Unitary Quantum Lattice Algorithms For Classical and Quantum Turbulence - part 2

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OVERVIEW

1. Computational journey of our research group

2. Lattice Boltzmann Algorithms - Gordon Bell finalists 2005 (Earth Simulator)

3. QLA for NLS, KdV - 1D. : exactly soluble - solitons

4. QLA for MHD-Burgers : NMR Expt. Burgers Eq.

5. **QLA for GP/NLS for scalar BEC : quantum vortex - 2D and 3D Quantum Turbulence**

6. **QLA for Spin-2 BECs : non-Abelian vortices**

7. **QLA for Maxwell Equations**

• Mean field theory for scalar Bose-Einstein Condensates

collective s-wave bosonic interactions : $i\dfrac{\partial\psi(\mathbf{x},t)}{\partial t}=\left[-\nabla^2+V_{ext}+g\left|\psi(\mathbf{x},t)\right|^2\right]\psi(\mathbf{x},t)$

GP/NLS equation: Hamiltonian $\langle H\rangle=\int d^3x\left[\psi^*\left(-\nabla^2+V_{ext}\right)\psi+\frac{1}{2}g\left|\psi\right|^4\right]$ -non-integrable in 2D, 3D

Superfluid Equations (Madelung transformation)

→ $\dfrac{\partial\rho}{\partial t}+\nabla\bullet\left(\rho\mathbf{v}_{BEC}\right)=0$ *with mean density* $\rho=\psi\psi^*$

superfluid velocity $\Rightarrow$ $\rho\mathbf{v}_{BEC}=i\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right)$

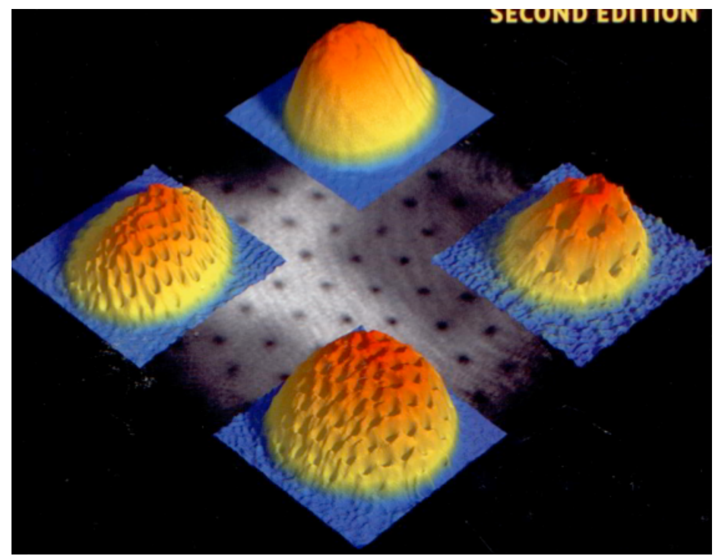
→ momentum eq: inviscid-Euler with singular "quantum pressure" term

$\psi(\mathbf{x},t)=\sqrt{\rho(\mathbf{x},t)}\,\exp\left[i\,n_w\,\varphi(\mathbf{x},t)\right]$ ➡ $\mathbf{v}_{BEC}=2\,n_W\nabla\varphi(\mathbf{x},t)$

if simply connected domain : $\oint_C d\vec{\ell}\bullet\mathbf{v}_{BEC}=0$ - no circulation

➡ multi-connected domain $\Rightarrow$ $\exists$ topological singularities: $\rho=0$ at core of (scalar) quantum vortices

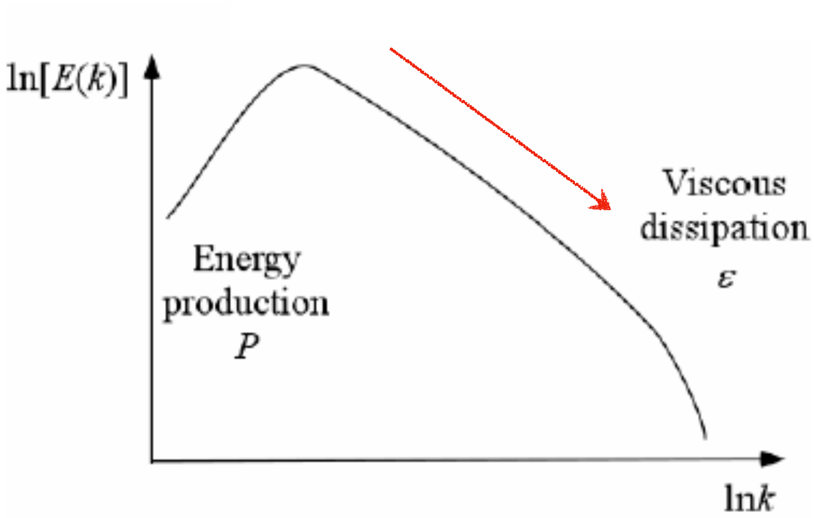
quantization of circulation $\oint d\vec{\ell}\bullet\mathbf{v}_{BEC}=n_w\kappa$



rotating BEC : steady state density exhibits a lattice of quantum vortices

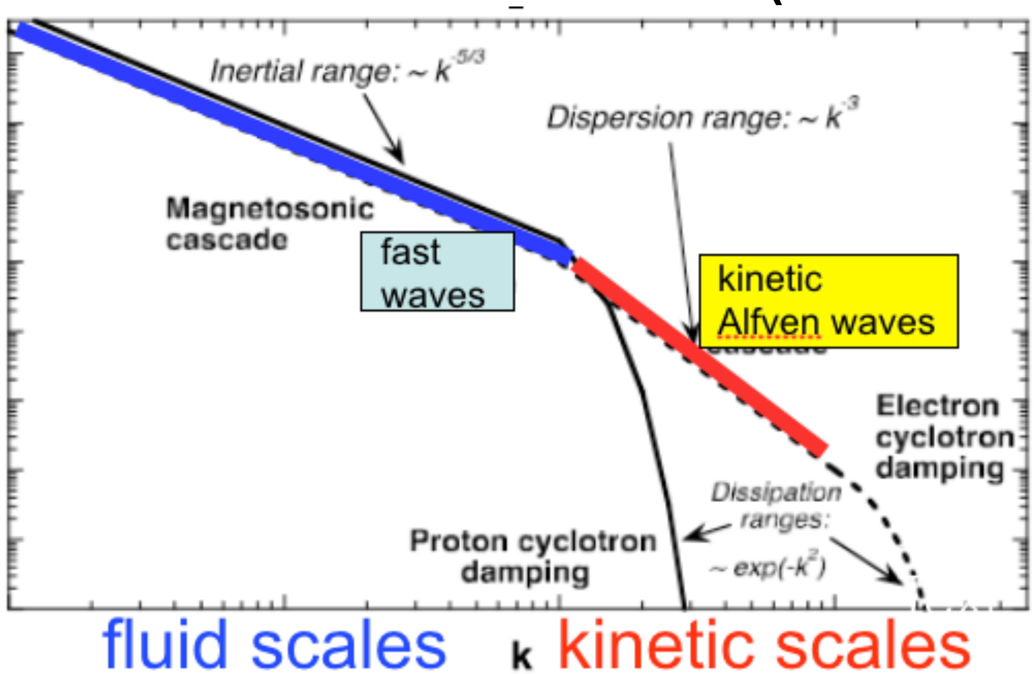
- *Feynman* : quantum turbulence -- tangled quantum vortices

→ *Classical 3D Fluid Turbulence* : incompressible , Kolmogorov $k^{-5/3}$ inertial range



- **Viscosity critical for vortex reconnection**

→ **Plasmas - dual cascades (solar wind magnetic energy spectrum)**



- DUAL CASCADES : multi-scale physics

[I] fluid scales : MHD cascade $k^{-5/3}$

[II] kinetic Alfven wave cascade k^{-3}

(ion kinetic to electron kinetic scales)

3D GP Eq. $i\frac{\partial\psi(\mathbf{x},t)}{\partial t}=\left[-\nabla^2+V_{ext}+g\left|\psi(\mathbf{x},t)\right|^2\right]\psi(\mathbf{x},t)$ **- 2 qubits/spatial node**

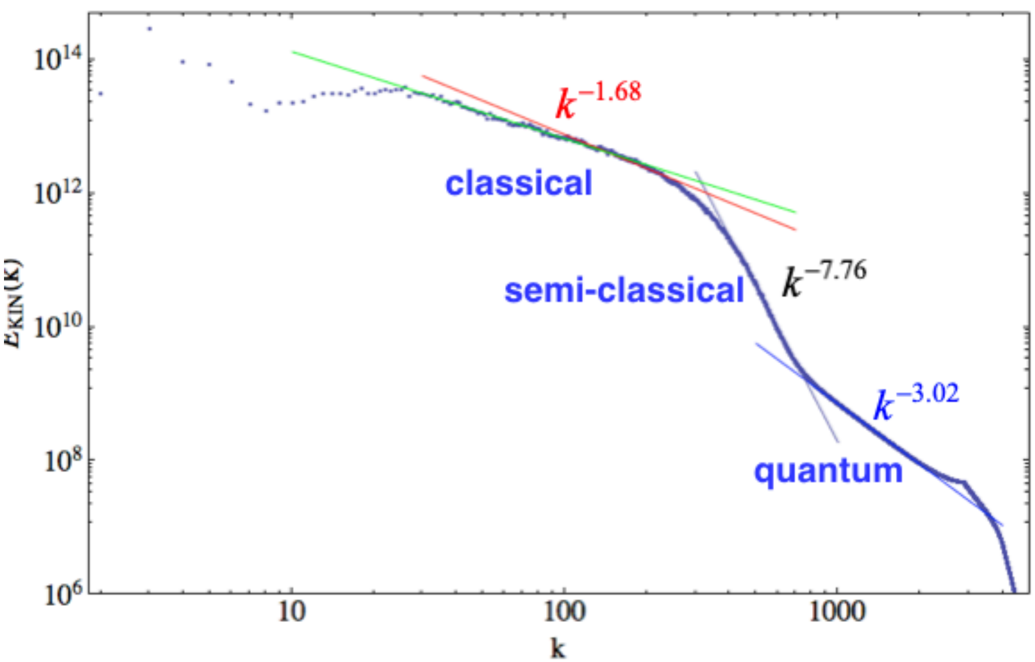
Mesoscopic Lattice Algorithm $\left|\phi(\mathbf{x},t+\Delta t)\right\rangle=\hat{U}[\mathbf{x},\Omega]\left|\phi(\mathbf{x},t)\right\rangle$,

where $\hat{U}[\mathbf{x},\Omega]\equiv\hat{I}_{x0}^2\,\hat{I}_{y1}^2\,\hat{I}_{z0}^2\,\hat{I}_{z1}^2\,\hat{I}_{y0}^2\,\hat{I}_{x1}^2$ *with* $\hat{I}_{x0}=\hat{S}_{-\Delta x,0}.\hat{C}_D.\hat{S}_{+\Delta x,0}.\hat{C}_D$

Unitary Collision Operator $C_D=\begin{pmatrix}\cos\theta(\mathbf{x}) & -i\sin\theta(\mathbf{x})\\ -i\sin\theta(\mathbf{x}) & \cos\theta(\mathbf{x})\end{pmatrix}$, $\theta(\mathbf{x})=\frac{\pi}{4}-\frac{1}{24}\Omega(\mathbf{x})$

CAP-2 (Einstein 2009, 12 288 cores; MRAP 2009)

Total Kinetic Energy Spectrum *grid* 5760^3



$$E_{TOT}=E_{KE}+E_{int}+E_{qu}=const.$$

$$E_{KE}=E_{incomp}+E_{comp}$$

- **Multi-Scale Physics**

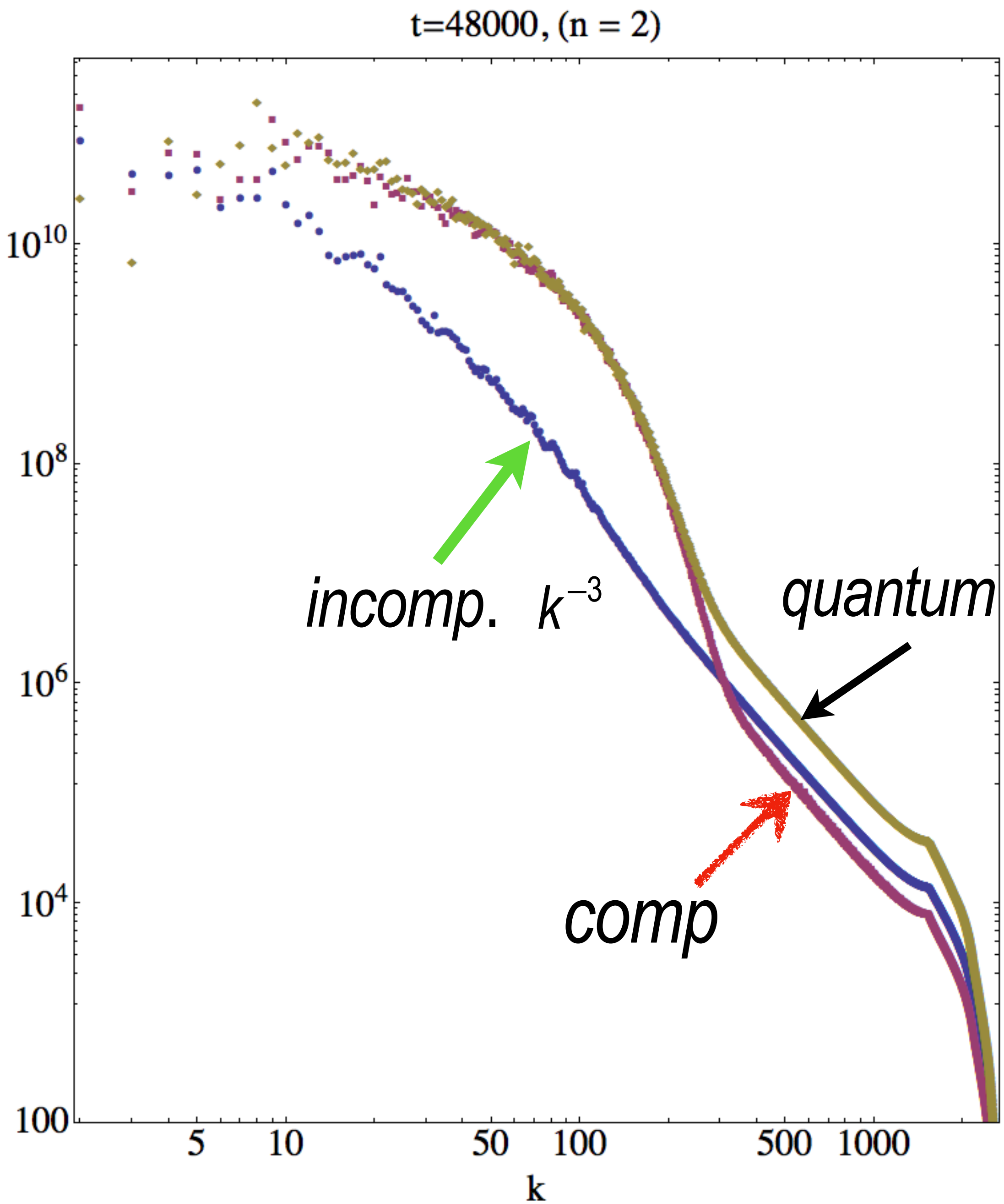
Triple Cascade Regions:

small k : Kolmogorov-like classical

medium k : semi-classical regime

large k : quantum vortex spectrum

- more detailed spectral analysis on 3072^3 grid



standard CFD simulations of quantum turbulence

$$\left[i-\gamma\left(\mathbf{x},t\right)\right]\frac{\partial\psi}{\partial t}=-\nabla^2\psi+\left[g\left|\psi\right|^2-\mu\right]\psi$$

dissipation for numerical stabilization

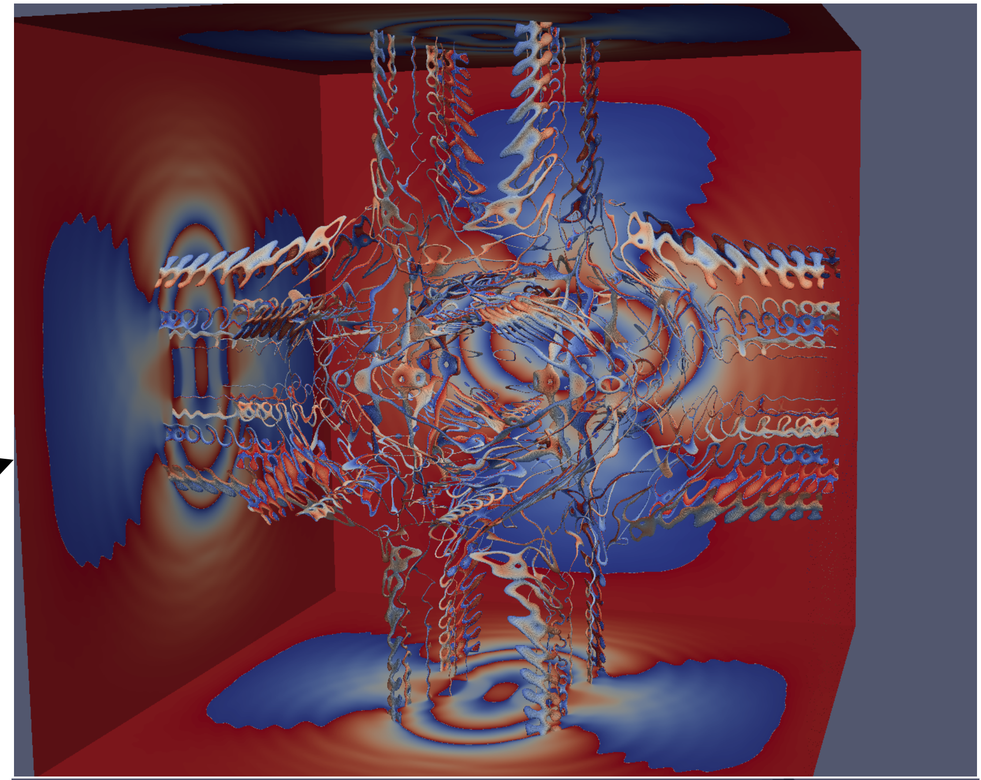
To recover energy conservation must inject appropriate energy ...

Quantum Line Vortex Core Isosurfaces (n=5)
- energetically more favorable to split into 5 non-deg vortices

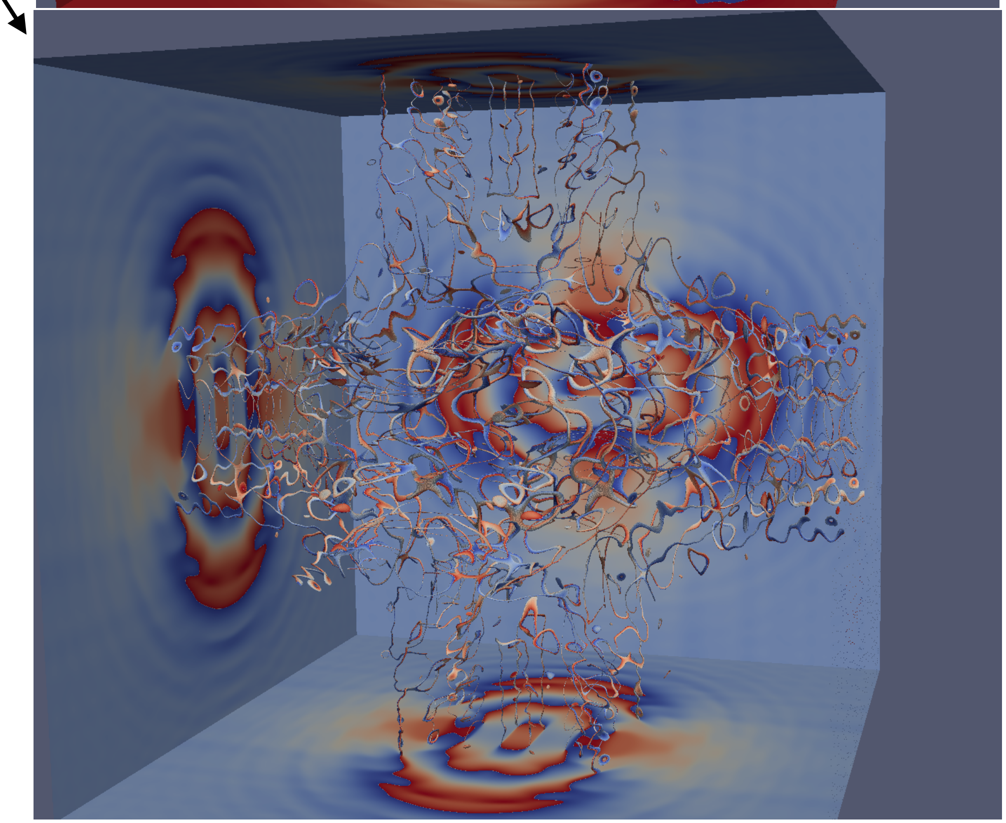
$phase: \phi = 0 - blue$

$\phi = 2\pi - red$

$t = 3000$

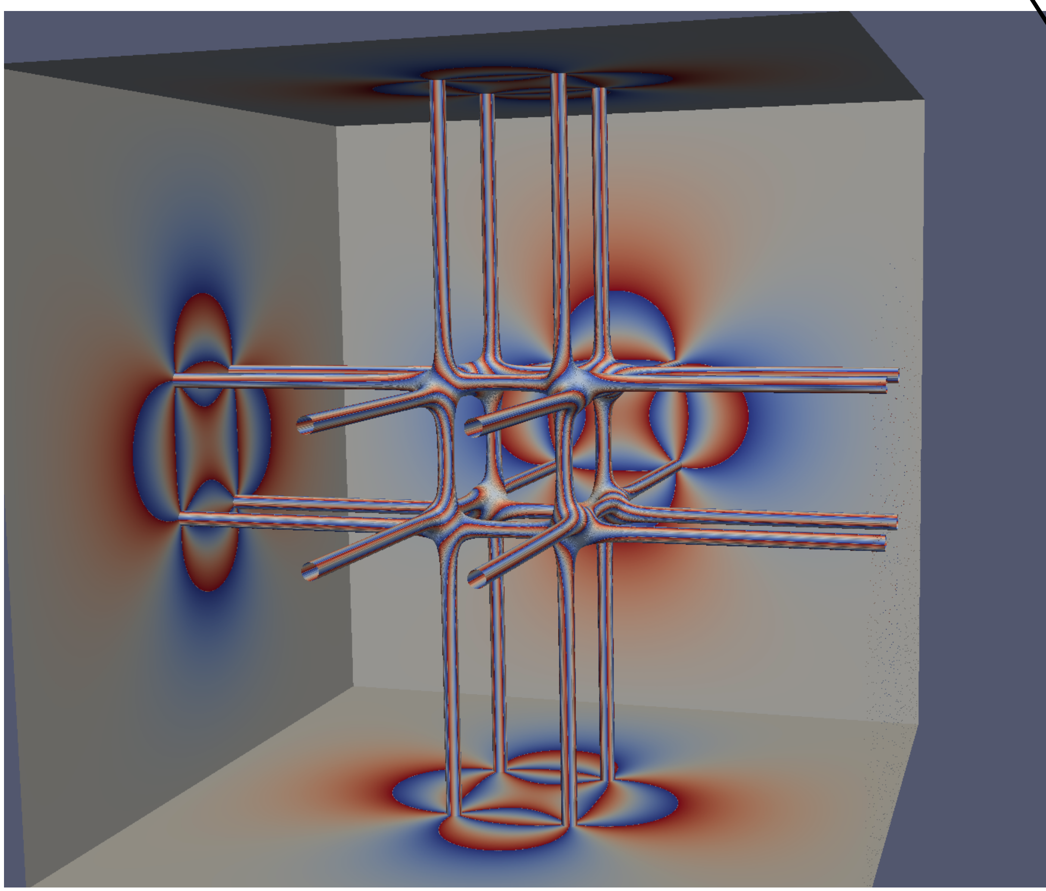


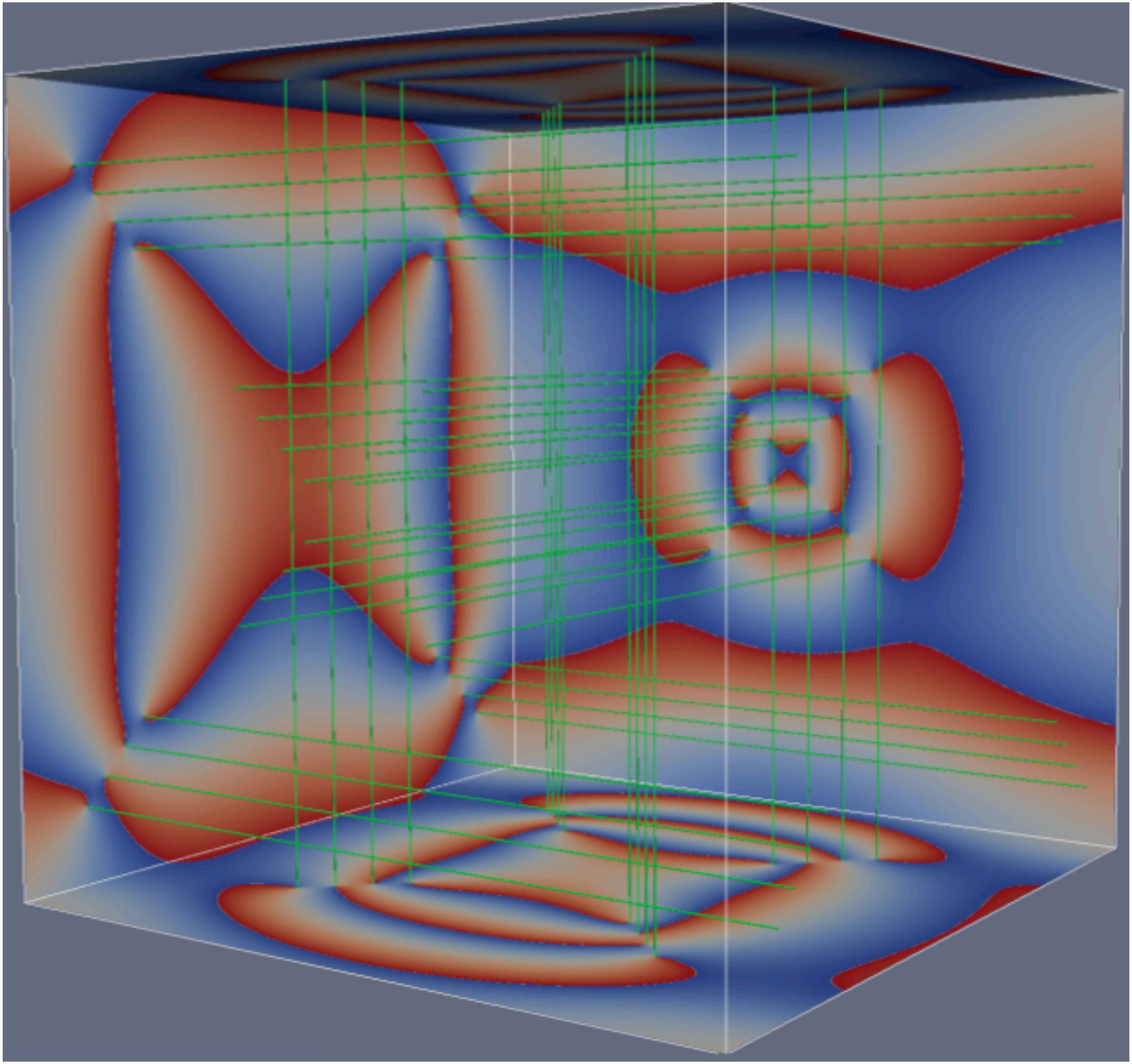
$t = 9000$



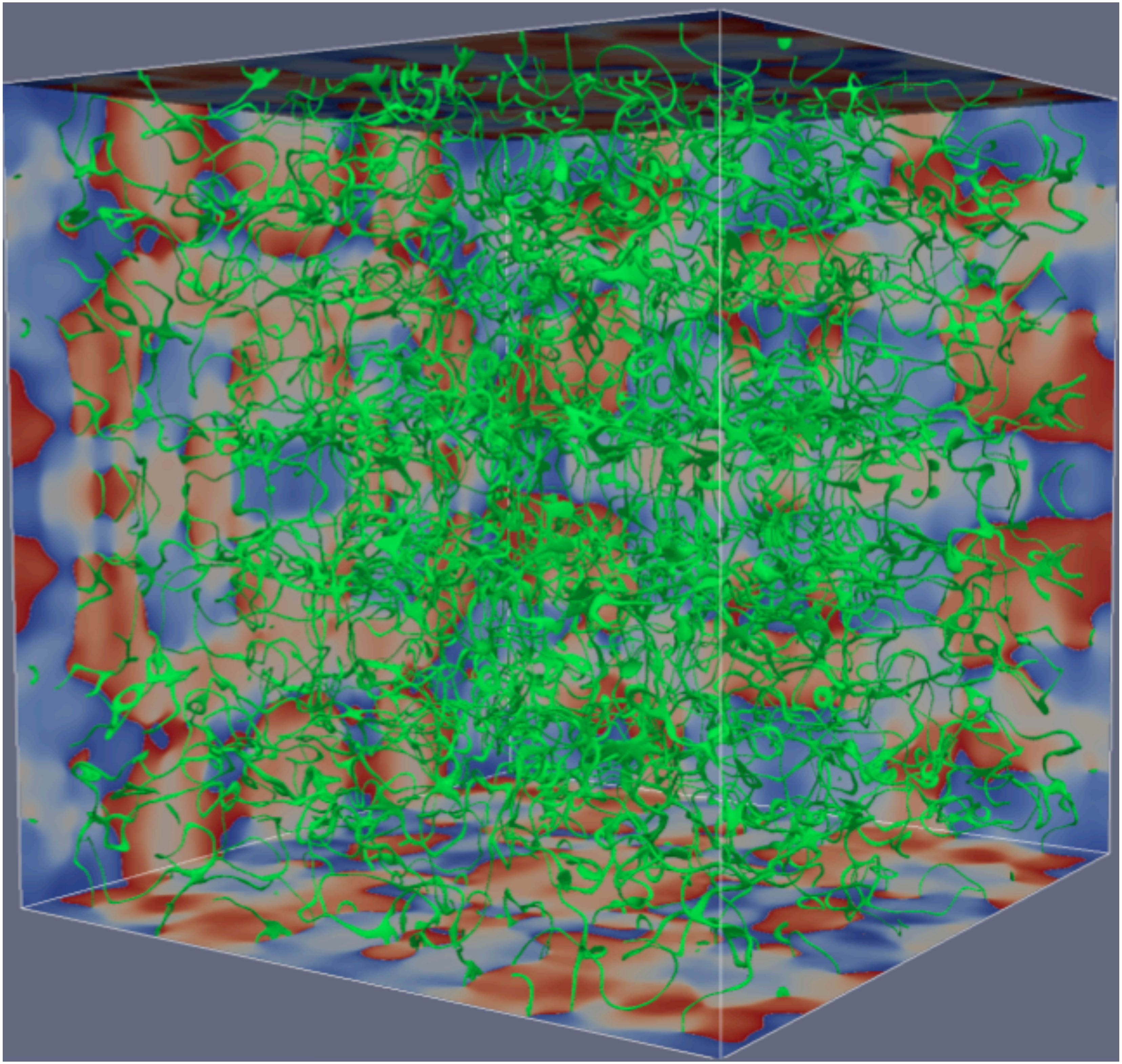
Core Isosurfaces of order parameter

$t = 0$

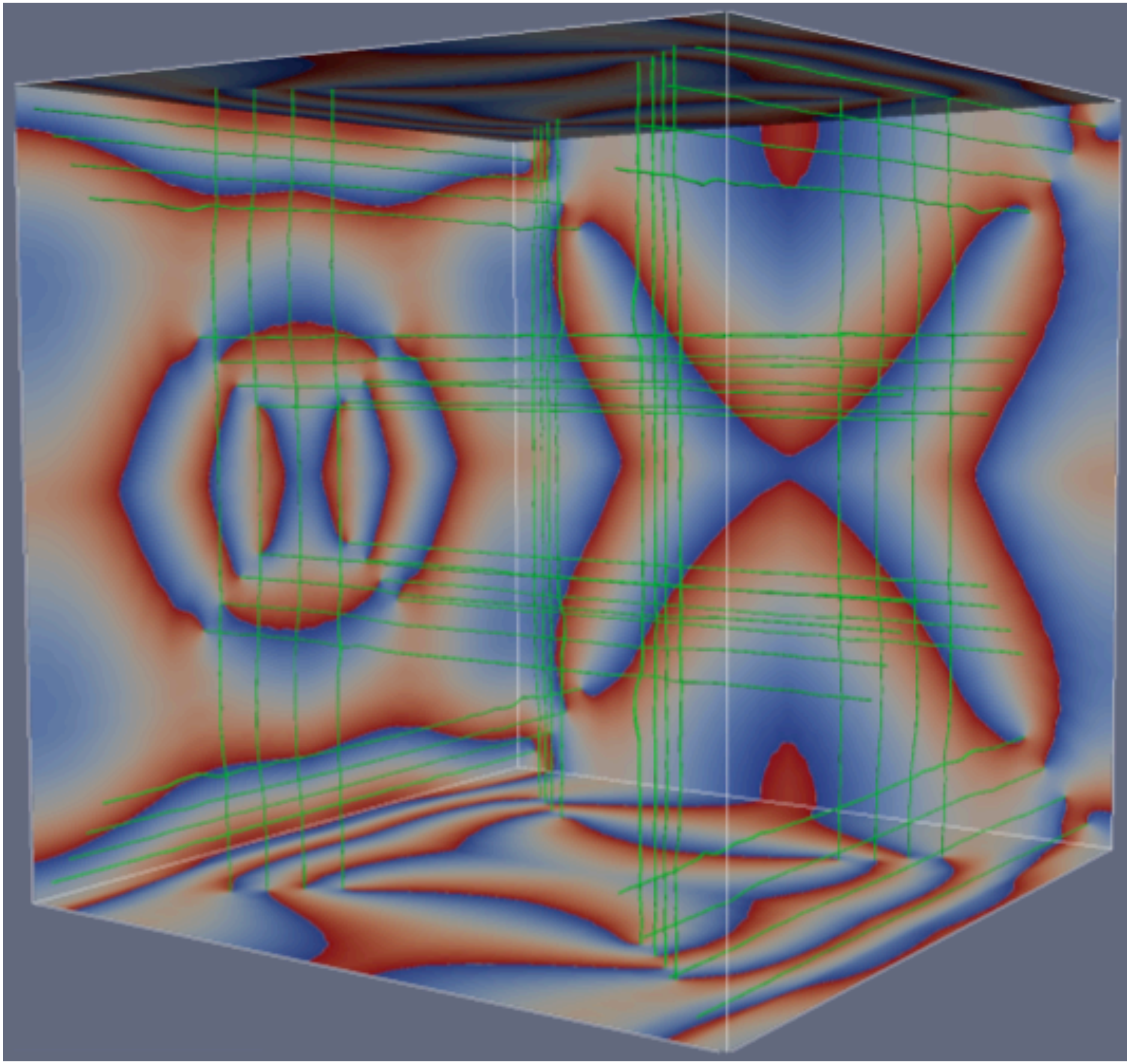




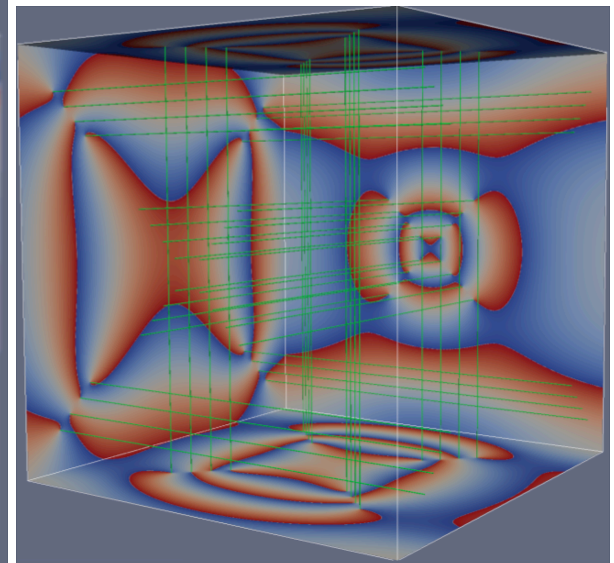
t = 0
3 x 16 line
Vortices



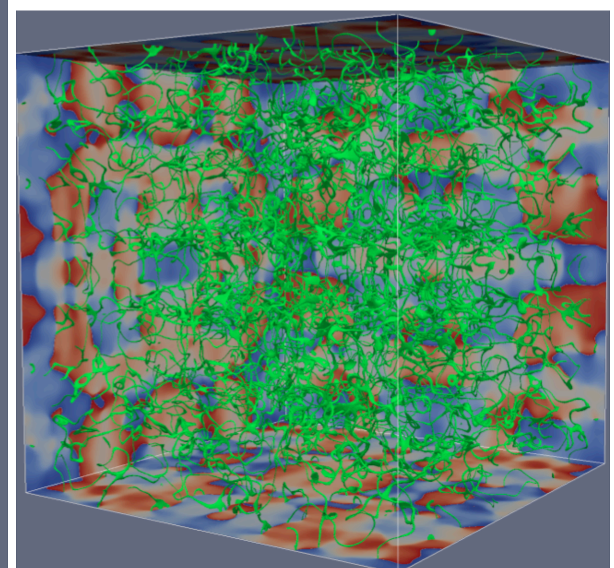
t = 84000
Vortex reconnection - quantum turbulence



t = 0

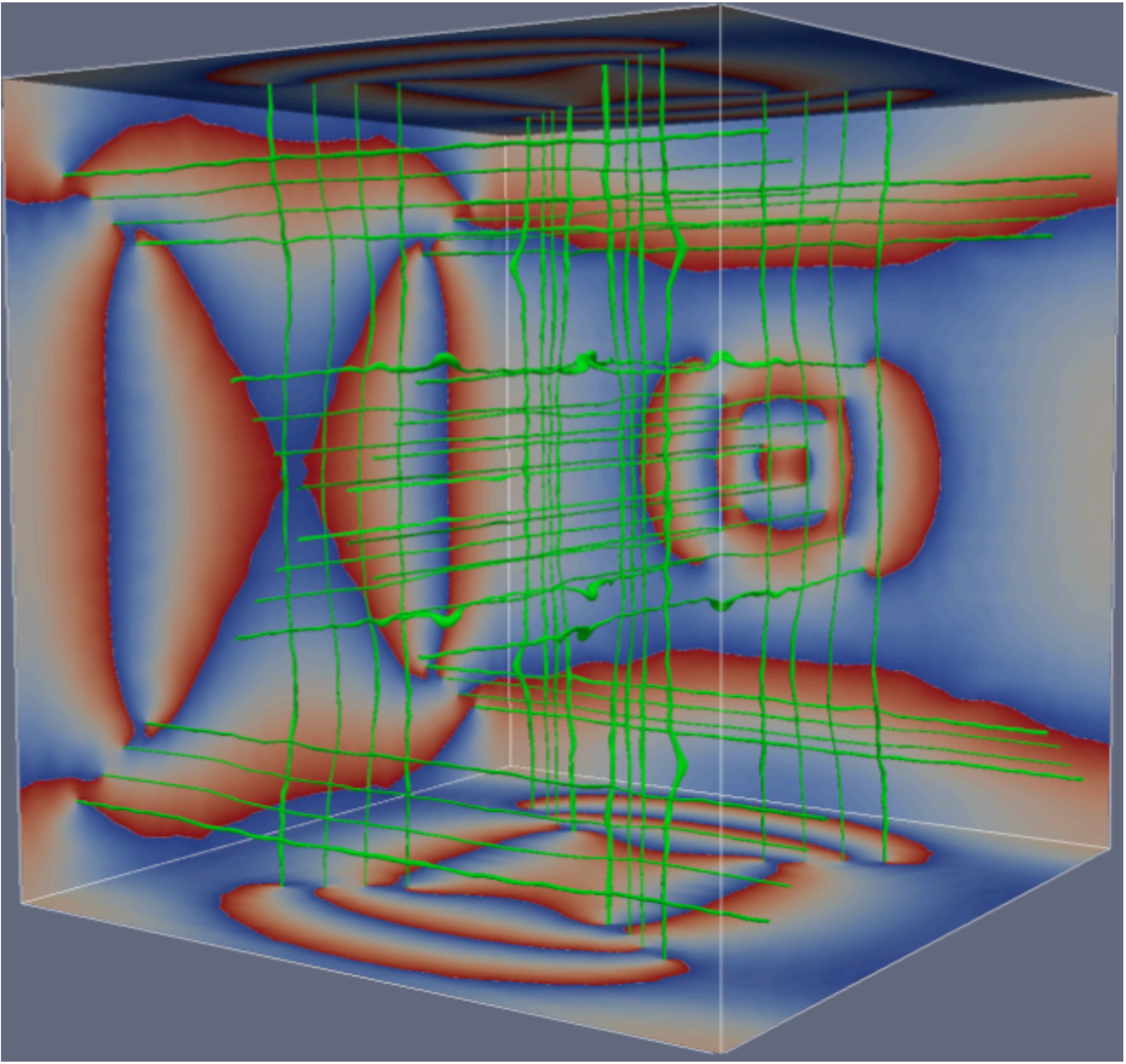


t = 84,000

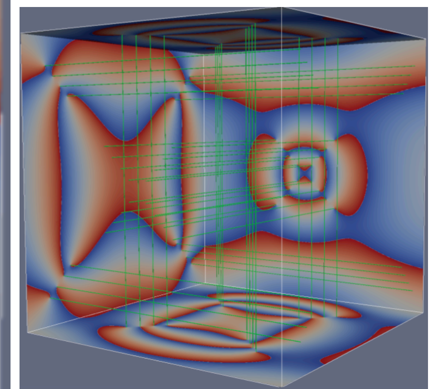


t = 115,000. Half-recurrence Time (line inversion)

C.f., Arnold cat map



$t = 0$



$t = 230{,}000$

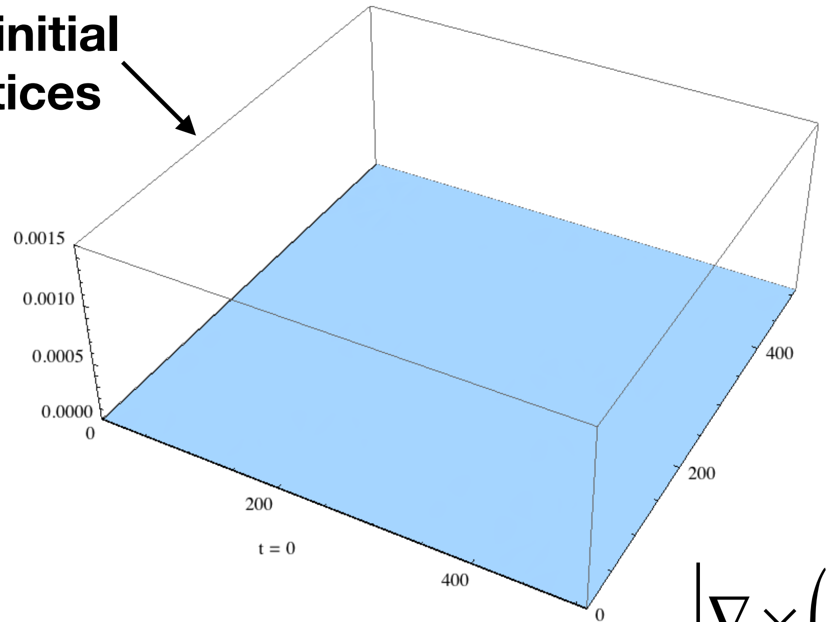
Is this Poincare recurrence
or
Fermi-Pasta-Ulam-Tsingou ?

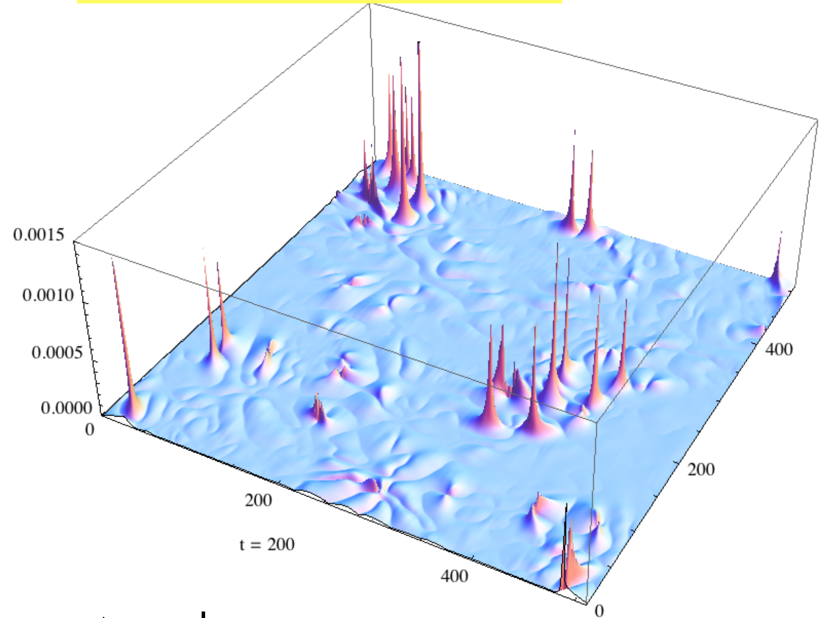
2D Quantum Turbulence (GP Eq.)

$t = 0: \ \rho = const., \ \phi - random$

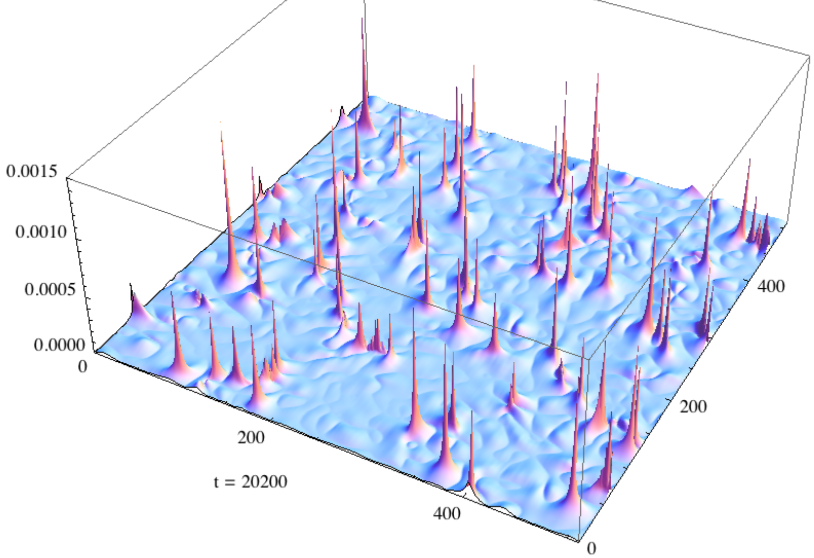
Poincare Recurrence
or
Fermi-Pasta-Ulam-Tsingou ?

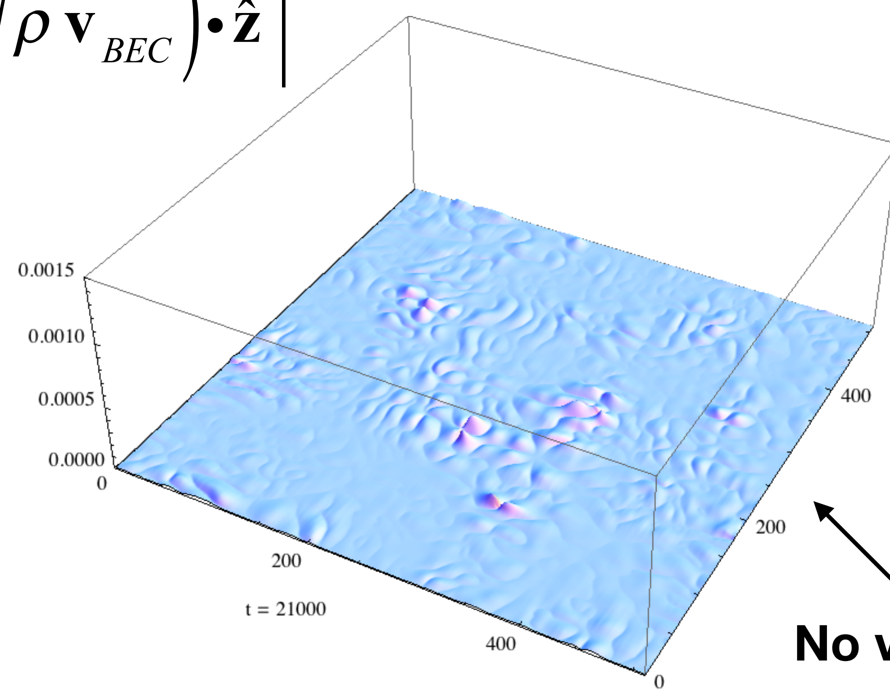
No initial vortices





$$\left| \nabla \times \left(\sqrt{\rho}\, \mathbf{v}_{BEC} \right) \bullet \hat{\mathbf{z}} \right|$$





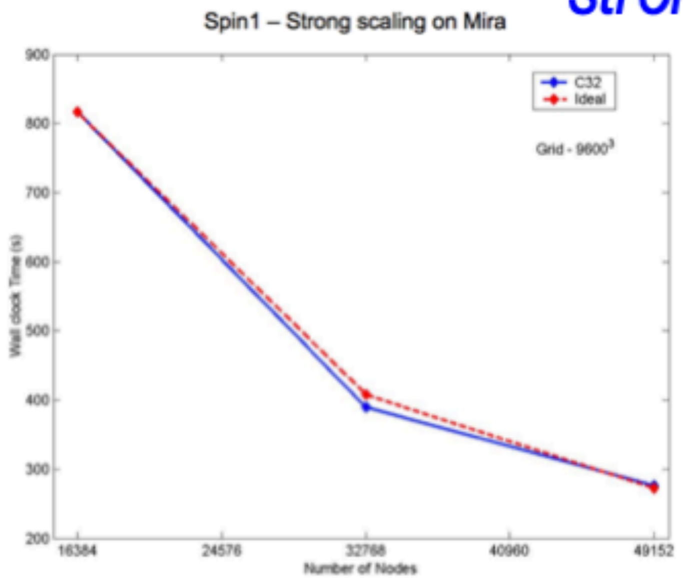
No vortices

• Mira (IBM BG/Q : 786,432 cores , 10 PF)

Table 2. Strong Scaling: Grid 9600^3 to the full 48 racks on IBM/BG Q (Mira)

#nodes	Ranks – Mode C32	Time (s)	Speed-up [ideal]
16 384	524 288	816.1	1.0 [1.0]
32 768	1 048 576	389.7	2.1 [2.0]
49 152	1 572 864	275.8	3.0 [3.0]

Fig. 14 Strong scaling of spinor BEC algorithm on Mira, using 2 MPI ranks/core with 16 cores/node (blue curve). The red dashed curve is ideal scaling up to the full 786 432 cores available on Mira. The multiple MPI ranks/core gives the benefit of multiple instruction issue by multiple threads on the BG/Q chip while running the code in pure MPI mode.



strong scaling to the full 786,432 cores

parallelization efficiency 98.6%

Table 3. Weak Scaling: Spin1- code on IBM/BlueGeneQ (Mira) : 50 iterations

(a) 1 MPI rank/core

Grid	Nodes	Ranks – Mode C16	Time (s)
800^3	32	512	323.4
1600^3	256	4096	323.4
3200^3	2048	32 768	323.7
6400^3	16 384	262 144	326.5

(b) 4 MPI ranks/core

Grid	Nodes	Ranks – Mode C64	Time (s)
800^3	32	2048	203.7
1600^3	256	16 384	197.1
3200^3	2048	131 072	197.8
6400^3	16 384	1 048 576	209.6

Weak scaling

Table 5. Strong Scaling , OpenMP Timings, Grid 5120^3 - to 32 racks

	4 racks	8 racks	16 racks	32 racks
Wallclock (s)	406.11	203.62	106.58	53.94
Cores	65 536	131 072	262 144	524 288
Parallel efficiency	100%	99.7%	95.3%	94.1%
L1 d-cache	88.64%	89.13%	89.11%	88.79%
DDR	2.59%	2.51%	2.56%	2.63%
GFlops/node	38.42	38.35	36.34	36.12
PFlops	0.156	0.311	0.595	1.174

On 32 racks (out of max 48) :

1.17 Peta Flops

parallel efficiency 94.1%

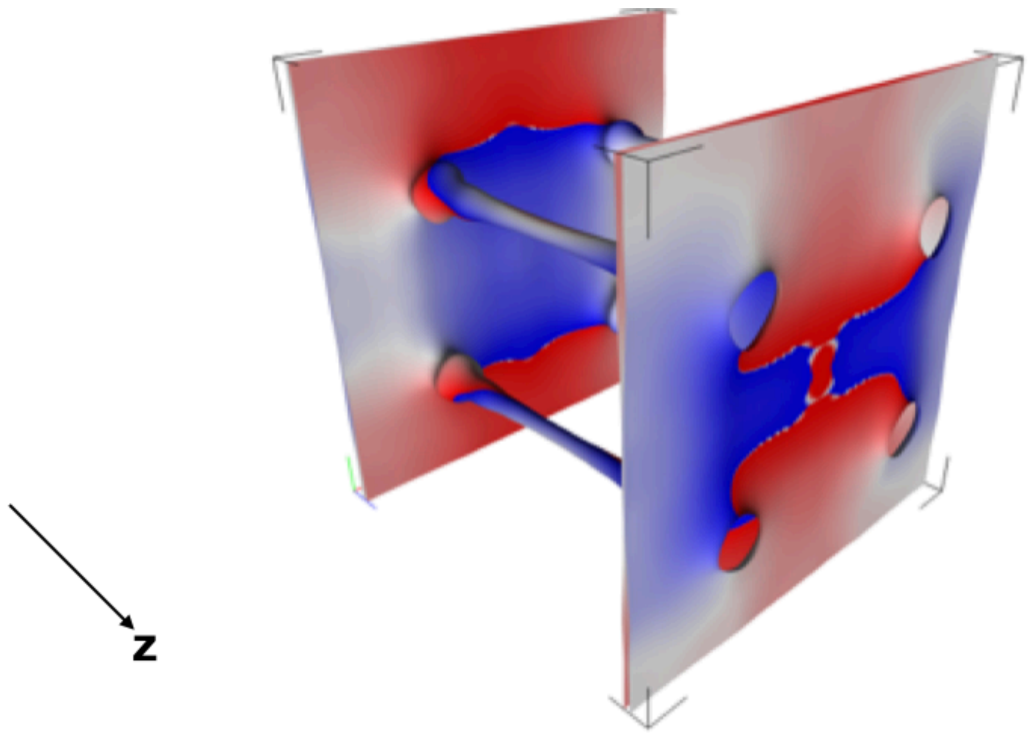
QLA for 3D Vortex Solitons in Hyperbolic Self-Defocusing Nonlinear Media

- Efremidis et. al. (2007) : stable vortex structures in 3D nonlinear optics

$$i\frac{\partial\psi}{\partial t}+\frac{1}{2}\nabla^2\psi-|\psi|^2\psi=0 \longrightarrow i\frac{\partial\psi}{\partial t}+\frac{1}{2}\left(\nabla_\perp^2\psi-\frac{\partial^2\psi}{\partial z^2}\right)-|\psi|^2\psi=0$$

elliptic *hyperbolic*

$$C_E\rightarrow\begin{pmatrix}\cos\theta_E & -i\sin\theta_E\\ -\sin\theta_E & \cos\theta_E\end{pmatrix} \quad \theta_E=\frac{\pi}{4}-\frac{1}{8}\left|\sqrt{2}\,\psi\right|^2 \longrightarrow \theta_H=\frac{3\pi}{4}-\frac{1}{8}\left|\sqrt{2}\,\psi\right|^2$$



#6. SPIN-2 BECs : Non-Abelian Vortices

Confine BEC in an optical trap

→ spin-2 BEC (^{87}Rb)

→ 5-coupled BECs

$$i\frac{\partial\psi_{\pm2}}{\partial t}=\left[-\nabla^2+c_0\,N\pm2c_1F_z-\mu\right]\psi_{\pm2}+c_1F_{\mp}\psi_{\pm1}+c_2A\psi^*_{\mp2}$$

$$i\frac{\partial\psi_{\pm1}}{\partial t}=\left[-\nabla^2+c_0\,N\pm c_1F_z-\mu\right]\psi_{\pm1}+c_1\left(\frac{\sqrt{6}}{2}F_{\mp}\psi_0+F_{\pm}\psi_{\pm2}\right)-c_2A\psi^*_{\mp1}$$

$$i\frac{\partial\psi_0}{\partial t}=\left[-\nabla^2+c_0\,N-\mu\right]\psi_{\pm2}+\frac{\sqrt{6}}{2}c_1\left(F_+\psi_1+F_-\psi_{-1}\right)+c_2A\psi^*_0$$

BEC density $N(\mathbf{x},t)=\sum_{j=-2}^{2}\left|\psi_j(\mathbf{x},t)\right|^2$

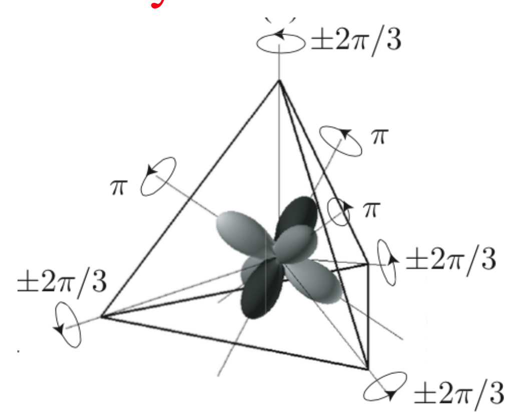
mean spin expectation $\mathbf{F}(\mathbf{x},t)=\sum_{m,n=-3}^{3}\psi^*_m(\mathbf{x},t)\,\mathbf{f}_{mn}\psi_{n(\mathbf{x},t)}$, $F_{\pm}=F_x\pm iF_y$

spin-singlet pair $A=\left(2\psi_2\psi_{-2}-2\psi_1\psi_{-1}+\psi_0^2\right)$

order parameter manifold of the cyclic phase : tetrahedral symmetry

-- non-Abelian vortices (homotopy group theory)

- **reconnection of different vortex classes is restricted**
- **energy spectrum of non-Abelian quantum turbulence?**



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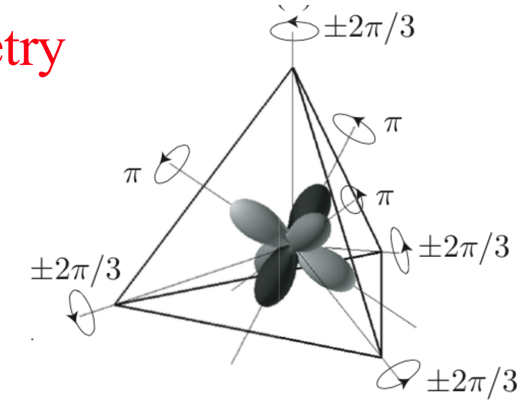


QLA for spin-2 BECs (Yepez....) : 10 qubits/node for 5-spinor $\vec{\psi}$

$$i\frac{\partial\vec{\psi}}{\partial t}=\left[\hat{H}_{diag}+\hat{H}_{non}\right]\vec{\psi} \quad , \quad \hat{H}_{non}\vec{\psi}=c_1\mathbf{F}\cdot\mathbf{f}\vec{\psi}+c_2\hat{A}\vec{\psi}$$

Evolution : $\vec{\psi}\left(t+\delta t\right)=\hat{U}_{non}\hat{U}_{diag}\vec{\psi}\left(t\right)$

can treat as in scalar BEC

$$\hat{U}_{non}=\exp\left[-ic_1\hat{N}_2F\delta t\right]\exp\left[-ic_2\hat{N}_AA\delta t\right]$$

$-$can we approximate these expressions by tridempotent operators

- $\hat{N}_{tri}^3=\hat{N}_{tri}$

$\exp\left[i\hat{N}_{tri}\right]$ – *can be summed to all orders*

$[c.f., \exp\left[i\theta\mathbf{n}\cdot\vec{\sigma}\right]=\hat{I}\cos\theta+i\left(\mathbf{n}\cdot\vec{\sigma}\right)\sin\theta]$

Current Research: how to generate initial conditions of non-Abelian line vortices in 3D spin-2 BECs ?

#7. QLA for Maxwell Equations

Uhlenbeck (1931), Oppenheimer (1931) : Dirac ⟷ Maxwell

$$\nabla \bullet \mathbf{D}(\mathbf{x},t) = \rho(\mathbf{x},t) \quad , \quad \nabla \bullet \mathbf{B}(\mathbf{x},t) = 0$$

$$\nabla \times \mathbf{H}(\mathbf{x},t) = \mathbf{J}(\mathbf{x},t) + \frac{\partial \mathbf{D}(\mathbf{x},t)}{\partial t} \ , \ \nabla \times \mathbf{E}(\mathbf{x},t) = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\mathbf{D}(\mathbf{x},t) = \varepsilon(\mathbf{x},t)\,\mathbf{E}(\mathbf{x},t)$$

$$\mathbf{B}(\mathbf{x},t) = \mu(\mathbf{x},t)\,\mathbf{H}(\mathbf{x},t)$$

Riemann-Silberstein vector $\mathbf{F}^{\pm} = \frac{1}{\sqrt{2}}\left[\sqrt{\varepsilon}\,\mathbf{E} \pm i\frac{\mathbf{B}}{\sqrt{\mu}}\right]$

Maxwell Eqs.
(Khan 2002, 2005)

$$i\frac{\partial \mathbf{F}^{\pm}}{\partial t} = \pm v \nabla \times \mathbf{F}^{\pm} \pm \frac{1}{2}\nabla v \times \mathbf{F}^{\pm} \pm \frac{v}{2h}\nabla h \times \mathbf{F}^{\mp} + \frac{i}{2}\left(\frac{\partial \ln v}{\partial t}\mathbf{F}^{\pm} + \frac{\partial \ln h}{\partial t}\mathbf{F}^{\mp}\right) - i\sqrt{\frac{vh}{2}}\,\mathbf{J}$$

$$\nabla \bullet \mathbf{F}^{\pm} = \frac{1}{2v}\nabla v \bullet \mathbf{F}^{\pm} + \frac{1}{2h}\nabla h \bullet \mathbf{F}^{\mp} + \sqrt{\frac{vh}{2}}\,\rho$$

$$v(\mathbf{x},t) = \frac{1}{\sqrt{\varepsilon\mu}} \ , \ h(\mathbf{x},t) = \sqrt{\frac{\mu}{\varepsilon}}$$

- **coupling of polarizations through derivatives on h(x,t)**

• Maxwell into Dirac Form

8-component spinors

$$\Psi^{\pm}=\begin{pmatrix}-F_x^{\pm}\pm iF_y^{\pm}\\ F_z^{\pm}\\ F_z^{\pm}\\ F_x^{\pm}\pm iF_y^{\pm}\end{pmatrix}\quad,\quad W^{\pm}=\frac{1}{\sqrt{2\varepsilon}}\begin{pmatrix}-J_x\pm iJ_y\\ J_z-v\rho\\ J_z+v\rho\\ J_x\pm iJ_y\end{pmatrix}$$

$$v(\mathbf{x},t)=\frac{1}{\sqrt{\varepsilon\mu}}\ ,\ h(\mathbf{x},t)=\sqrt{\frac{\mu}{\varepsilon}}$$

$$\sigma_x=\begin{pmatrix}0&1\\1&0\end{pmatrix}\ ,\ \sigma_y=\begin{pmatrix}0&-i\\i&0\end{pmatrix}\ ,\ \sigma_z=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

$$\mathbf{M}=\vec{\sigma}\otimes I_2 \qquad M_z=\sigma_z\otimes I_2$$

$$\vec{\alpha}=\begin{pmatrix}0&\vec{\sigma}\\ \vec{\sigma}&0\end{pmatrix} \qquad \vec{\Sigma}=\begin{pmatrix}\vec{\sigma}&0\\0&\vec{\sigma}\end{pmatrix}$$

$$\frac{\partial}{\partial t}\begin{pmatrix}\Psi^+\\ \Psi^-\end{pmatrix}-\frac{1}{2}\frac{\partial\ln v}{\partial t}\begin{pmatrix}\Psi^+\\ \Psi^-\end{pmatrix}+\frac{iM_z\alpha_y}{2}\frac{\partial\ln h}{\partial t}\begin{pmatrix}\Psi^-\\ \Psi^-\end{pmatrix}$$

$$=-v\begin{pmatrix}\mathbf{M}\bullet\nabla+\vec{\Sigma}\bullet\frac{\nabla v}{2v} & -iM_z\vec{\Sigma}\bullet\frac{\nabla h}{h}\alpha_y\\ -iM_z\vec{\Sigma}^*\bullet\frac{\nabla h}{h}\alpha_y & \mathbf{M}^*\bullet\nabla+\vec{\Sigma}^*\bullet\frac{\nabla v}{2v}\end{pmatrix}\begin{pmatrix}\Psi^+\\ \Psi^-\end{pmatrix}-\begin{pmatrix}W^+\\ W^-\end{pmatrix}$$

Homogeneous Media

$$\frac{\partial\Psi^+}{\partial t}=-v\,\mathbf{M}\bullet\nabla\Psi^+-W^+$$

Recovery of Maxwell Eqs.

$$\Psi^+=\begin{pmatrix}-F_x^++iF_y^+\\ F_z^+\\ F_z^+\\ F_x^++iF_y^+\end{pmatrix}\quad,\quad \mathbf{F}^+=\frac{1}{\sqrt{2}}\left[\sqrt{\varepsilon}\,\mathbf{E}+i\frac{\mathbf{B}}{\sqrt{\mu}}\right]$$

(a) sum 1st and 4th rows $\rightarrow \frac{\partial}{\partial t}\left[\mathrm{E}_y,B_y\right]$

(b) difference of 1st and 4th rows $\rightarrow \frac{\partial}{\partial t}\left[\mathrm{E}_x,B_x\right]$

(c) sum of 2nd and 3rd rows $\rightarrow \frac{\partial}{\partial t}\left[\mathrm{E}_z,B_z\right]$

(d) diff. of 2nd and 3 rows $\rightarrow \nabla\bullet\left[\mathbf{E},\mathbf{B}\right]$

$$\Psi^+ = \begin{pmatrix} -F_x^+ + iF_y^+ \\ F_z^+ \\ F_z^+ \\ F_x^+ + iF_y^+ \end{pmatrix} \equiv \begin{pmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{pmatrix}$$

Maxwell Eqs.

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

Dirac for massless particle

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

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

2D Maxwell : vacuum

4 qubits/node

$$C_X = \begin{pmatrix} \cos\theta & 0 & \sin\theta & 0 \\ 0 & \cos\theta & 0 & \sin\theta \\ -\sin\theta & 0 & \cos\theta & 0 \\ 0 & -\sin\theta & 0 & \cos\theta \end{pmatrix}, \quad C_Y = \begin{pmatrix} \cos\theta & 0 & i\sin\theta & 0 \\ 0 & \cos\theta & 0 & i\sin\theta \\ i\sin\theta & 0 & \cos\theta & 0 \\ 0 & i\sin\theta & 0 & \cos\theta \end{pmatrix}$$

$$S_{\pm X}^{01}\begin{pmatrix} q_0(x,y,t) \\ q_1(x,y,t) \\ q_2(x,y,t) \\ q_3(x,y,t) \end{pmatrix} = \begin{pmatrix} q_0(x\pm 1,y,t) \\ q_1(x\pm 1,y,t) \\ q_2(x,y,t) \\ q_3(x,y,t) \end{pmatrix} \qquad S_{\pm X}^{23}\begin{pmatrix} q_0(x,y,t) \\ q_1(x,y,t) \\ q_2(x,y,t) \\ q_3(x,y,t) \end{pmatrix} = \begin{pmatrix} q_0(x,y,t) \\ q_1(x,y,t) \\ q_2(x\pm 1,y,t) \\ q_3(x\pm 1,y,t) \end{pmatrix}$$

provided $\theta = \frac{\varepsilon}{4}$

QLA for Maxwell to 2nd order

$$U_X = S_{-X}^{01} C_X S_{+X}^{01} C_X^{\dagger} . S_{+X}^{23} C_X S_{-X}^{23} C_X^{\dagger}$$

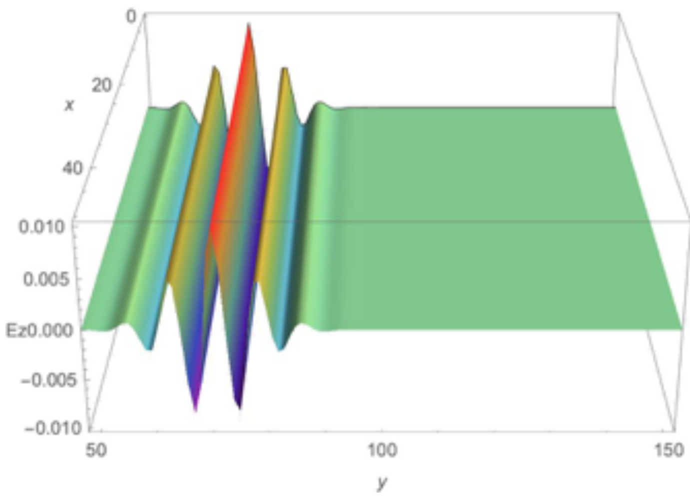
$$U_X^{adj} = S_{+X}^{01} C_X^{\dagger} S_{-X}^{01} C_X . S_{-X}^{34} C_X^{\dagger} S_{+X}^{34} C_X$$

$$U_Y = S_{-Y}^{23} C_Y S_{+Y}^{23} C_Y^{\dagger} . S_{+Y}^{01} C_Y S_{-Y}^{01} C_Y^{\dagger}$$

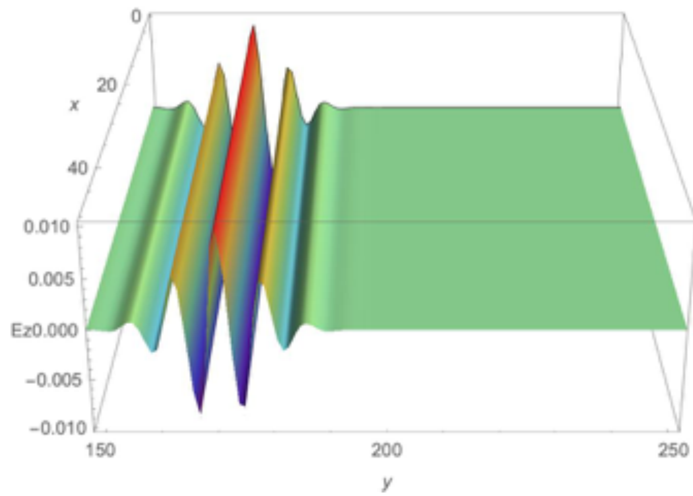
$$U_Y^{adj} = S_{+Y}^{23} C_Y^{\dagger} S_{-Y}^{23} C_Y . S_{+Y}^{01} C_Y^{\dagger} S_{-Y}^{01} C_Y$$

$$\begin{pmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{pmatrix}_{t+\delta t} = U_Y^{adj} U_Y U_X^{adj} U_X \begin{pmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{pmatrix}_t$$

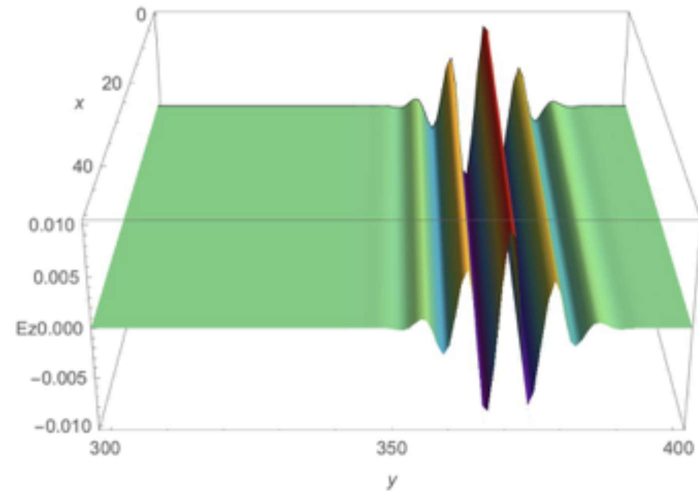
E_z



t = 0



t = 1k



t = 30k + periodicity

1D normal incidence onto dielectric interface

$$E_z \, , B_x \, , n(y)$$

8-spinor

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

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

$$\begin{pmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \\ q_4 \\ q_5 \\ q_6 \\ q_7 \end{pmatrix} = \begin{pmatrix} -F_x^+ + iF_y^+ \\ F_z^+ \\ F_z^+ \\ F_x^+ + iF_y^+ \\ -F_x^- - iF_y^- \\ F_z^- \\ F_z^- \\ F_x^- - iF_y^- \end{pmatrix} \quad , \quad with \;\; \mathbf{F}^{\pm} = \frac{1}{\sqrt{2}}\left[\sqrt{\varepsilon}\,\mathbf{E} \pm i\frac{\mathbf{B}}{\sqrt{\mu}}\right]$$

$$C_Y(\theta) = \begin{pmatrix} \cos\theta & 0 & i\sin\theta & 0 & 0 & 0 & 0 & 0 \\ 0 & \cos\theta & 0 & i\sin\theta & 0 & 0 & 0 & 0 \\ i\sin\theta & 0 & \cos\theta & 0 & 0 & 0 & 0 & 0 \\ 0 & i\sin\theta & 0 & \cos\theta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos\theta & 0 & -i\sin\theta & 0 \\ 0 & 0 & 0 & 0 & 0 & \cos\theta & 0 & -i\sin\theta \\ 0 & 0 & 0 & 0 & -i\sin\theta & 0 & \cos\theta & 0 \\ 0 & 0 & 0 & 0 & 0 & -i\sin\theta & 0 & \cos\theta \end{pmatrix} \qquad \theta = \frac{\varepsilon}{4n(y)}$$

$$V_{22} = \begin{pmatrix} \cos\alpha & 0 & 0 & 0 & 0 & 0 & -\sin\alpha & 0 \\ 0 & \cos\alpha & 0 & 0 & 0 & 0 & 0 & -\sin\alpha \\ 0 & 0 & \cos\alpha & 0 & \sin\alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & \cos\alpha & 0 & \sin\alpha & 0 & 0 \\ 0 & 0 & -\sin\alpha & 0 & \cos\alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & -\sin\alpha & 0 & \cos\alpha & 0 & 0 \\ \sin\alpha & 0 & 0 & 0 & 0 & 0 & \cos\alpha & 0 \\ 0 & \sin\alpha & 0 & 0 & 0 & 0 & 0 & \cos\alpha \end{pmatrix}$$

$$V_{11} = \begin{pmatrix} \cos\alpha & \sin\alpha & 0 & 0 & 0 & 0 & 0 & 0 \\ -\sin\alpha & \cos\alpha & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos\alpha & \sin\alpha & 0 & 0 & 0 & 0 \\ 0 & 0 & -\sin\alpha & \cos\alpha & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos\alpha & -\sin\alpha & 0 & 0 \\ 0 & 0 & 0 & 0 & \sin\alpha & \cos\alpha & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cos\alpha & -\sin\alpha \\ 0 & 0 & 0 & 0 & 0 & 0 & \sin\alpha & \cos\alpha \end{pmatrix} \qquad = -i\varepsilon^2\frac{n'(y)}{2n^2(y)}$$

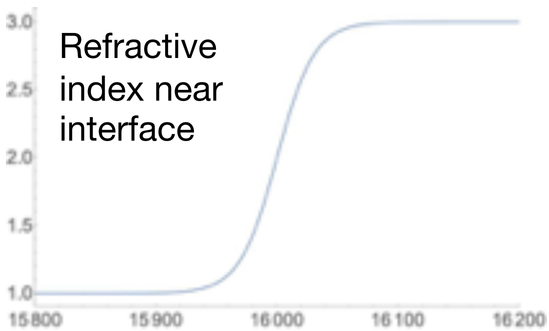
$$U_{YY} = S_{-Y}^{23,67}\, C_Y(\theta) S_{+Y}^{23,67}\, C_Y^{\dagger}(\theta) . S_{+Y}^{01,45}\, C_Y(\theta) S_{-X}^{01,45}\, C_Y^{\dagger}(\theta)$$

$$U_{YY}^{adj} = S_{+Y}^{23,67}\, C_Y^{\dagger}(\theta) S_{-Y}^{23,67}\, C_Y(\theta) . S_{+Y}^{01,45}\, C_Y^{\dagger}(\theta) S_{-Y}^{01,45}\, C_Y(\theta)$$

QLA to 2nd order:

$$\vec{\mathbf{q}}(t+\delta t) = V_{11}\, V_{22}\, U_{YY}^{adj}\, U_{YY}\, \vec{\mathbf{q}}(t)$$

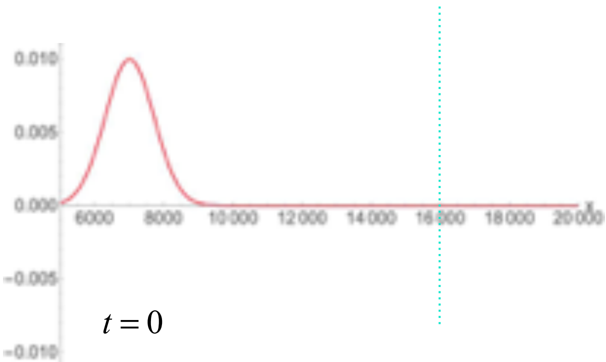
1D normal incidence onto dielectric interface

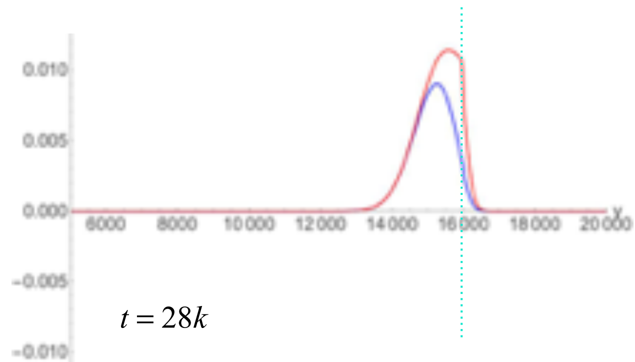


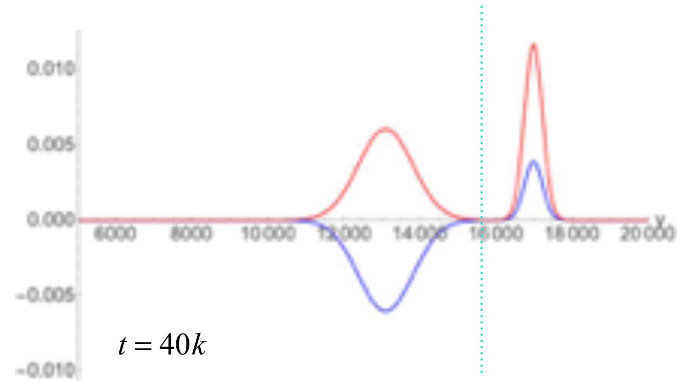
Medium 1: $0 < L < 16000$, Medium 2 : $16000 < L < 32000$

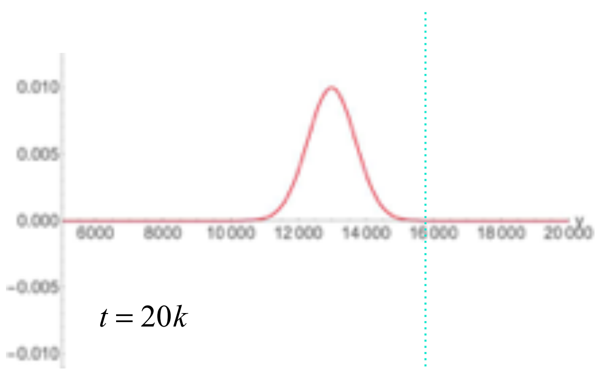
No boundary conditions are applied at interface

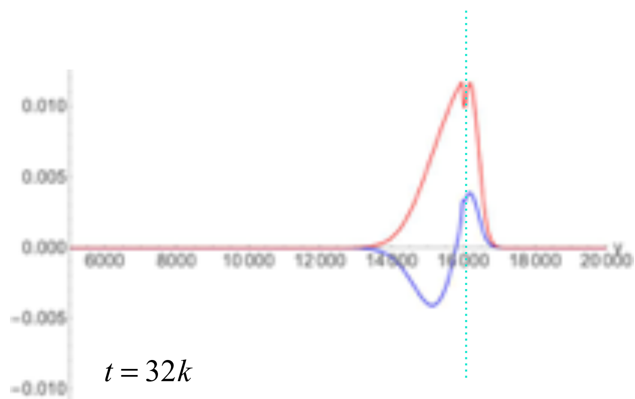
Case 1 : $n_1 = 1 \rightarrow n_2 = 3$ $E_z(blue)$, $B_x(red)$

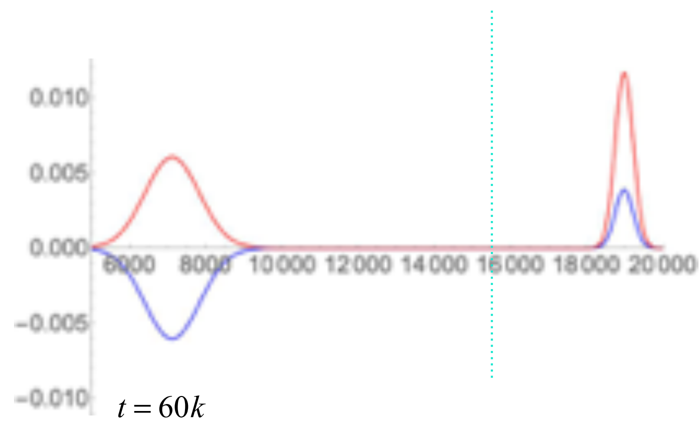






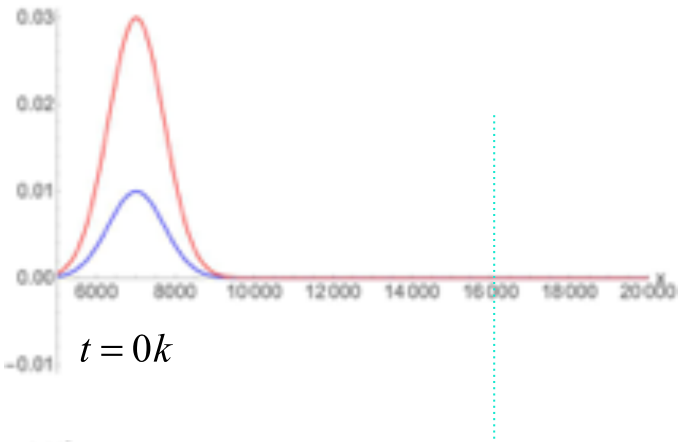


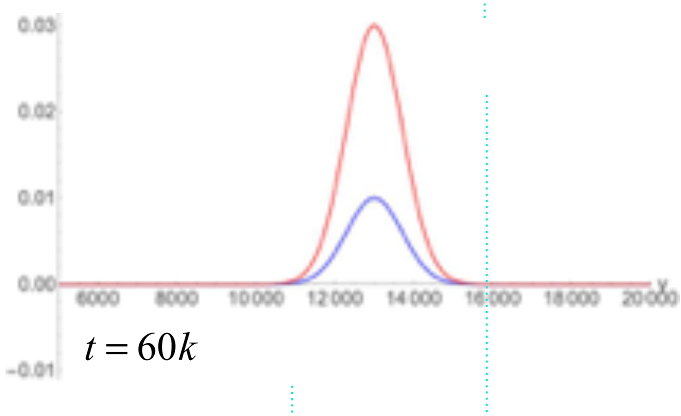


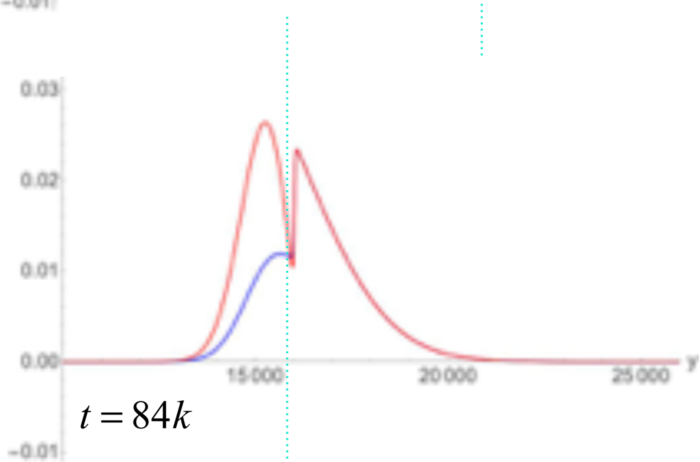


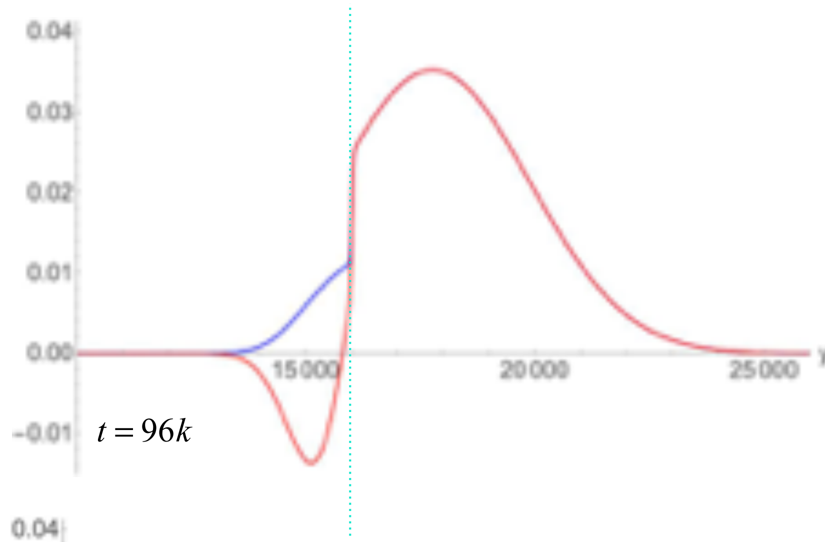
$$Physics: \frac{B_x}{E_z} = n_{med} \text{ , } E_z \text{ phase change , pulse speed \& width in } n_2 \text{ reduced by } \frac{n_1}{n_2}$$

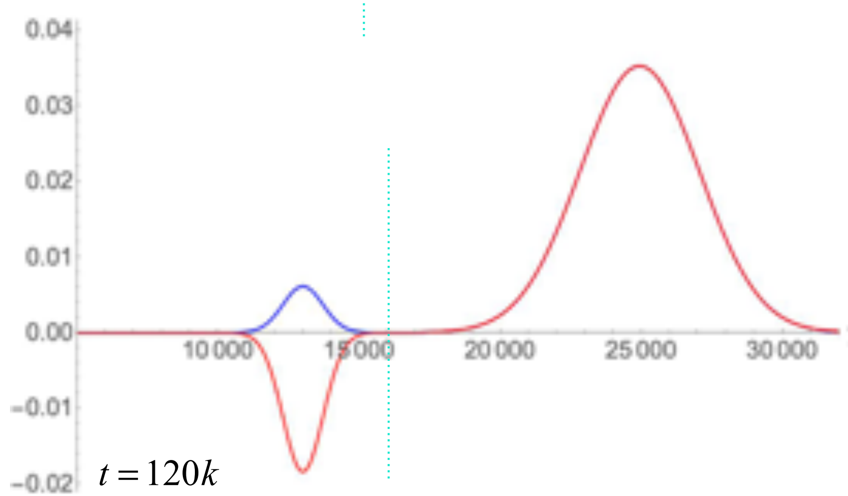
Case II : $n_1 = 3 \rightarrow n_2 = 1$ $E_z(blue)$, $B_x(red)$





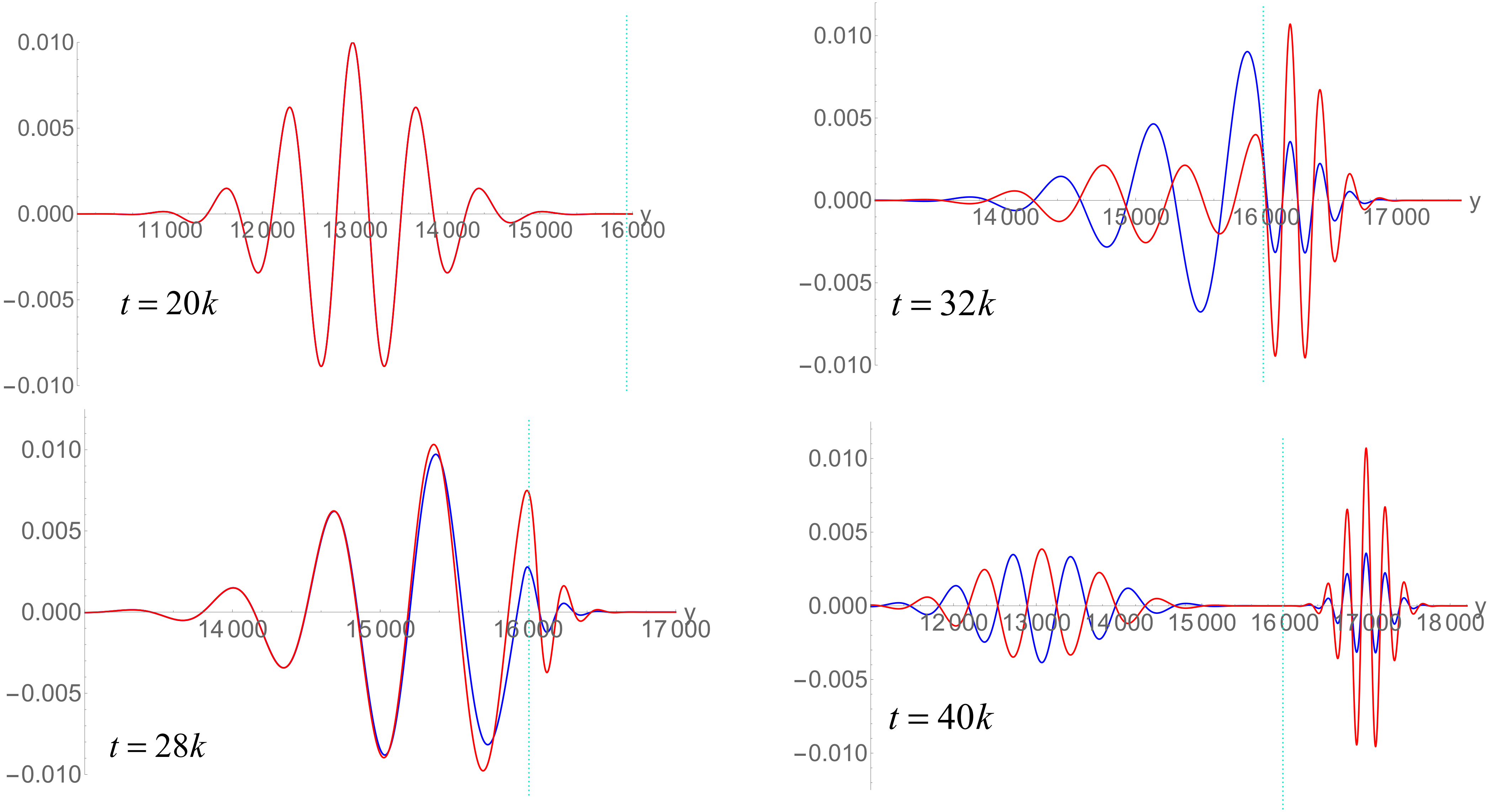






Case III : $n_1 = 1 \rightarrow n_2 = 3$ $E_z(blue)$, $B_x(red)$

Gaussian wave packet



$t = 24k$

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