Qubit Lattice Algorithms (QLA) - 2D Electromagnetic Scattering from tensor dielectric objects

George Vahala, Physics, William & Mary, Williamsburg, VA
Min Soe, Mathematics and Physical Sciences, Rogers State University, Claremore, OK
Linda Vahala, Electrical & Computer Engineering, Old Dominion University, Norfolk, VA
Abhay K. Ram, Plasma Science and Fusion Center, MIT, Cambridge, MA
Efstratios Koukoutsis, National Technical University of Athens
Kyriakos Hizanidis, National Technical University of Athens

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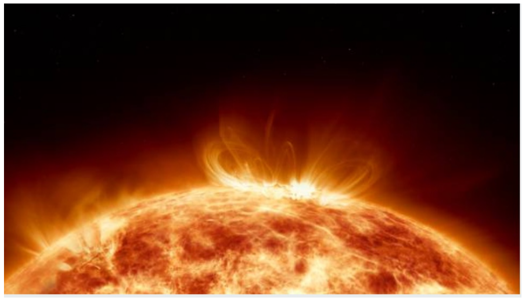
Fusion from Magnetic Confinement



- Sun : plasma flares - nuclear fusion (gravitational forces)

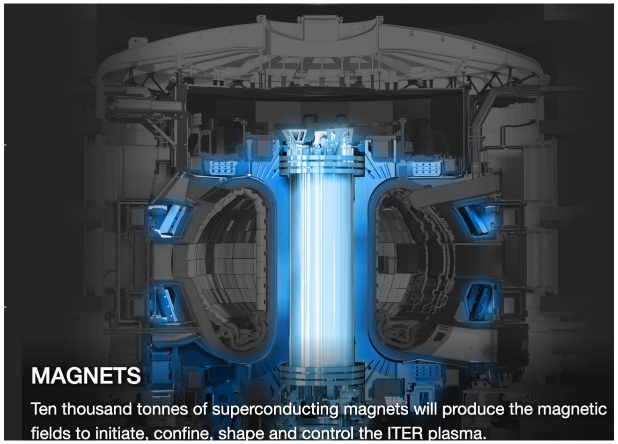
- EARTH : magnetic confinement

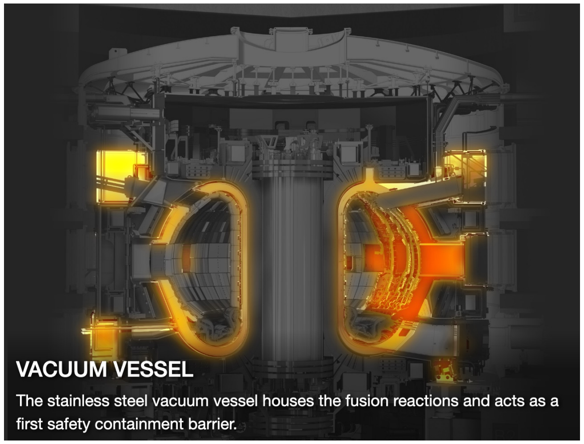
D + T → n + α

3 parameters (Lawson criteria) :
density, temperature, confinement time

ITER : weight 23,000 tonnes

Vacuum vessel – heavier than Eiffel Tower





- particle motion in **E, B** - fields
- collective effects of plasma in **E, B** - fields

MAXWELL EQUATIONS

$$\nabla \times \overline{E} = -\frac{\partial \overline{B}}{\partial t}$$

$$\nabla \times \overline{H} = \overline{J} + \frac{\partial \overline{D}}{\partial t}$$

$$\nabla \bullet \bar{D} = \rho$$

$$\nabla \bullet \overline{B} = 0$$

Closure : constitutive equations describe the effects of the fields on the plasma medium self-consistently

$$\overline{D} = \epsilon \overline{E}$$

Simplest model: $\overline{B} = \mu \overline{H}$

$$\overline{J} = \sigma \overline{E}$$

SOLUTION TECHNIQUE :

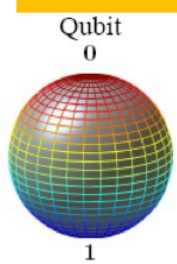
(a) classical supercomputers - parallelization critical

(b) quantum computer -- unitary evolution on a qubit basis

(c) unitary algorithm but also ideal for classical supercomputers

Classical

Quantum



$$Qubit : |q_1\rangle = a_0|0\rangle + a_1|1\rangle$$

$$\text{with} \quad |a_0|^2 + |a_1|^2 = 1$$

QUANTUM ENTANGLEMENT

Tensor product of 2-qubits :

$$|q_1\rangle \otimes |q_2\rangle = [a_0|0\rangle + a_1|1\rangle] \otimes [b_0|0\rangle + b_1|1\rangle]$$

$$|q_1 q_2\rangle = a_0 b_0|00\rangle + a_0 b_1|01\rangle + a_1 b_0|10\rangle + a_1 b_1|11\rangle$$

will NEVER recover the state

$$\frac{1}{\sqrt{2}}[|01\rangle - |10\rangle]$$

- entangled state
- a Bell state

- **Quantum Parallelization**

3 (classical) bit register

000 = “0”
001 = “1”
010 = “2”
011 = “3”
100= “4”
101 = “5”
110 = “6”
111 = “7”

A classical register can be in only ONE unique state, at any given time instant:
e.g., |011> = “3”

$Qubit : |q\rangle = a_0|0\rangle + a_1|1\rangle \quad \text{with} \quad |a_0|^2 + |a_1|^2 = 1$

Consider the 3-qubit state ”3” : $|011\rangle = |0\rangle \otimes |1\rangle \otimes |1\rangle$

Apply the Hadamard gate to each qubit :

$$H|0\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \quad , \quad H|1\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

$$H|0\rangle \otimes H|1\rangle \otimes H|1\rangle = \frac{"0" - "1" - "2" + "3" + "4" - "5"' - "6" + "7"}{\sqrt{8}}$$

i.e., we can create a quantum register in which we can simultaneously and independently store ALL 8 possible basis states at the same time instant.

Spin-1 BECs

3 coupled NLS eqs. $\hat{\psi} = (\,\psi_{-1}\ \ \psi_0\ \ \psi_1)^T$

$$i\frac{\partial\hat{\psi}}{\partial t} = \left(-\nabla^2 - \hat{\mu} + g\hat{\psi}^{\dagger}\hat{\psi}\right)\hat{\psi} + c_1 \mathbf{F}\bullet\mathbf{f}\hat{\psi} \equiv \left(\hat{T} + \hat{V}_{diag}\right)\hat{\psi} + c_1\hat{V}_{nondiag}\hat{\psi}$$

- Time evolution :

$$\hat{\psi}\left(\mathbf{x}, t+\delta t\right) = Exp\left[-i\left(\hat{T} + \hat{V}_{diag} + c_1\hat{V}_{nondiag}\right)\delta t\right]\hat{\psi}\left(\mathbf{x}, t\right)$$

tri-idempotent operator

Baker-Campbell-Hausdorff (lowest order) :

$$Exp\left[-i\left(\hat{H}_{diag} + \hat{V}_{nondiag}\right)\delta t\right] = Exp\left[-\frac{i\hat{V}_{nondiag}\delta t}{2}\right] Exp\left[-i\hat{H}_{diag}\delta t\right] Exp\left[-\frac{i\hat{V}_{nondiag}\delta t}{2}\right] + ...$$

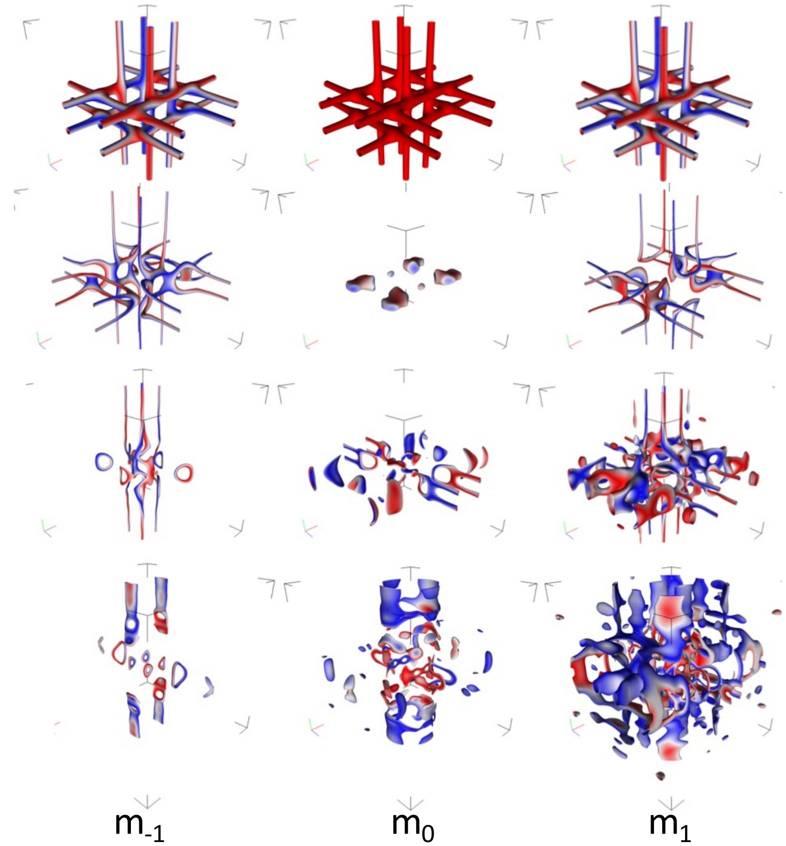
summable to all orders

QLA : fully unitary, 6 qubits/lattice node

t = 0: 12 line Vortices/m_s

Formation of Quantum loop vortices

Grid 864^3



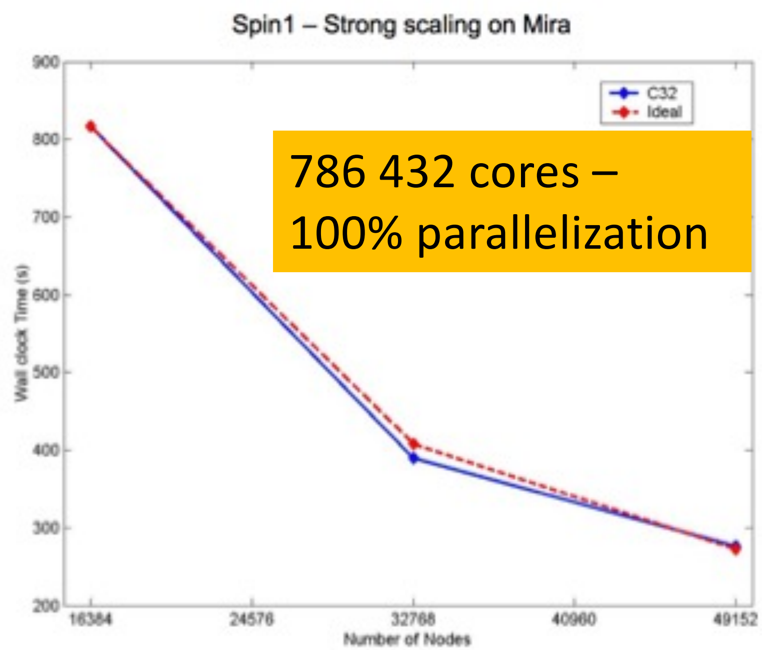
Time	Probability	Unitarity	Energy
0	2.394440389827002E-004	1.197220194913501E-004	2.399237643177138E-004
1000	2.394440386082502E-004	1.197220194910103E-004	2.399177921934308E-004
3200	2.394440225580082E-004	1.197220194905830E-004	2.399082131416646E-004
4500	2.394435073214831E-004	1.197220194903661E-004	2.399107356071618E-004

Parallelization of QLA on Classical Supercomputers *(Mira) [2016]*

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.



786 432 cores – 100% parallelization

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

94.1% parallel efficiency

1.174 PetaFlops (Tim Williams)

2D ELECTROMAGNETIC SCATTERING from TENSOR DIELECTRIC OBJECTS

6 qubits/lattice node

$$\mathbf{U} = \left(n_x E_x, n_y E_y, n_z E_z, \mu_0^{1/2}\mathbf{H}\right)^T \equiv \mathbf{Q}.$$

Pde's

$$\frac{\partial q_0}{\partial t} = \frac{1}{n_x}\frac{\partial q_5}{\partial y}, \qquad \frac{\partial q_1}{\partial t} = -\frac{1}{n_y}\frac{\partial q_5}{\partial x}, \qquad \frac{\partial q_2}{\partial t} = \frac{1}{n_z}\left[\frac{\partial q_4}{\partial x} - \frac{\partial q_3}{\partial y}\right]$$

$$\frac{\partial q_3}{\partial t} = -\frac{\partial (q_2/n_z)}{\partial y}, \qquad \frac{\partial q_4}{\partial t} = \frac{\partial (q_2/n_z)}{\partial x}, \qquad \frac{\partial q_5}{\partial t} = -\frac{\partial (q_1/n_y)}{\partial x} + \frac{\partial (q_0/n_x)}{\partial y}$$

C_X – Unitary Collision Operator forms 2-qubit entanglements

$$C_X = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & cos\,\theta_1 & 0 & 0 & 0 & -sin\,\theta_1 \\ 0 & 0 & cos\,\theta_2 & 0 & -sin\,\theta_2 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & sin\,\theta_2 & 0 & cos\,\theta_2 & 0 \\ 0 & sin\,\theta_1 & 0 & 0 & 0 & cos\,\theta_1 \end{bmatrix}$$

Coupling q1 – q5
q2 – q4

C_Y – Unitary Collision Operator forms 2-qubit entanglements

$$\widehat{C}_Y = \begin{bmatrix} \cos\theta_0 & 0 & 0 & 0 & 0 & \sin\theta_0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos\theta_2 & \sin\theta_2 & 0 & 0 \\ 0 & 0 & -\sin\theta_2 & \cos\theta_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ -\sin\theta_0 & 0 & 0 & 0 & 0 & \cos\theta_0 \end{bmatrix}.$$

Coupling q0 – q5
q2 – q3

$$\mathbf{U_X} = S_{25}^{+x}.C_X^{\dagger}.S_{25}^{-x}.C_X.S_{14}^{-x}.C_X^{\dagger}.S_{14}^{+x}.C_X.S_{25}^{-x}.C_X.S_{25}^{+x}.C_X^{\dagger}.S_{14}^{+x}.C_X.S_{14}^{-x}.C_X^{\dagger}$$

$$\mathbf{U_Y} = S_{25}^{+y}.C_Y^{\dagger}.S_{25}^{-y}.C_Y.S_{03}^{-y}.C_Y^{\dagger}.S_{03}^{+y}.C_Y.S_{25}^{-y}.C_Y.S_{25}^{+y}.C_Y^{\dagger}.S_{03}^{+y}.C_Y.S_{03}^{-y}.C_Y^{\dagger}$$

$$\theta_0 = \frac{\delta}{4n_x}, \qquad \theta_1 = \frac{\delta}{4n_y}, \qquad \theta_2 = \frac{\delta}{4n_z},$$

Non-unitary
External potentials

$$V_X = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -sin\,\beta_2 & 0 & cos\,\beta_2 & 0 \\ 0 & sin\,\beta_0 & 0 & 0 & 0 & cos\,\beta_0 \end{bmatrix}$$

$$\beta_0 = \delta^2 \frac{\partial n_y/\partial x}{n_y^2} \quad , \quad \beta_1 = \delta^2 \frac{\partial n_x/\partial y}{n_x^2} \quad , \quad \beta_2 = \delta^2 \frac{\partial n_z/\partial x}{n_z^2} \quad , \quad \beta_3 = \delta^2 \frac{\partial n_z/\partial y}{n_z^2}$$

$$V_Y = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & o \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \cos\,\beta_3 & \sin\,\beta_3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ -sin\,\beta_1 & 0 & 0 & 0 & 0 & cos\,\beta_1 \end{bmatrix}$$

Can rewrite V_X and V_Y as a linear sum of unitary matrices (LCU method - Childs et. al.)

QLA : $\mathbf{Q}(t+\Delta t) = V_Y.V_X.\mathbf{U_Y}.\mathbf{U_X}.\mathbf{Q}(t)$

2^{nd} order accurate scheme

under diffusion ordering, $\Delta t \approx \delta^2$.

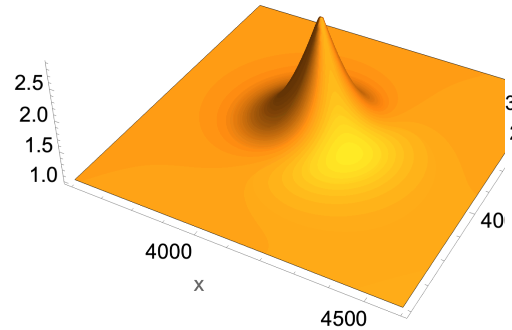
- in principle QLA, as an initial value problem, could be run on an error-correcting qubit quantum computer.

Scattering of a 1D Electromagnetic Pulse off of scalar dielectric object:

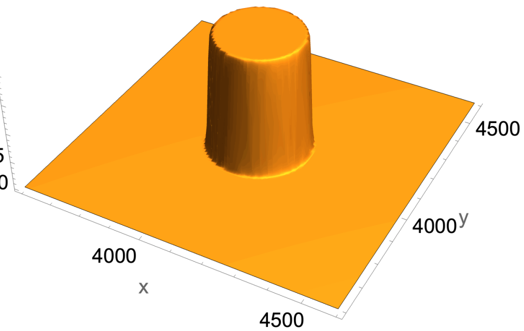
- dielectric cone
- dielectric cylinder

Grid: 8192^2

Cone



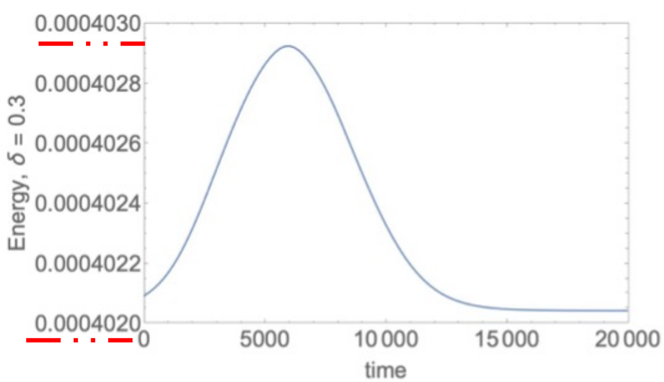
Cylinder



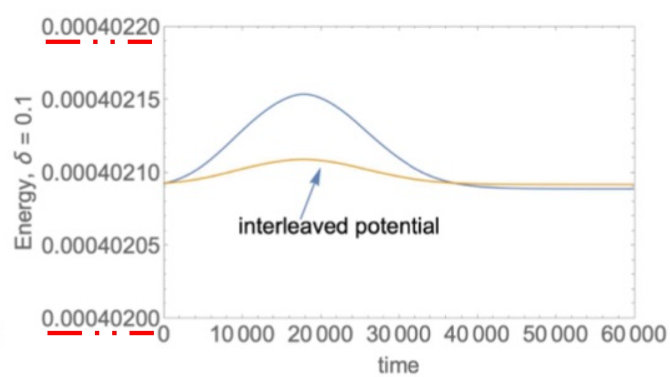
No internal boundary conditions : initial value problem

Conservation of Energy

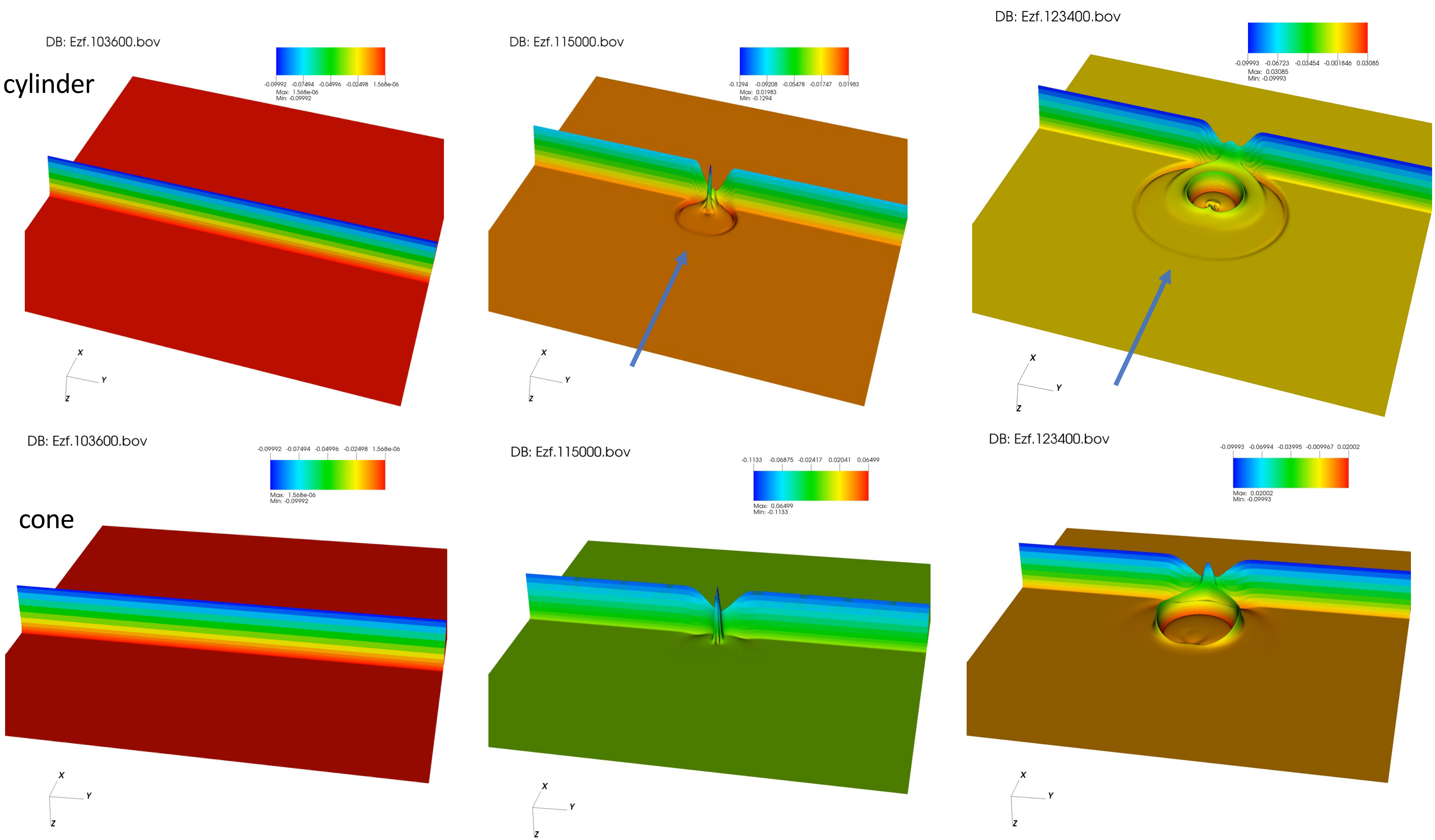
$$\mathcal{E}(t) = \frac{1}{L^2}\int_0^L\int_0^L dxdy\left[n_x^2E_x^2 + n_y^2E_y^2 + n_z^2E_z^2 + \mathbf{B}^2\right] = \frac{1}{L^2}\int_0^L\int_0^L dxdy\mathbf{Q}\cdot\mathbf{Q}$$

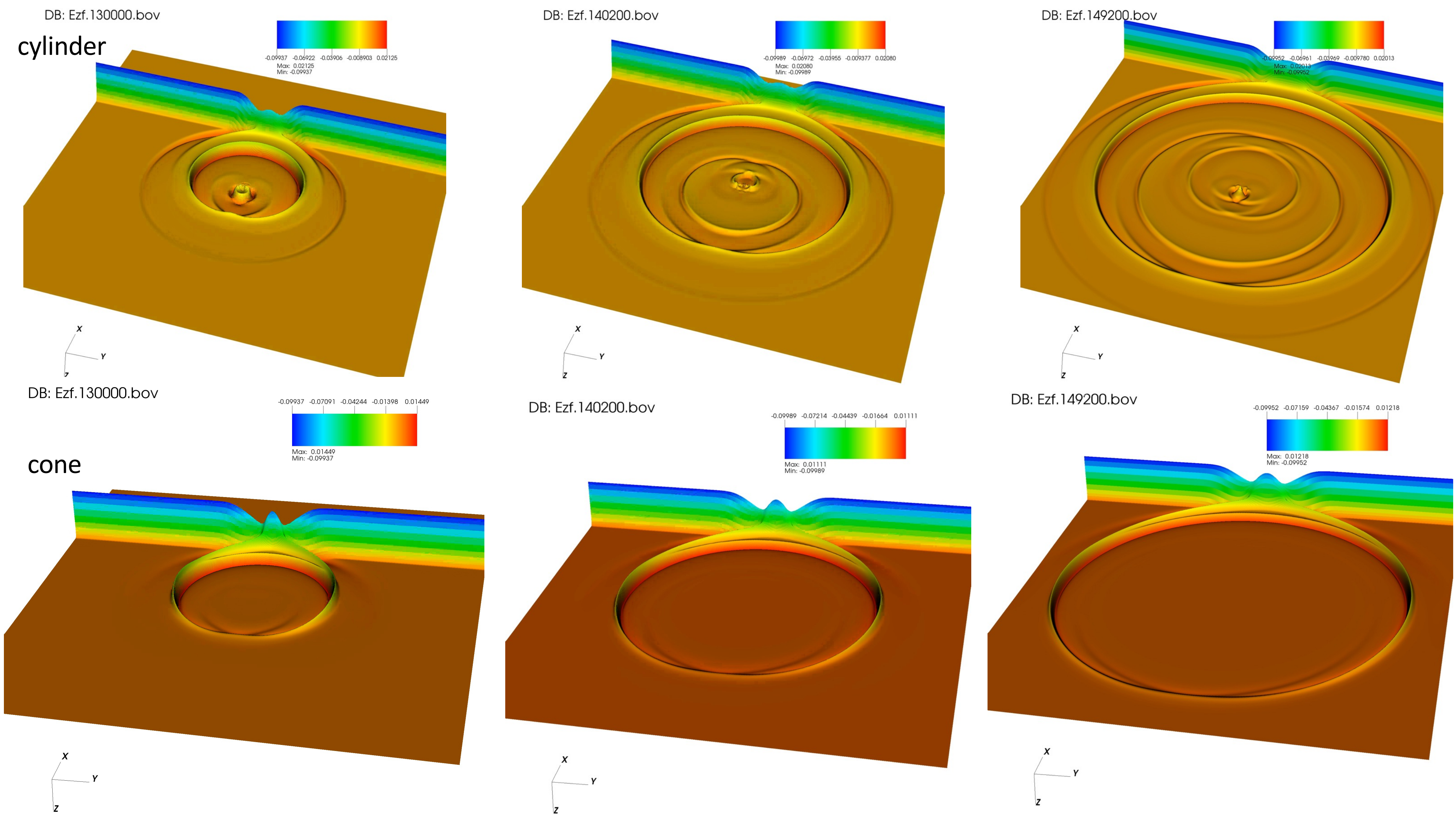


(a) $\mathcal{E}(t)$, $\delta = 0.3$,



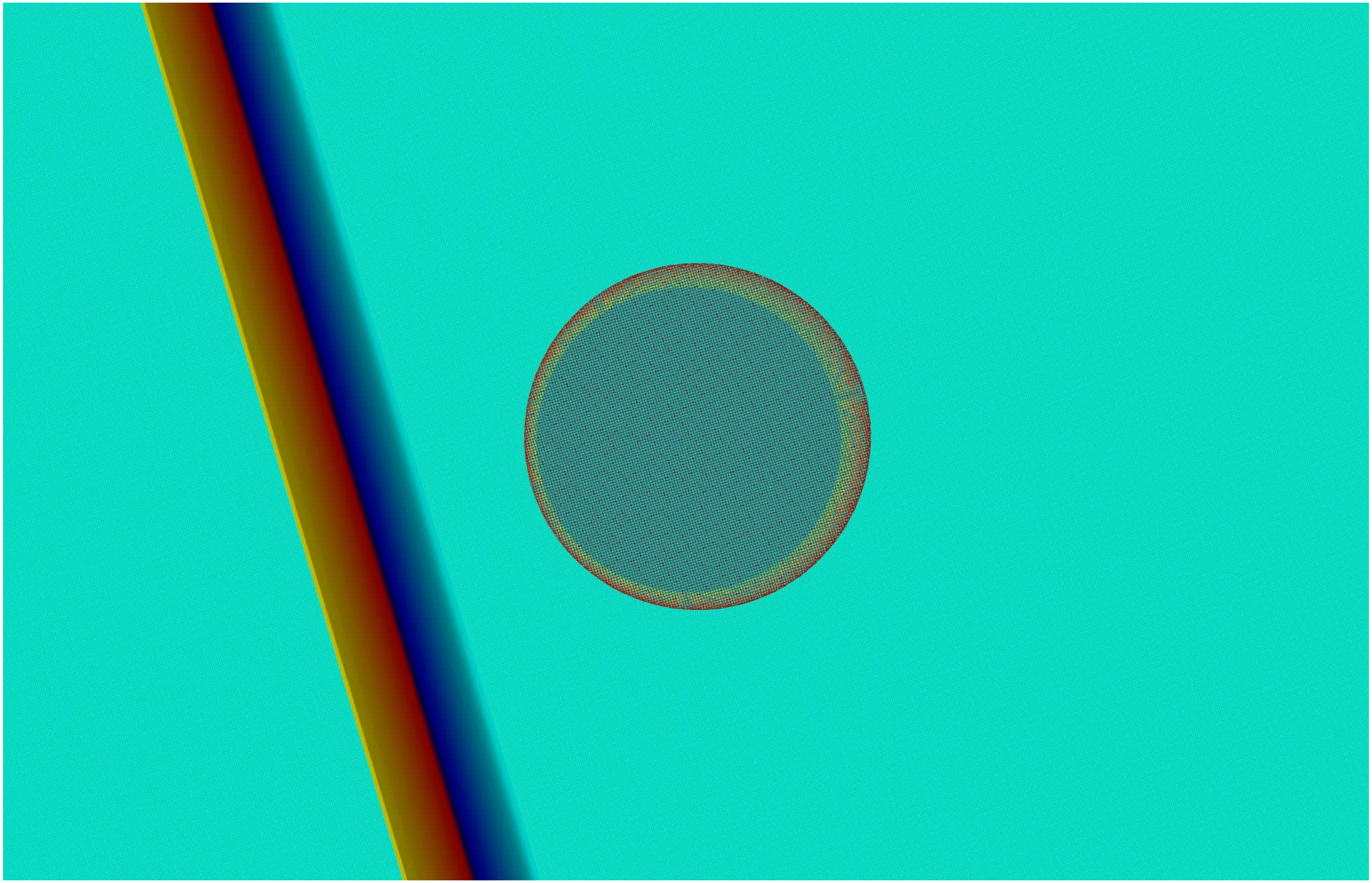
(b) $\mathcal{E}(t)$, $\delta = 0.1$


DB: Ezf.103600.bov
cylinder
-0.09992 -0.07494 -0.04996 -0.02498 1.568e-06
Max: 1.568e-06
Min: -0.09992
DB: Ezf.115000.bov
-0.1294 -0.09208 -0.05478 -0.01747 0.01983
Max: 0.01983
Min: -0.1294
DB: Ezf.123400.bov
-0.09993 -0.06723 -0.03454 -0.001846 0.03085
Max: 0.03085
Min: -0.09993
DB: Ezf.103600.bov
-0.09992 -0.07494 -0.04996 -0.02498 1.568e-06
Max: 1.568e-06
Min: -0.09992
cone
DB: Ezf.115000.bov
-0.1133 -0.06875 -0.02417 0.02041 0.06499
Max: 0.06499
Min: -0.1133
DB: Ezf.123400.bov
-0.09993 -0.06994 -0.03995 -0.009967 0.02002
Max: 0.02002
Min: -0.09993
X
Y
Z



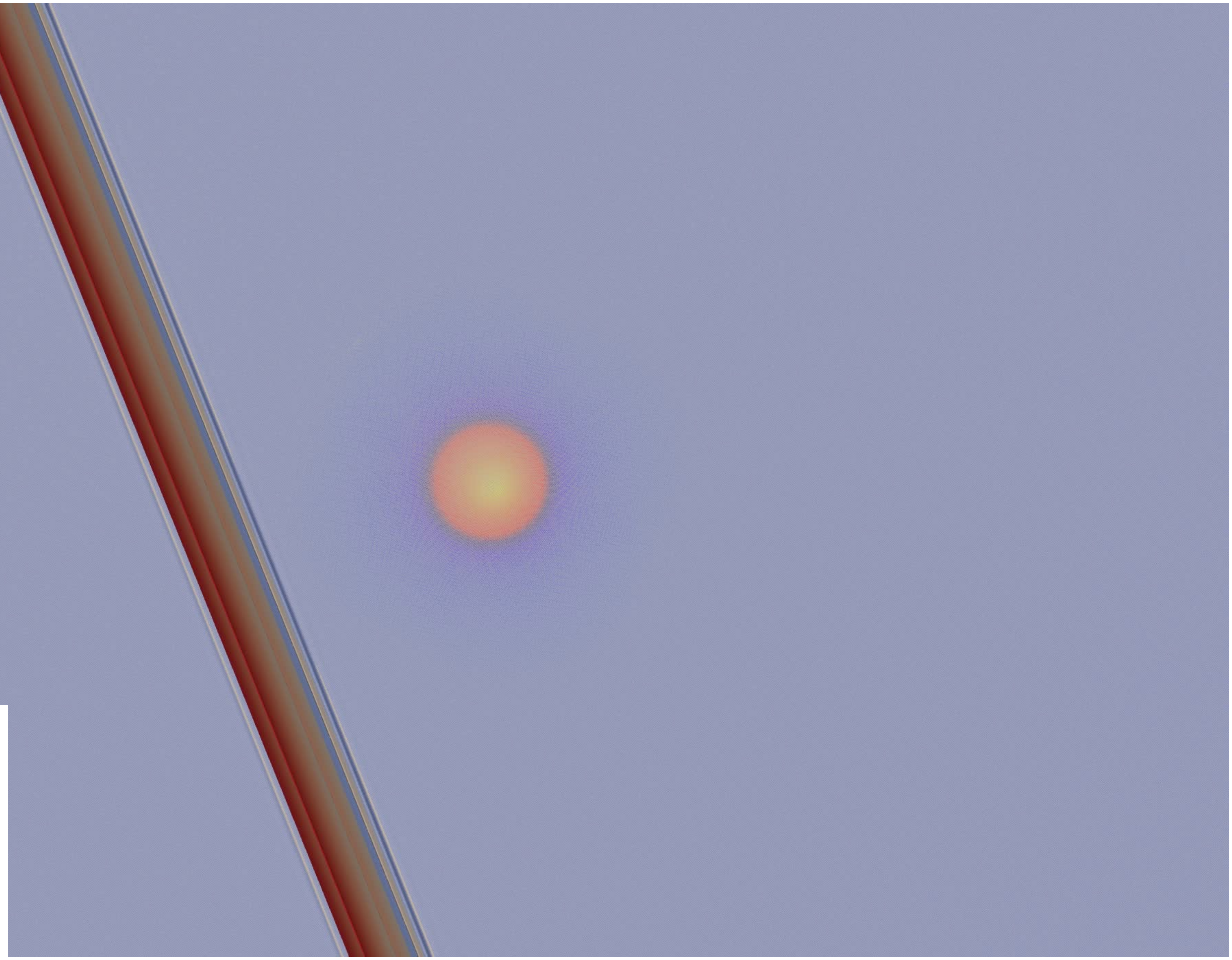
DB: Ezf.130000.bov
cylinder
DB: Ezf.140200.bov
DB: Ezf.149200.bov
DB: Ezf.130000.bov
cone
DB: Ezf.140200.bov
DB: Ezf.149200.bov

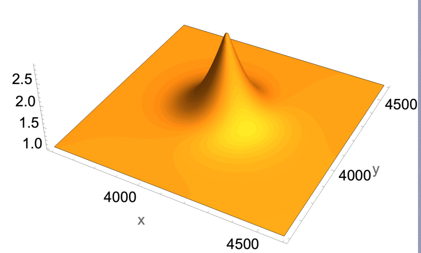
i.v.p
Gaussian
Pulse
Scattering
from circular
dielectric

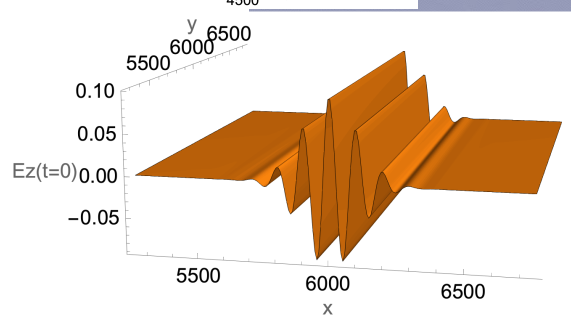


Refr. Index
$n_1=1$
$n_2=3$

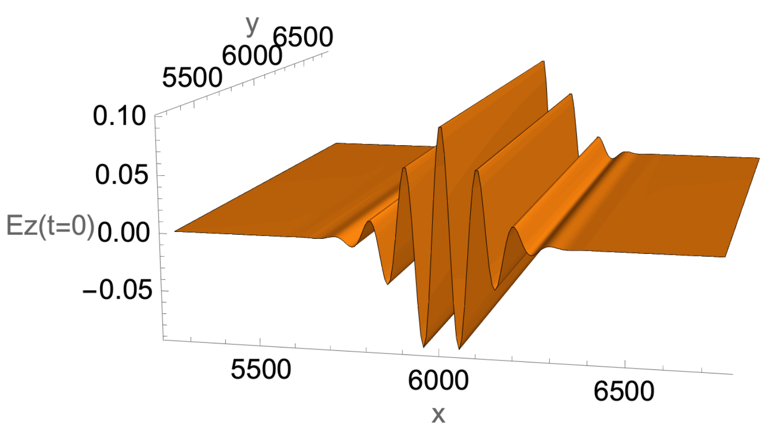
i.v.p
Wave packet
scattering from
cone







Initial Value Problem,
Gaussian wavepacket
scattering from an
elliptical dielectric cyinder



Refractive index

$n_1=1$

$n_2=2$ (ellipse)

#1. PT - Hamiltonians (Bender 1998)

- **Quantum Mechanics: real, bounded energy spectra of a system**

$$i\frac{\partial\psi}{\partial t}=\hat{H}\psi \qquad \psi(\mathbf{x},t)=\psi(\mathbf{x})e^{-iEt} \qquad \hat{H}\psi = E\psi$$

- **usual assumption:** $\hat{H}=\hat{H}^{\dagger}$ **- Hermitian Hamiltonian**

- **Bender (1998) : to recover real eigenvalues one does NOT need to assume Hermitian operator**

- **PT-symmetry can be sufficient. [P - parity, T - time reversal]**

$$\hat{P}\psi(\mathbf{x},t)=\psi(-\mathbf{x},t) \qquad \hat{T}\psi(\mathbf{x},t)=\psi^{*}(\mathbf{x},-t)$$

$$anti-linear \quad \hat{T}(\lambda\psi)=\lambda^{*}\hat{T}\psi$$

$$\hat{T}\, i = -i$$

• **PT-Symmetric Hamiltonian** $\left[\hat{P}\hat{T},\hat{H}\right]=0$

Bender & Boetcher, 1998

$$\hat{H}(\varepsilon)=\hat{p}^2+\hat{x}^2(ix)^\varepsilon$$

$$\left[\hat{P},\hat{H}\right]\neq 0 \;\; but \;\; \left[\hat{P}\hat{T},\hat{H}\right]=0$$

$$\varepsilon=0:\hat{H}(0)=\hat{p}^2+\hat{x}^2=\hat{H}^\dagger(0)$$

- harmonic oscillator, Hermitian

$$E_n=2n+1$$

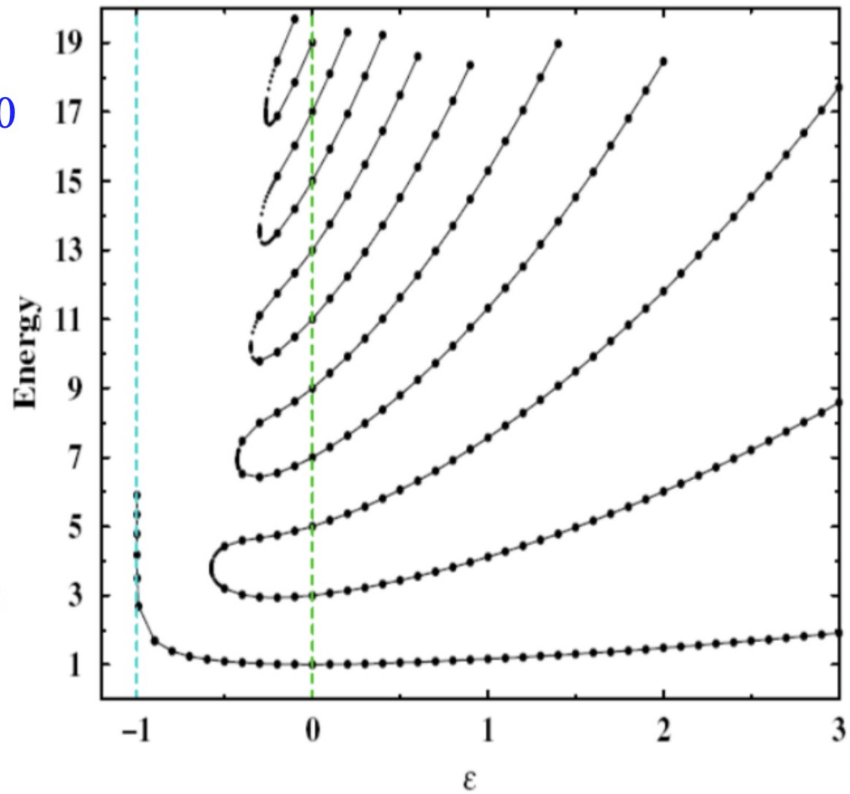
Energy Spectrum:

$\varepsilon\geq 0$ real, discrete, like analytic cont. of s.h.o

$-1<\varepsilon<0$: finite # real > 0

+ infinite # ccomplex conj. pairs

$\varepsilon<-1$: *no real eigenvalues*



broken PT symmetry $\varepsilon<0$

unbroken PT symmetry: $\varepsilon\geq 0$

$$\hat{H}\psi=E\psi\;\;,\;\;\hat{P}\hat{T}\psi=\lambda\psi$$

FUTURE WORK

(1) QLA for scattering from 3D objects

(2) Tensor dielectric – dispersive, dissipative (collisional cold plasma)

- treat classical dissipative system as an “open-quantum” system : non-unitary system
- introduce appropriate Kraus operators
- treat the environment as a single qubit-system
  (c.f., quantum amplitude channel for vector spontaneous emission)
- find the dilated Hilbert space in which the resultant dynamics is now unitary
  [Koukoutsis et. al., arXiv:2308.00056v1]
- develop QLA for this higher dimensional Hilbert space unitary systems

(3) Nonlinear 2 fluid equations + Maxwell : Madelung transformation on the GP BEC-equations
- quaternions to eliminate quantum pressure terms, nonsingular classical vortices

Theory: Unitary Algorithm for Maxwell Equations in Anisotropic Dielectric Media

Basic Fields **u = (E, H)^T**

Derived Fields **d = (D , B)^T**

Constitutive Equation $\mathbf{D} = \overline{\overline{\varepsilon}}(\mathbf{x}) \cdot \mathbf{E}$, $\mathbf{B} = \mu_0 \mathbf{H}$ ➔ **W** Hermitian $\mathbf{W} = \begin{bmatrix} \overline{\overline{\varepsilon}}(\mathbf{x}) & 0_3 \\ 0_3 & \mu_0 I_3 \end{bmatrix}$.

➔ **d = W u**

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \quad \nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t}.$$

➔ Maxwell i.v.p $i\frac{\partial \mathbf{d}}{\partial t} = \overline{\overline{\mathbf{M}}} \cdot \mathbf{u}$ with Hermitian operator $\mathbf{M} = \begin{bmatrix} 0_3 & i\nabla\times \\ -i\nabla\times & 0_3 \end{bmatrix}$

➔ $$i\frac{\partial \mathbf{u}}{\partial t} = \overline{\overline{\mathbf{W}}}^{-1}\overline{\overline{\mathbf{M}}} \cdot \mathbf{u}$$

- Homogeneous Media $\overline{\overline{\mathbf{W}}}^{-1}\overline{\overline{\mathbf{M}}}$ Is Hermitian ➔ {**u**} – basis for a unitary representation.
- **INHOMOGENEOUS MEDIA :** $\overline{\overline{\mathbf{W}}}^{-1}\overline{\overline{\mathbf{M}}}$ is not Hermitian , since $\overline{\overline{\mathbf{W}}}^{-1}\overline{\overline{\mathbf{M}}} \neq \overline{\overline{\mathbf{M}\mathbf{W}}}^{-1}$

➔ {**u**} **-** basis will not yield a unitary repr.

$$\mathbf{W} = \begin{bmatrix} \overline{\overline{\varepsilon}}(\mathbf{x}) & 0_3 \\ 0_3 & \mu_0 I_3 \end{bmatrix}.$$

DYSON MAP

Consider map : **u** → **U** s.t $\mathbf{U} = \overline{\overline{\rho}}\,\mathbf{u}$ with $\overline{\overline{\rho}} = \overline{\overline{\mathbf{W}}}^{+1/2}$

$$\rightarrow \quad i\frac{\partial \mathbf{u}}{\partial t} = \overline{\overline{\mathbf{W}}}^{-1}\overline{\overline{\mathbf{M}}}\cdot\mathbf{u}$$

$$i\frac{\partial \rho \mathbf{u}}{\partial t} = \overline{\overline{\rho}}\,\overline{\overline{\mathbf{W}}}^{-1}\overline{\overline{\mathbf{M}}}\cdot\mathbf{u}$$

$$= \overline{\overline{\rho}}\,\overline{\overline{\mathbf{W}}}^{-1}\overline{\overline{\mathbf{M}}}\left(\overline{\overline{\rho}}^{-1}\,\overline{\overline{\rho}}\right)\cdot\mathbf{u}$$

$$= \left(\overline{\overline{\rho}}\,\overline{\overline{\mathbf{W}}}^{-1}\overline{\overline{\mathbf{M}}}\,\overline{\overline{\rho}}^{-1}\right)\overline{\overline{\rho}}\mathbf{u}$$

$$\rightarrow \quad i\frac{\partial \mathbf{U}}{\partial t} = H_D \mathbf{U}$$

, but now H_D is Hermitian

$$\mathbf{U} = \begin{bmatrix} \sqrt{\epsilon_k}E_k \\ \sqrt{\mu_0}H_k \end{bmatrix}$$

$$H_D = \overline{\overline{\rho}}\,\overline{\overline{\mathbf{W}}}^{-1}\overline{\overline{\mathbf{M}}}\,\overline{\overline{\rho}}^{-1}$$

$$= \overline{\overline{\mathbf{W}}}^{-1/2}\,\overline{\overline{\mathbf{M}}}\,\overline{\overline{\mathbf{W}}}^{-1/2}$$