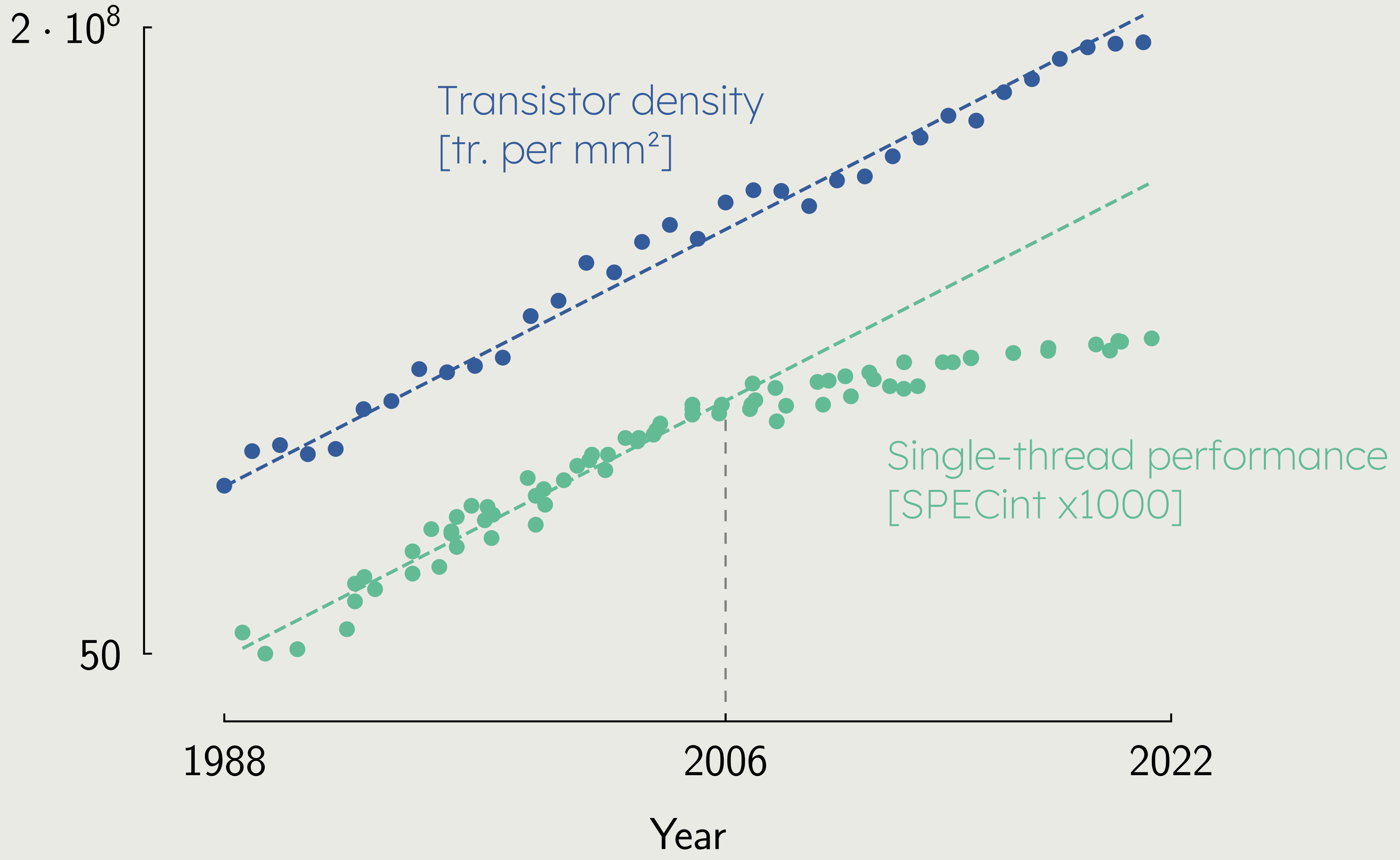
# Solving the Fully Coupled Time-Dependent Maxwell-Dirac System: A Second-Order Accurate Numerical Scheme

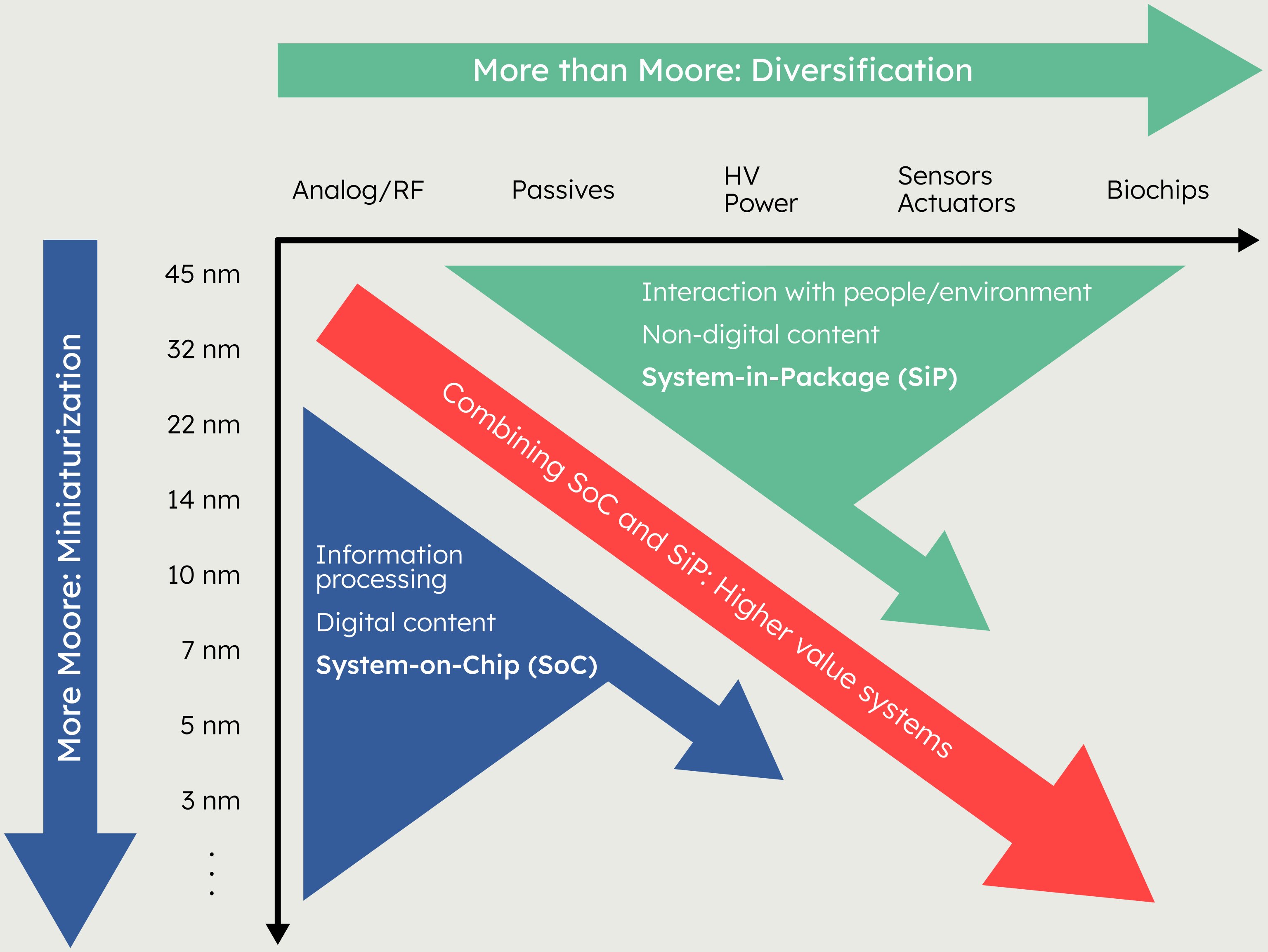
Jul Van den Broeck
Pieter Decleer
Emile Vanderstraeten
Dries Vande Ginste

quest.

# Device performance is lacking since 2006 with respect to Moore's law.

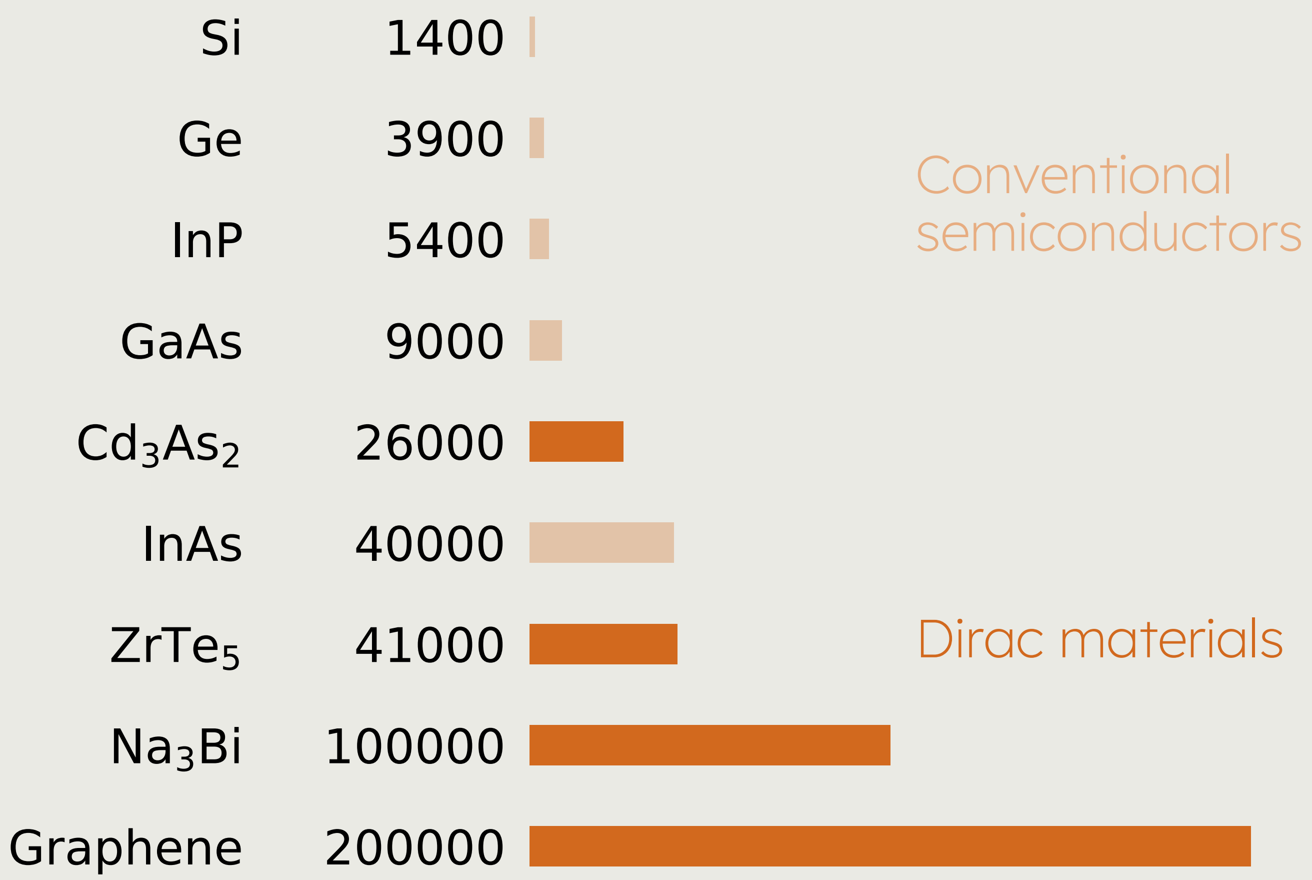


# Novel research paths are being explored.



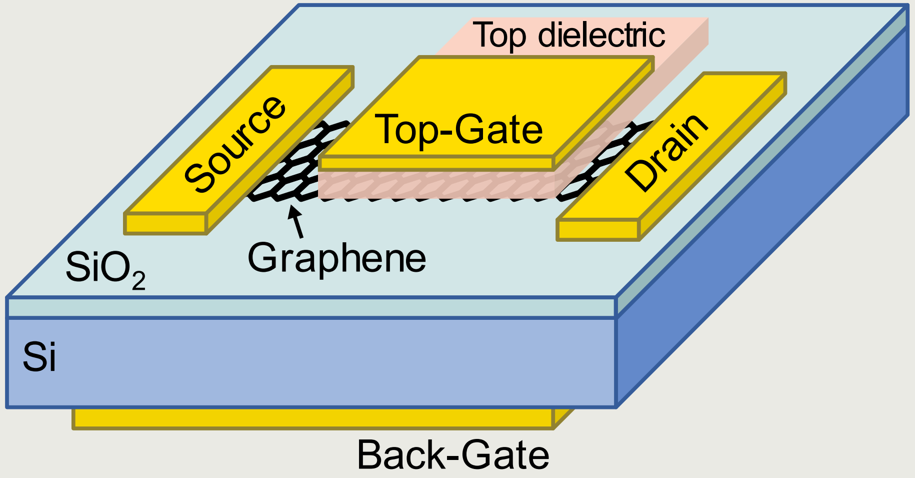
# Dirac materials have faster carrier transport compared to conventional semiconductors.

Electron mobility in $\mathrm{cm}^2/\mathrm{Vs}$

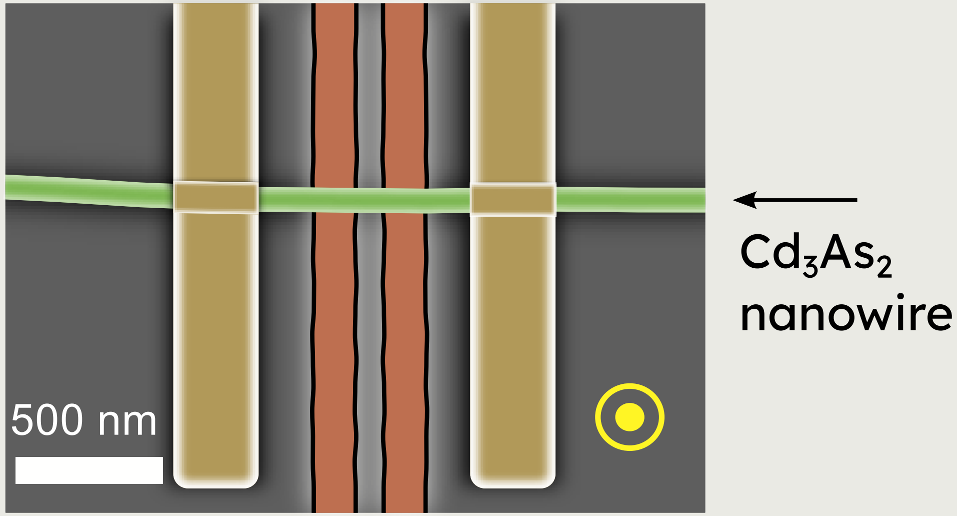


# Novel Dirac devices are gaining interest.

Graphene field-effect transistor [1]




Double-barrier $Cd_3As_2$ nanowire diode [2]




[1] J. R. Bayogan *et al.* 2020 *Nanotechnology* 31 205001

[2] F. Giubileo *et al.* 2017 *Progress in Surface Science* 92(3) 143-175

# Existing Maxwell-Dirac solvers are not suitable for the simulation of practical applications.

- EM potentials are solved for ➡ Not integrable into existing EM frameworks
- Dirac equation is discretized on collocated grid ➡ Fermion doubling problem
- Lorenz gauge ➡ Not satisfied numerically

# In quest, we developed a novel scheme that overcomes these problems.

| | | |
|---|---|---|
| • EM fields are included | → | Easy integration into existing EM code |
| • Staggered grid approach to discretize Dirac spinor | → | Less fermion doubling |
| • Lorenz gauge | → | Exactly satisfied on the discrete level |

Discretization of the Maxwell-Dirac equations

Properties of the novel method

Conservation laws

Simulation of $ZrTe_5$ waveguide

Future work

# The fully-coupled Maxwell-Dirac equations describe the time evolution of a charged fermion.

Dirac spinor

EM potentials

$$i\hbar\frac{\partial\Psi}{\partial t} = \left[c\boldsymbol{\alpha}\cdot(\hat{\boldsymbol{p}} - q\boldsymbol{a}) + mc^2\beta + q\phi\right]\Psi$$

# The fully-coupled Maxwell-Dirac equations describe the time evolution of a charged fermion.

Dirac spinor

EM potentials

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[ c\boldsymbol{\alpha} \cdot (\hat{\boldsymbol{p}} - q\boldsymbol{a}) + mc^2 \beta + q\phi \right] \Psi$$

Backward coupling
via quantum current density:

$$\boldsymbol{j}_q = q\Psi^\dagger c\boldsymbol{\alpha}\Psi$$

# The fully-coupled Maxwell-Dirac equations describe the time evolution of a charged fermion.

Dirac spinor

EM potentials

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[ c\boldsymbol{\alpha} \cdot (\hat{\boldsymbol{p}} - q\boldsymbol{a}) + mc^2 \beta + q\phi \right] \Psi$$

Backward coupling
via quantum current density:

$$\boldsymbol{j}_q = q\Psi^\dagger c\boldsymbol{\alpha}\Psi$$

$$\begin{cases} \nabla \times \boldsymbol{e} = \mu_0 \frac{\partial \boldsymbol{h}}{\partial t} \\ \nabla \times \boldsymbol{h} = \epsilon_0 \frac{\partial \boldsymbol{e}}{\partial t} + \boldsymbol{j}_{\text{ex}} + \boldsymbol{j}_q \end{cases}$$

EM fields

# The fully-coupled Maxwell-Dirac equations describe the time evolution of a charged fermion.

Dirac spinor

EM potentials

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[ c\boldsymbol{\alpha} \cdot (\hat{\boldsymbol{p}} - q\boldsymbol{a}) + mc^2 \beta + q\phi \right] \Psi$$

Backward coupling
via quantum current density:

$$\boldsymbol{j}_q = q\Psi^\dagger c\boldsymbol{\alpha}\Psi$$

$$\begin{cases} \nabla \times \boldsymbol{e} = \mu_0 \frac{\partial \boldsymbol{h}}{\partial t} \\ \nabla \times \underbrace{\boldsymbol{h}}_{\text{EM fields}} = \epsilon_0 \frac{\partial \boldsymbol{e}}{\partial t} + \boldsymbol{j}_{\text{ex}} + \boldsymbol{j}_q \end{cases}$$

EM potentials

$$\begin{cases} \boldsymbol{e} = -\nabla\phi - \frac{\partial \boldsymbol{a}}{\partial t} \\ \nabla \cdot \boldsymbol{a} + \frac{1}{c^2}\frac{\partial \phi}{\partial t} = 0 \end{cases}$$

Lorenz gauge

# The fully-coupled Maxwell-Dirac equations describe the time evolution of a charged fermion.

Dirac spinor

EM potentials

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[c\boldsymbol{\alpha} \cdot (\hat{\boldsymbol{p}} - q\boldsymbol{a}) + mc^2\beta + q\phi\right]\Psi$$

Forward coupling
via minimal coupling

Backward coupling
via quantum current density:

$$\boldsymbol{j}_q = q\Psi^\dagger c\boldsymbol{\alpha}\Psi$$

$$\begin{cases} \boldsymbol{e} = -\nabla\phi - \frac{\partial \boldsymbol{a}}{\partial t} \\ \nabla \cdot \boldsymbol{a} + \frac{1}{c^2}\frac{\partial \phi}{\partial t} = 0 \end{cases}$$

Lorenz gauge

EM potentials

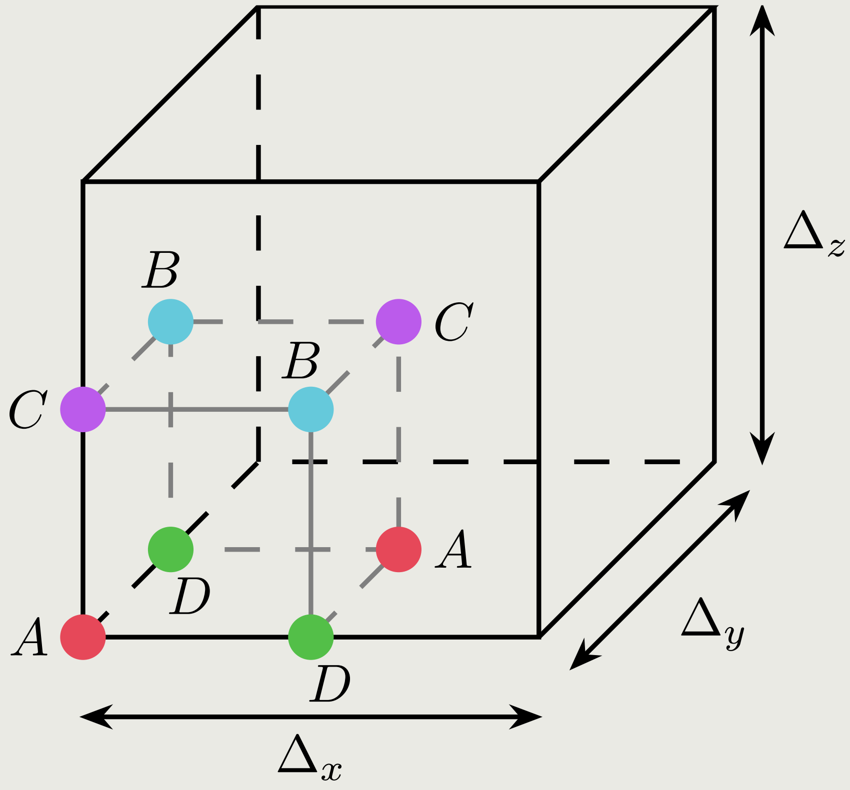
$$\begin{cases} \nabla \times \boldsymbol{e} = \mu_0 \frac{\partial \boldsymbol{h}}{\partial t} \\ \nabla \times \boldsymbol{h} = \epsilon_0 \frac{\partial \boldsymbol{e}}{\partial t} + \boldsymbol{j}_{\mathrm{ex}} + \boldsymbol{j}_q \end{cases}$$

EM fields

# The stencil presented by R. Hammer is chosen to discretize the Dirac spinor.

$$\Psi = \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix}$$

Discretization

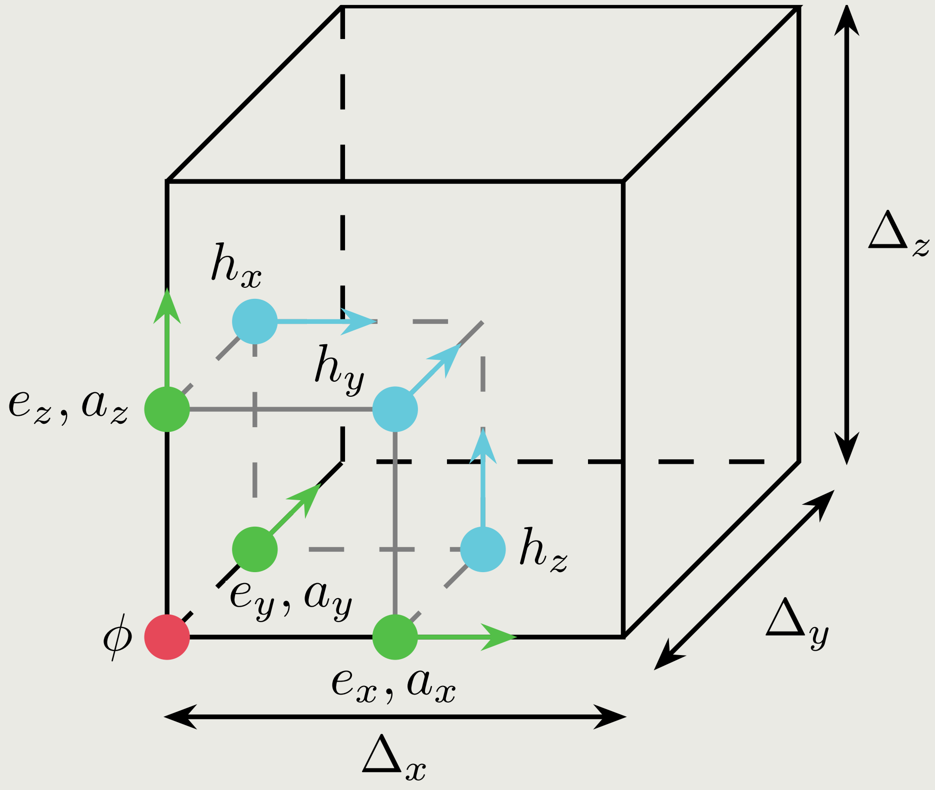


# Yee's method for Maxwell's equations is well-established and versatile.

EM fields $\tilde{e}$ and $\hat{h}$

EM potentials $\tilde{a}$ and $\phi$

Discretization



# The final scheme is easily conceptualized with a flowchart.

$$
\begin{tikzcd}
{} \arrow[r, "\text{Initialization}"] & \phi^{n+\frac{1}{2}} \arrow[r, "\text{Interpolate } \boldsymbol{a} \text{ and } \boldsymbol{\phi}"] & A^{n+\frac{1}{2}}, B^{n+\frac{1}{2}} \arrow[r, "\text{Interpolate } \boldsymbol{\Psi}"] & \tilde{\boldsymbol{\jmath}}_q^{\,n} \arrow[d] \\
C^{n+1}, D^{n+1} \arrow[u] & & \hat{\boldsymbol{h}}^{n+1}, \tilde{\boldsymbol{a}}^{n+1} \arrow[ll, "\text{Interpolate } \boldsymbol{a} \text{ and } \boldsymbol{\phi}"'] & \tilde{\boldsymbol{e}}^{n+\frac{1}{2}} \arrow[l]
\end{tikzcd}
$$

Discretization of the Maxwell-Dirac equations

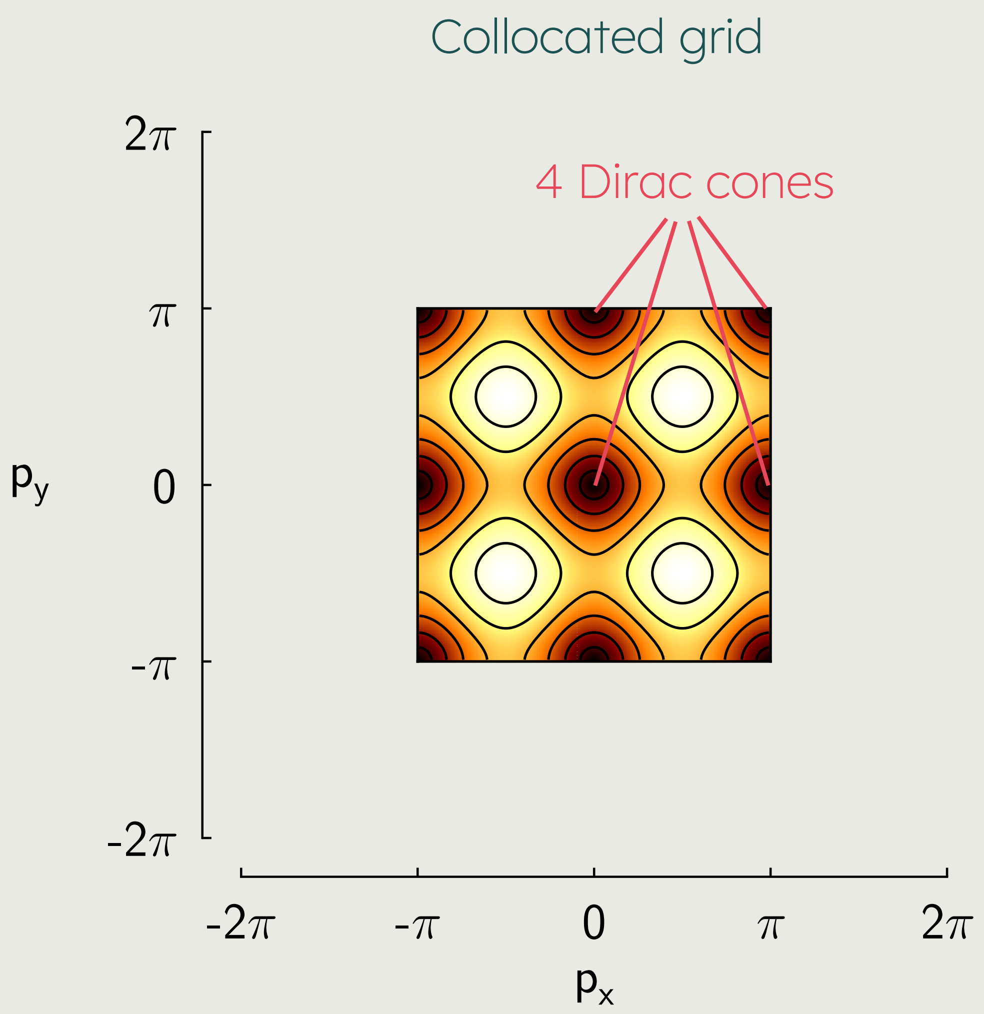
Properties of the novel method

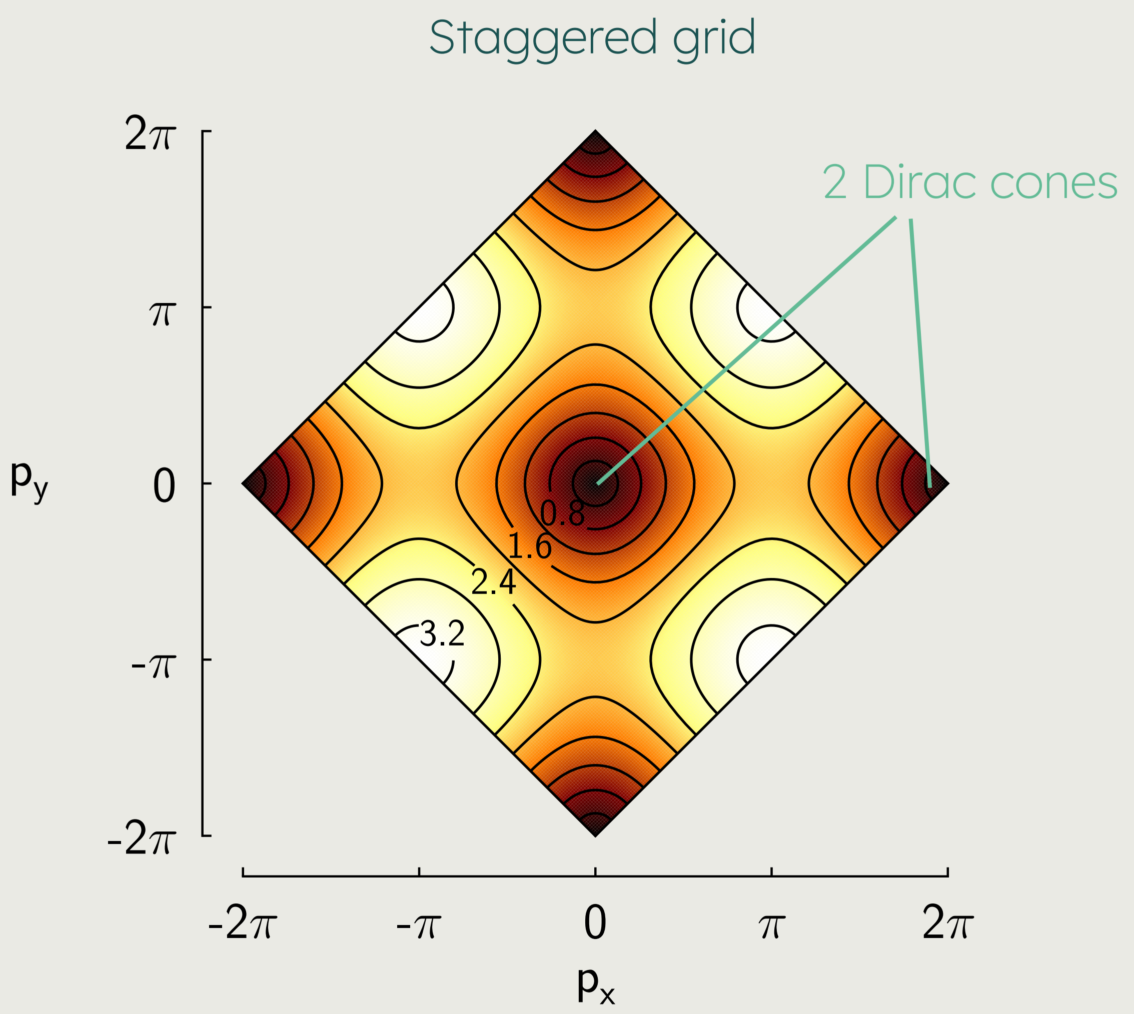
Conservation laws

Simulation of $ZrTe_5$ waveguide

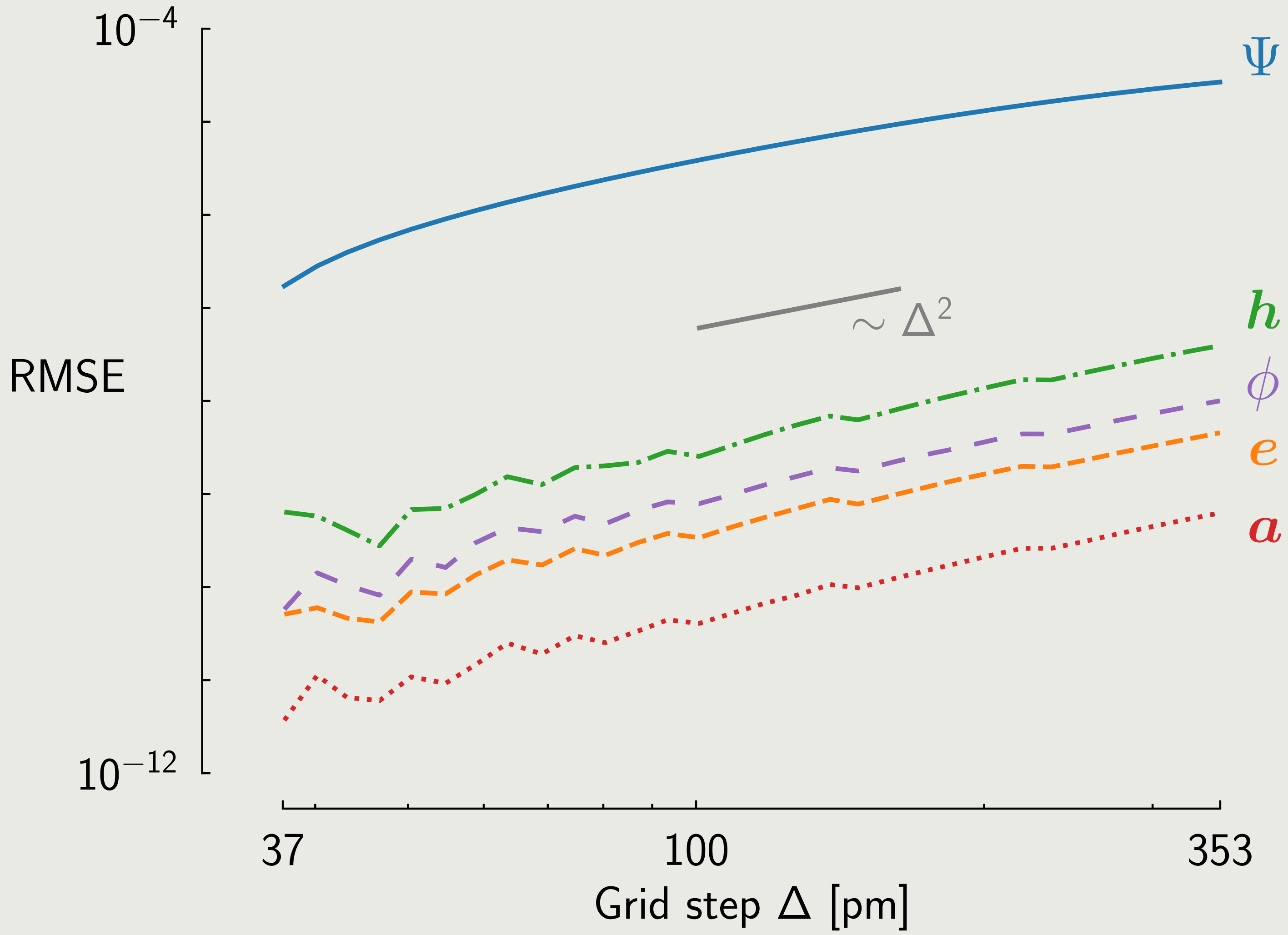
Future work

# The staggered grid alleviates the fermion doubling problem.



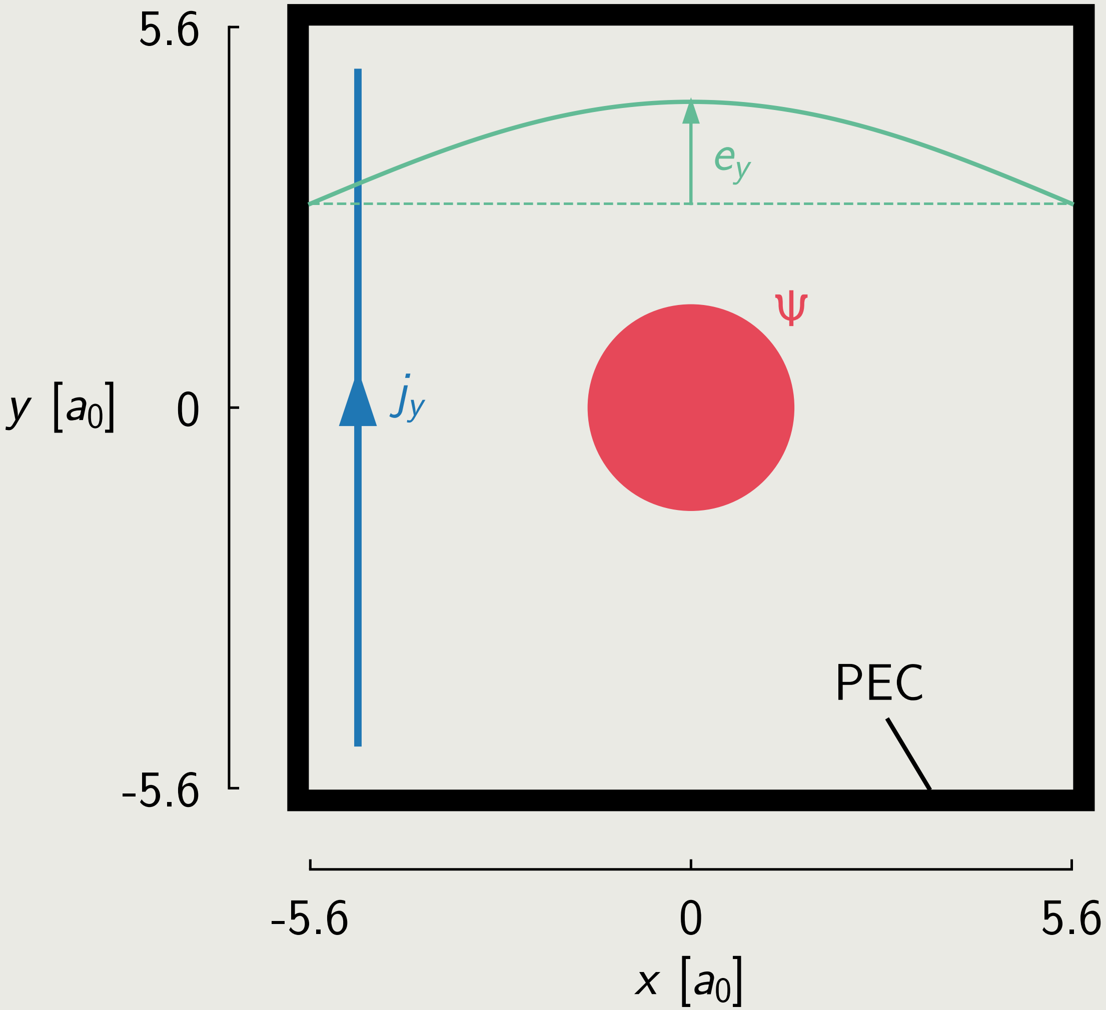
# The fully-coupled scheme is second-order accurate in both space and time.



# Our method neatly combines these schemes, while maintaining their properties.

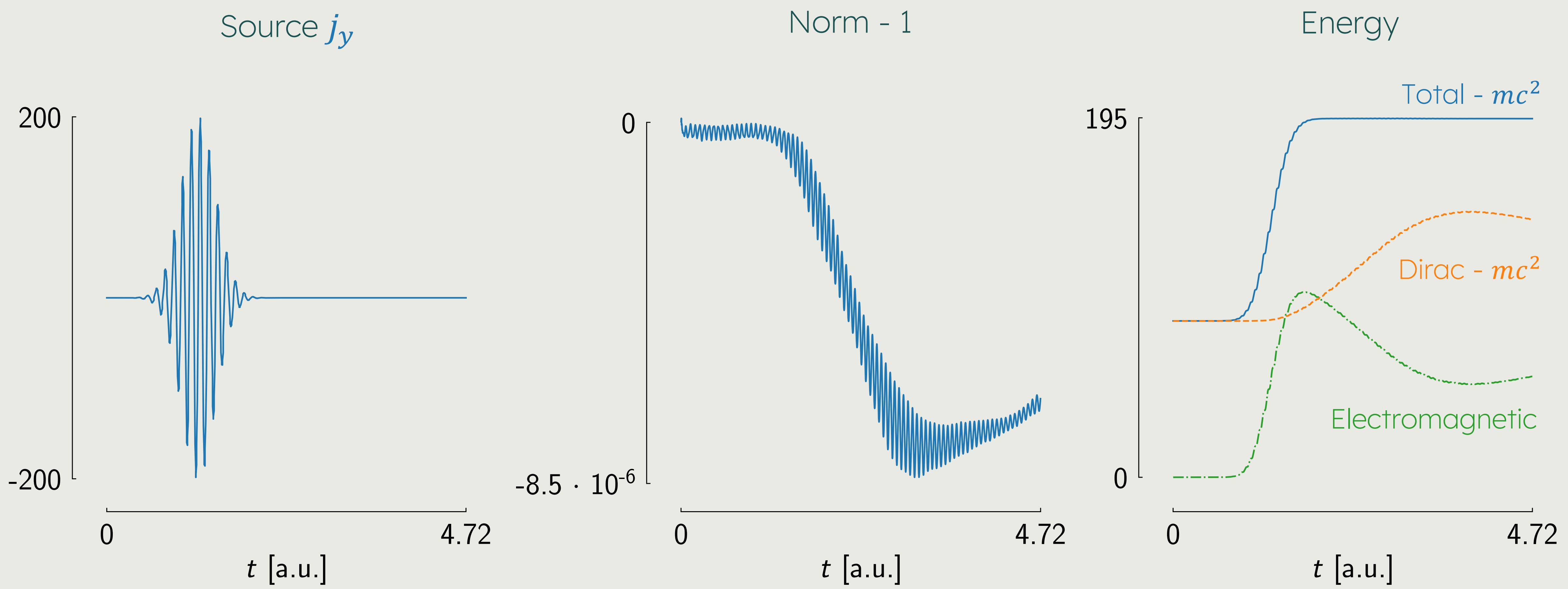
- Less fermion doubling
- Second-order accurate in space and time
- Integrable with existing CEM methods
- Exactly satisfying the Lorenz gauge
- Explicit method

# A Dirac particle is coupled to an EM cavity to demonstrate conservation of probability and energy.



# The results show the excellent conservation properties.

All quantities are expressed in Hartree atomic units.



Discretization of the Maxwell-Dirac equations

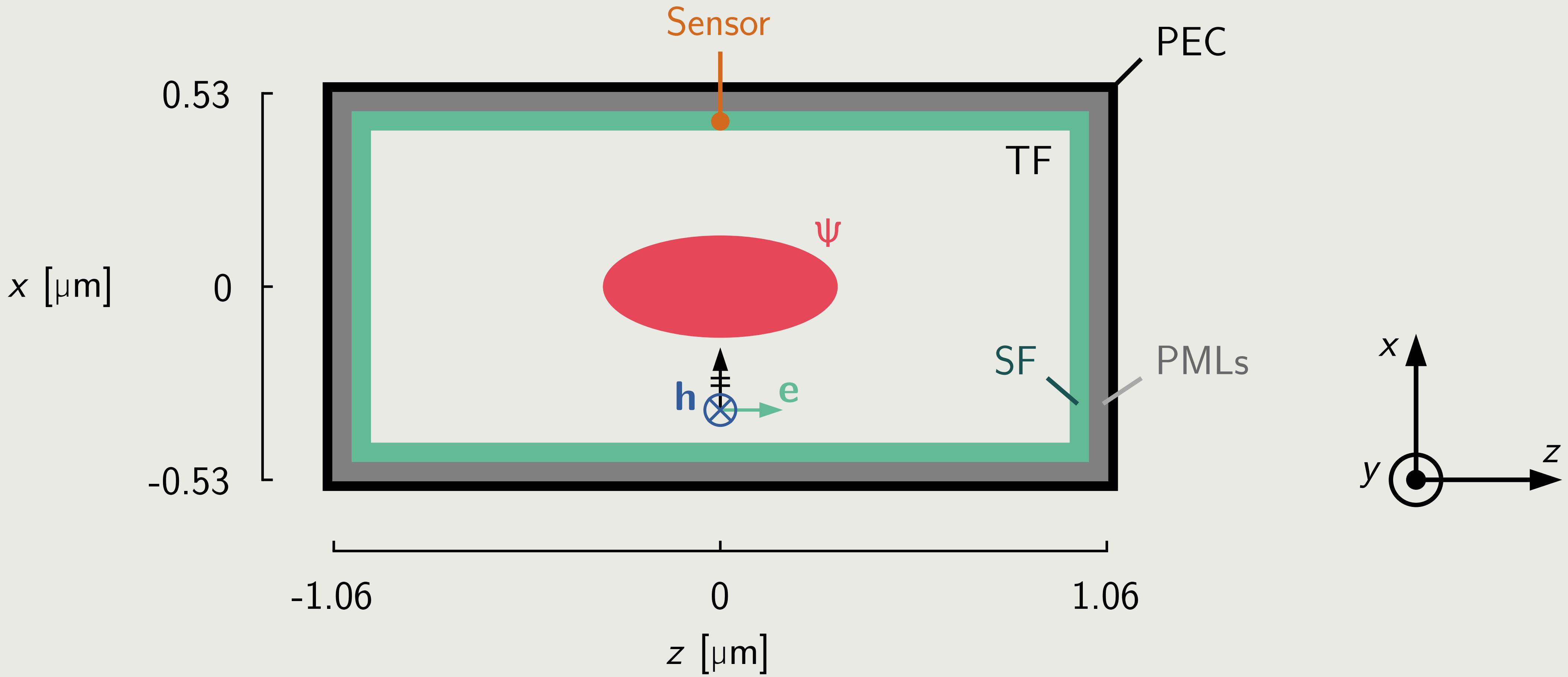
Properties of the novel method

Conservation laws

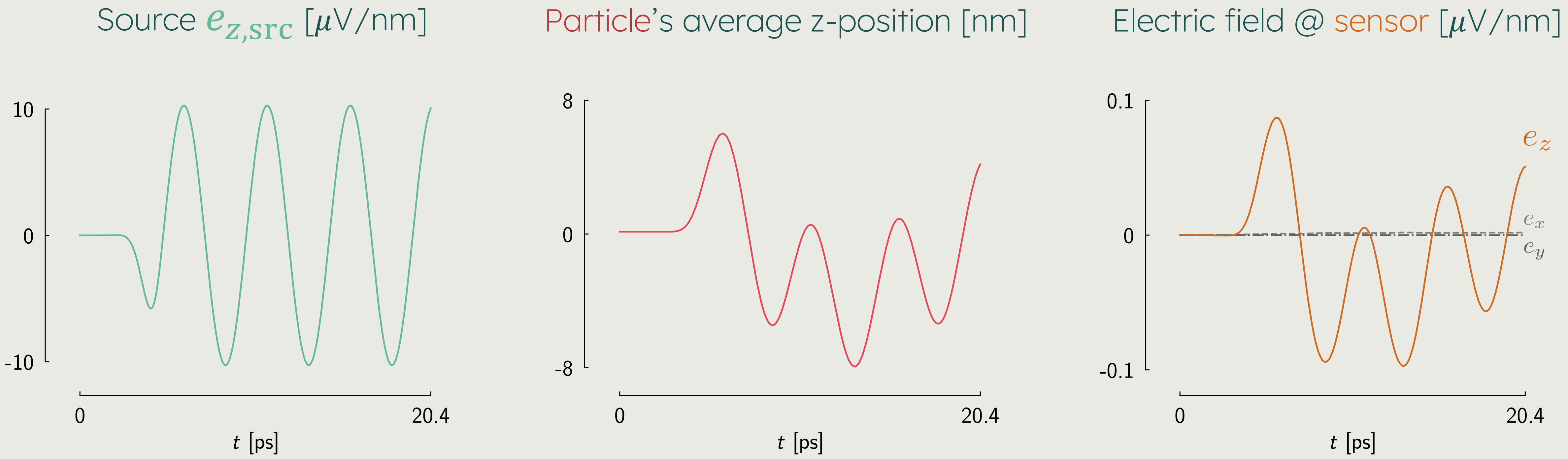
Simulation of a $ZrTe_5$ waveguide

Future work

# An EM plane wave impinging on a Dirac particle in a $ZrTe_5$ waveguide is simulated.



# The particle is quickly accelerated and generates its own electric field.



Discretization of the Maxwell-Dirac equations

Properties of the novel method

Conservation laws

Simulation of $ZrTe_5$ waveguide

Future work

# There is plenty of room for further progress.

- Dielectric materials
- (Ohmic) contacts
- More complex device structures
- Zeeman effect
- Chiral magnetic effect
- ...

Discretization of the Maxwell-Dirac equations

Properties of the novel method

Conservation laws

Simulation of $ZrTe_5$ waveguide

Future work

quest.

Quantum Mechanical &
Electromagnetic Systems
Modelling Lab

GHENT UNIVERSITY

imec

Technologiepark–Zwijnaarde 126, B-9052 Gent, Belgium
T +32 9 331 48 81 — **jul.vandenbroeck@ugent.be**
**www.questlab.be**

Jul Van den Broeck, PhD Researcher.