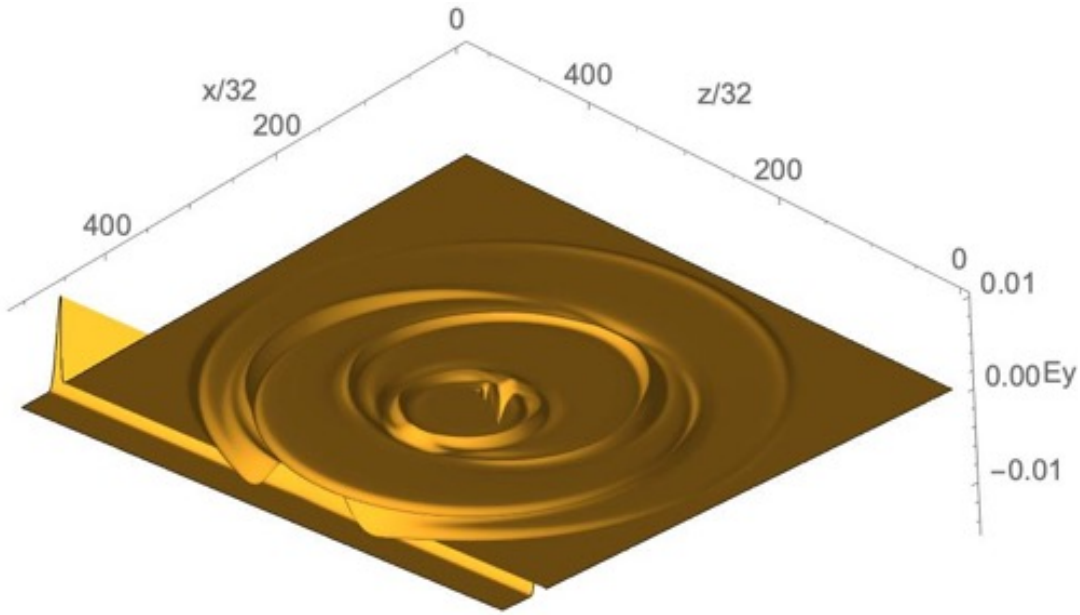












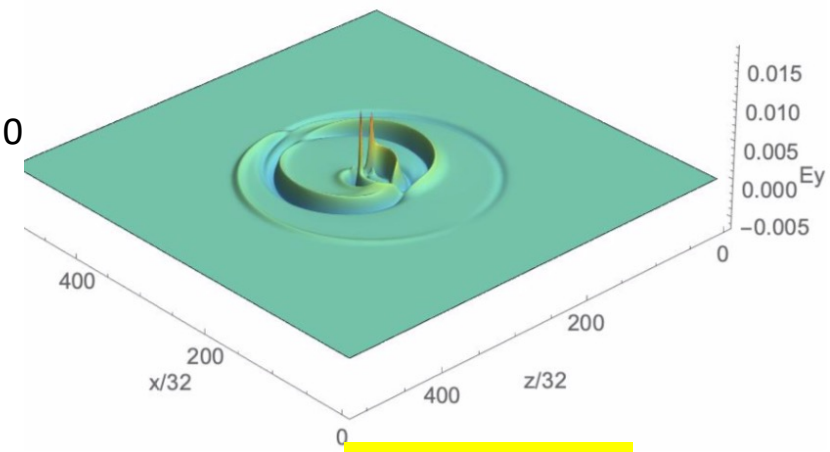
$E_y(x,z,\ t= 40k) > 0$

$E_y(x,z,\ t= 40k) < 0$

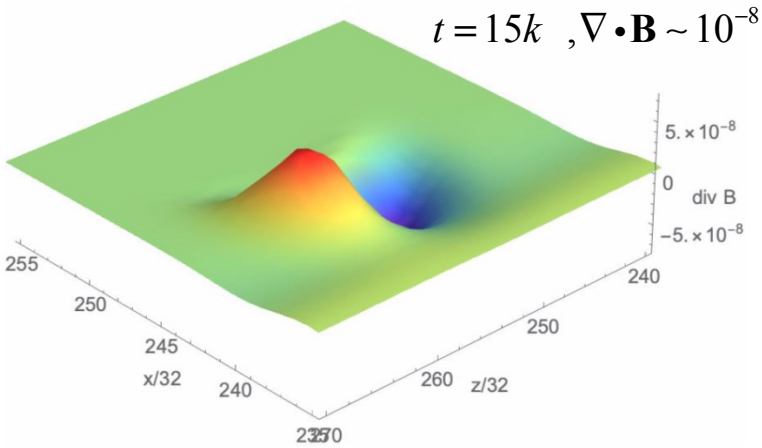
$B_x(x,z,t)$ is generated when pulse takes on 2D structure following interaction with dielectric cylinder

$\nabla \cdot \mathbf{B}$

Bx > 0

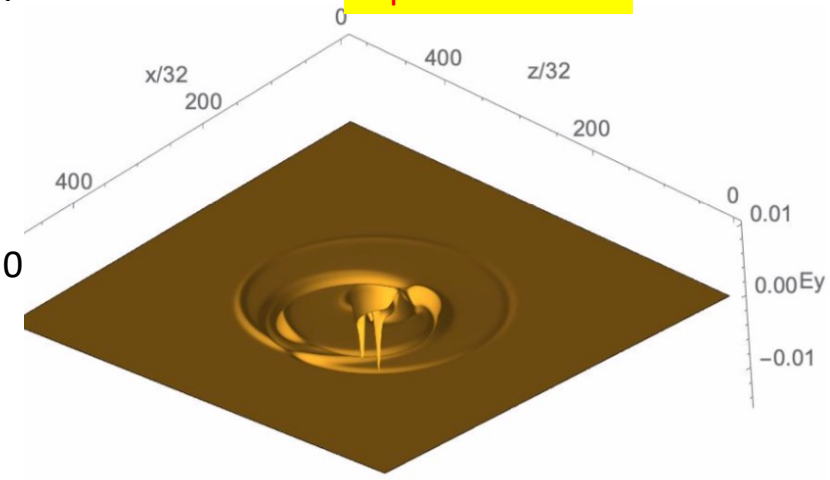


$t = 15k \quad ,\nabla \cdot \mathbf{B} \sim 10^{-8}$



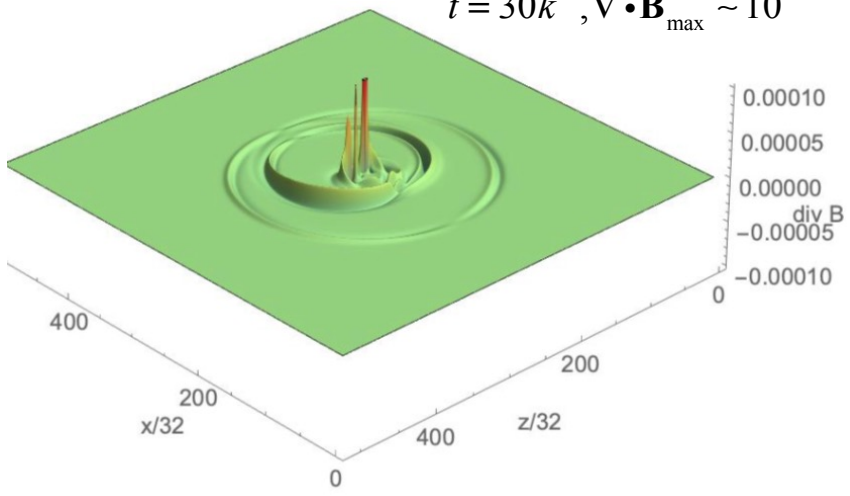
t = 30 k

dipole-structure

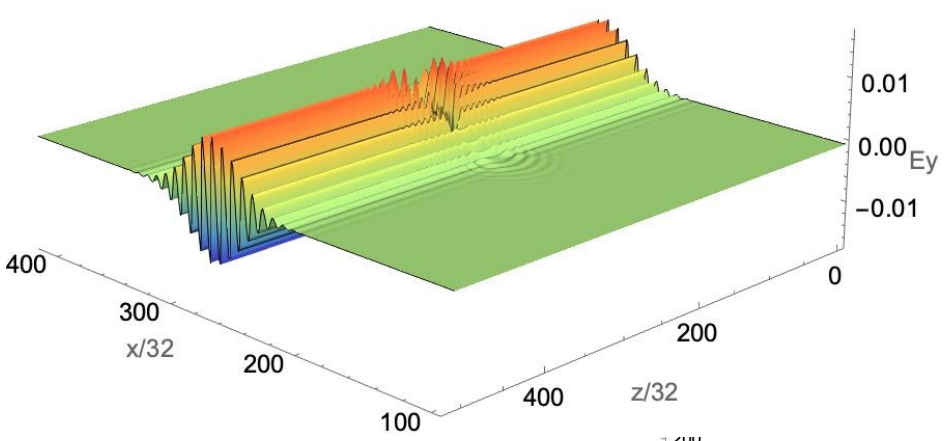


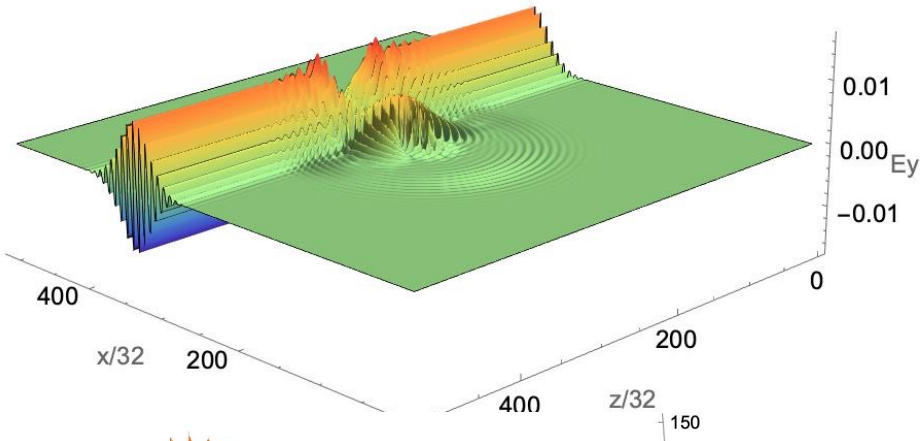
Bx < 0

$t = 30k \quad ,\nabla \cdot \mathbf{B}_{max} \sim 10^{-4}$

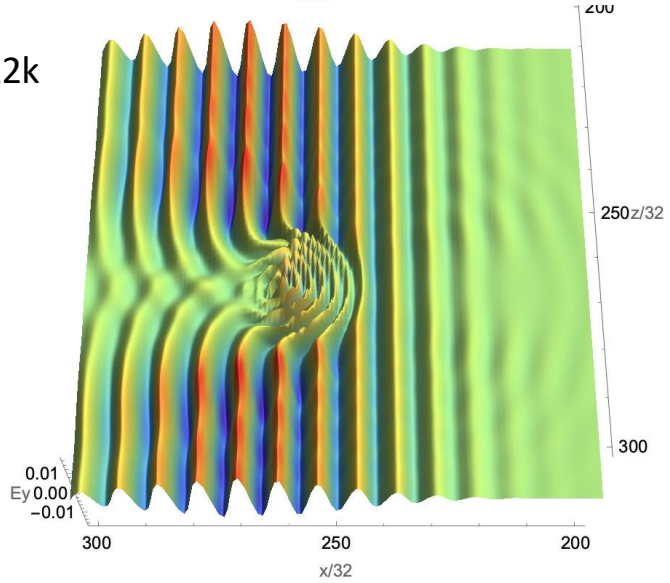


Gaussian Wave Packet : dielectric cylinder n_2=3 : 242 ≤ x'≤270

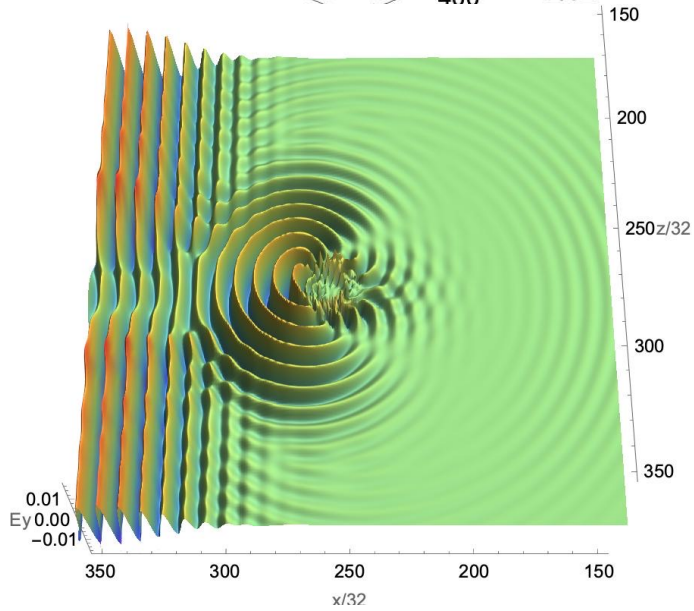




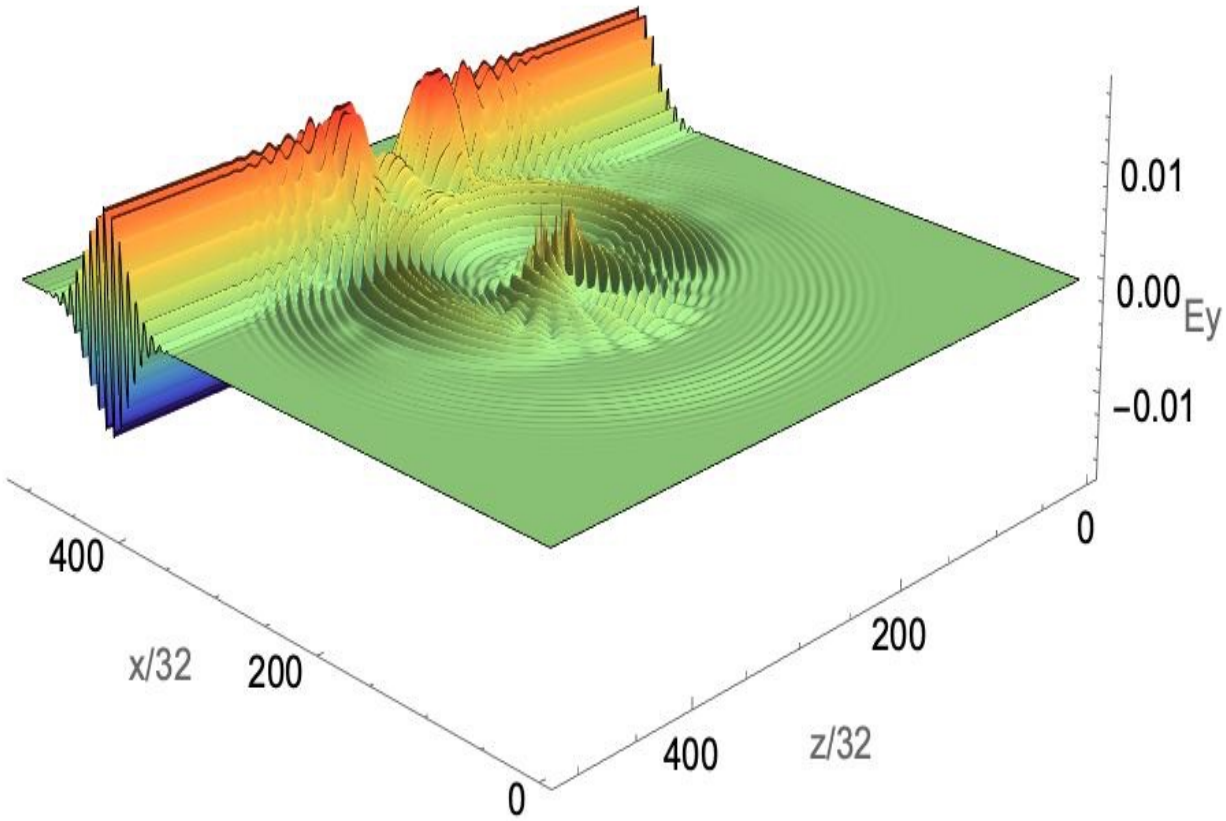
t = 12k



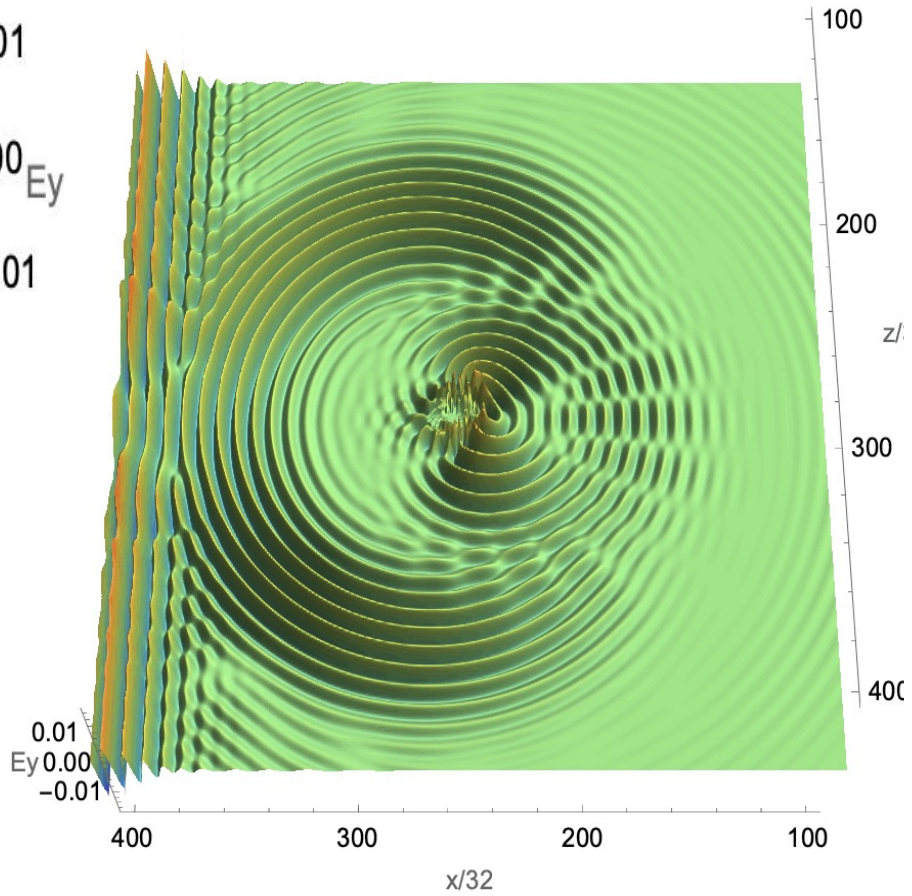
t = 20k



Gaussian Wave Packet : dielectric cylinder n_2=3 : 242 ≤ x'≤270



t = 28 k



SUMMARY

- developed a QLA for Maxwell Eqs. in scalar dielectric media (initial value code)
  - as its cousin QLA for spinor BECs, it is ideally parallelized to all available cores
  - a 3D simulation requires only 16 qubits/lattice site

- for 1D initial pulse
  - excellent conservation of energy
  - initial value code, no boundary conditions at dielectric interfaces
  - recover all the standard plane wave jump conditions except

$$\frac{E_{trans}}{E_{inc}} = \frac{2n_1}{n_1 + n_2}\sqrt{\frac{n_2}{n_1}}$$

  - a theory for Gaussian pulses at sharp boundaries has been developed

- QLA mesoscopic representation recovers Maxwell to $O\left(\varepsilon^2\right)$ where ε is a perturbation parameter introduced into the collision operators
  - ε is the (normalized) speed of light c in a vacuum
  - linear QLA is numerically stable for all $\varepsilon \le 1$

- QLA for Gaussian wave packet : diffraction/interference

- Extending QLA to tensor dielectric media and eventually to the cold plasma dielectric tensor.