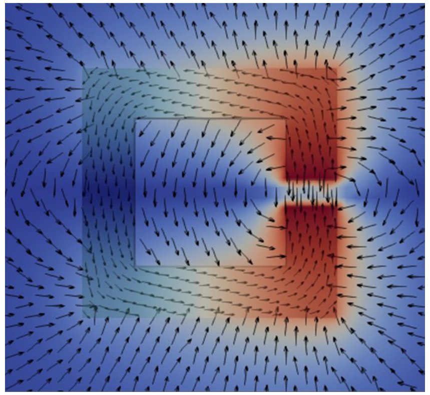
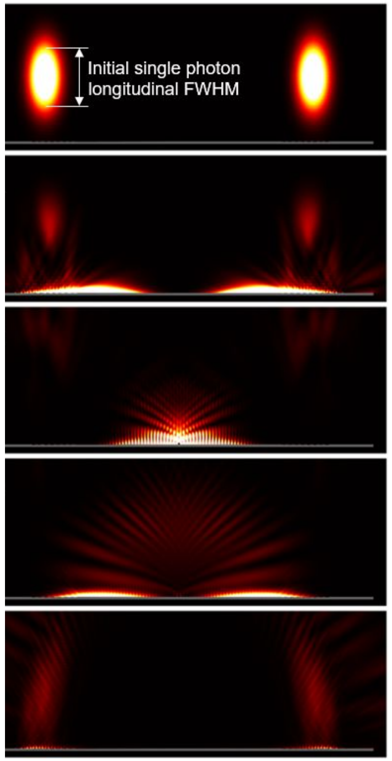
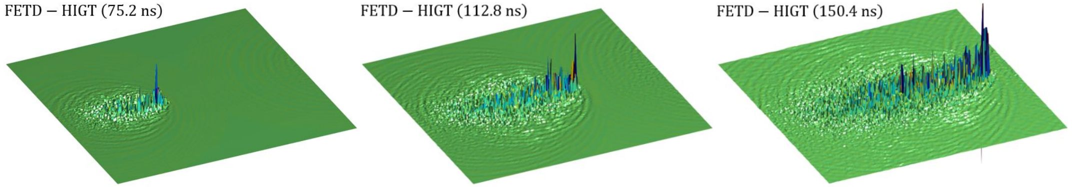
멀티피직스 전자기 수치해석 방법론: 고에너지 플라즈마 시스템 및 양자 전자기 현상 모델링

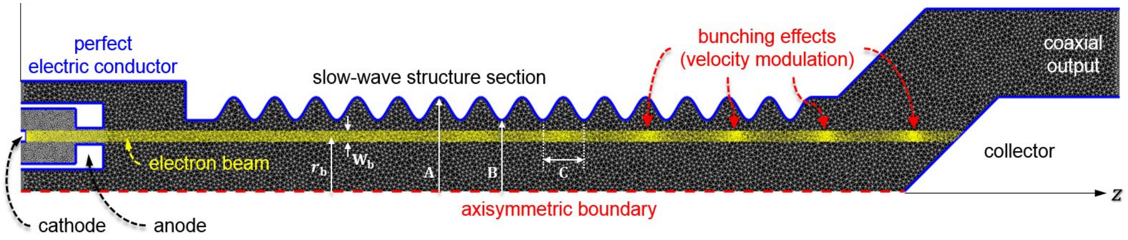
나동엽

포항공과대학교
전자전기공학과









2023년 한국전자파학회 하계종합학술대회 워크숍
(전자장해석) 2023년 8월 23일(수), 강원도 고성

Value Creating University
POSTECH

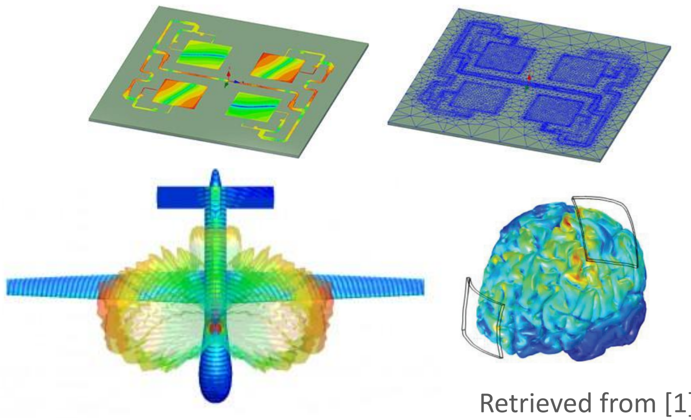
Outline

- ❑ **Computational Electromagnetics (CEM): Current state and challenges**

- ❑ **Research Experience**
  - ➢ **Research topic 1: 'Multiphysics' Electromagnetics**
    - Particle-in-Cell algorithms for high energy plasma modeling
  - ➢ **Research topic 2: 'Multiscale' Electromagnetics**
    - Lorenz-gauged $\mathbf{A} - \Phi$ solver stable over ultra-wideband (DC-to-Optics)
  - ➢ **Research topic 3: Quantum Electromagnetics/Optics**
    - Canonical quantization via numerical mode decomposition / Langevin noise formalism

- ❑ **Concluding Remarks**

Current State and Challenges of Computational Electromagnetics (CEM)

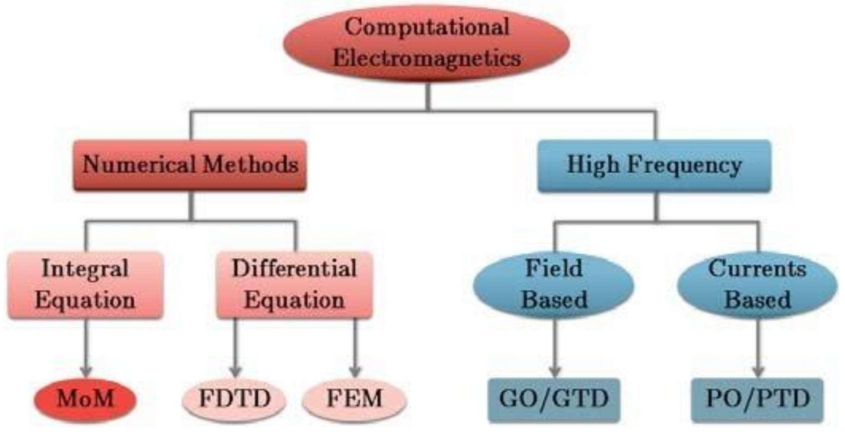


Retrieved from [1]

"Efficiency and Efficacy"

Maxwell's equations ⟶ Linear systems $\bar{\mathbf{A}} \cdot \mathbf{x} = \mathbf{b}$

- ✔ Differential equations
- ✔ Integral equations
- ✔ High frequency approximation



Reproduced from [2]

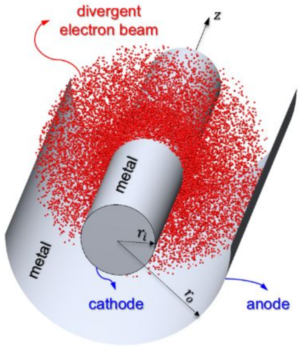
Challenges

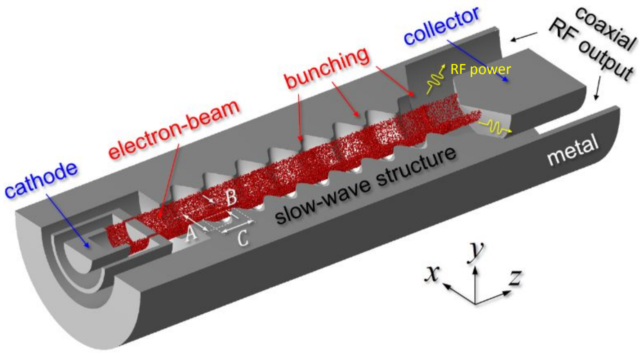
- Modern wireless devices are **highly integrated**, exhibiting the significant difference in the **characteristic scale**.
- **Non-classical** effect-related issues (uncertainty, superposition, or entanglement) need to be addressed in quantum information science technology.
- In the state-of-the-art EM technology, **multiphysics** comes into an important play, e.g., kinematics, thermodynamics, etc.

[1] https://www.inas.ro/en/ansys-electronics-hfss, S. N. Makarov *et al.*, *IEEE reviews in biomedical engineering*, vol. 10, pp. 95-121 (2017)
[2] J. Moreno *et al.*, *IEEE Aerospace and Electronic Systems Magazine*, vol. 34, no. 7, pp. 18-31 (2019).

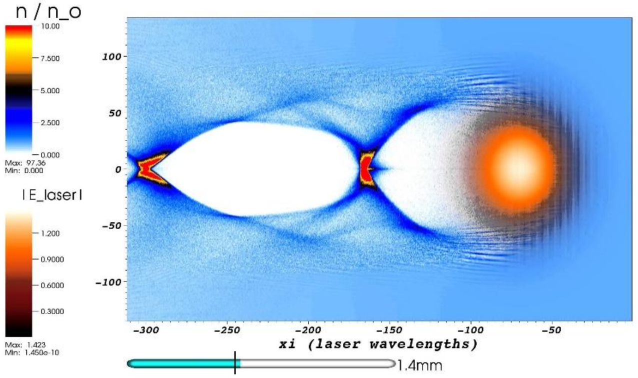
Applications of High Energy Plasmas

High-power microwave devices



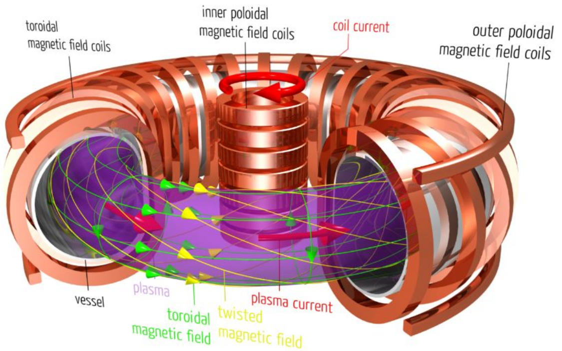


Particle accelerators



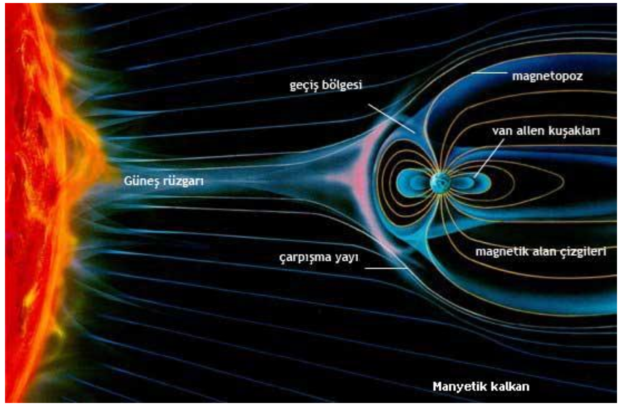
Reproduced from [4]

Fusion devices



Retrieved from [3]

Astronomical/ atmospheric effects



Reproduced from [5]

[3] https://acee.princeton.edu/acee-news/10-facts-about-fusion-energy-via-magnetic-confinement/
[4] https://shvets.ph.utexas.edu/research/laser-wakefield
[5] http://www.theapproachinghour.com/earth/magnetic_shield/the_magnetic_shield_protecting_earth_magnetosphere.asp

고에너지 플라즈마 모델링 방법

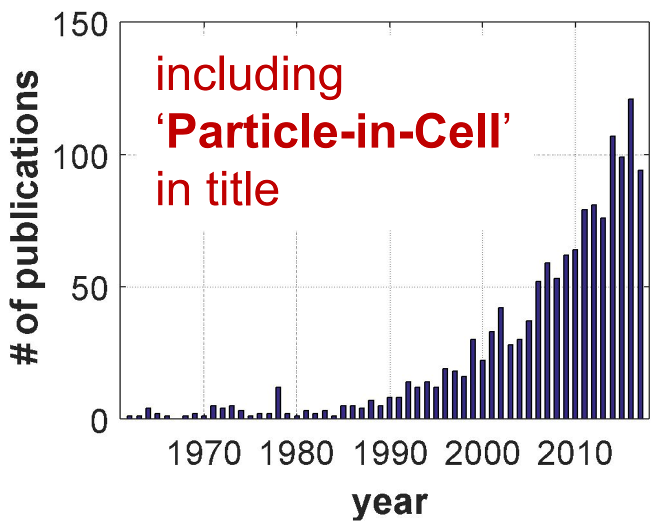
[1]

	Magnetohydrodynamics	Two Fluids	Gyrokinetics	Kinetics	Everything
Description	The plasma is one continuous fluid - ions have all the mass, but electron carry all the current.	Break the ions & electrons into two continuous, mingling fluids.	Only track superparticles straight motion - and ignore the corkscrewing.	Assign particles a speed and location based on a distribution. Track super particles through space.	Track every particle, at all times.
Strengthens	Easily solved.	Simple bulk effects like drift waves & reconnection can be understood.	Captures most of kinetic model, but much easier to solve - can model an entire Tokamak.	Many things captured, can get powerful results like the linear velocity-space instabilities.	Most accurate model possible.
Weakness	Most things not captured: most plasma waves, leakage, kinetic instabilities, structures etc.	Many things not captured: plasma instabilities, large effects & non-equilibrium effects. Assumes bell curves.	Non-physical behavior over long times: resonances & adiabatic invariants can be lost.	Tough to solve: hard to apply to full size reactors. Loses some effects:	Typically impossible to solve.
Mathematics	Navier-stokes, Lorentz force, Maxwells' equations.	Navier-stokes, Lorentz force, Maxwells' equations.	Vlasov-Maxwell Expansion Equation	Collisionless Plasmas	Klimontovich Model

Plasma as a fluid (Chalkboard) — Plasma as a gas (Computer Required)

Simplicity — Detial

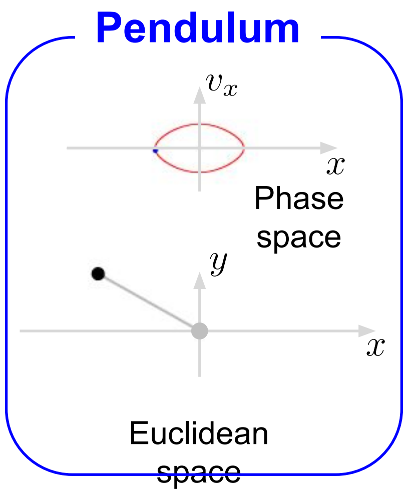
- **Particle-in-Cell** (1950)
  - Numerical technique for **Maxwell-Vlasov** eqn. (collisionless plasmsa)
  - Buneman, Dawson, Hockney, Birsall, Morse
  - `CST PARTICLE STUDIO`, `VSim`, `CONPIC` etc.
  - Plasma-based acceleration / fusion, High power microwaves, Astrophysics



[1] https://en.wikipedia.org/wiki/Plasma_modeling

Vlasov Equation

- Phase space distribution function: $f\left(\mathbf{x}, \mathbf{p}, t\right)$
  - Phase space consists of position and momentum (6-dim.).
  - It describes **states of an ensemble with many particles**.

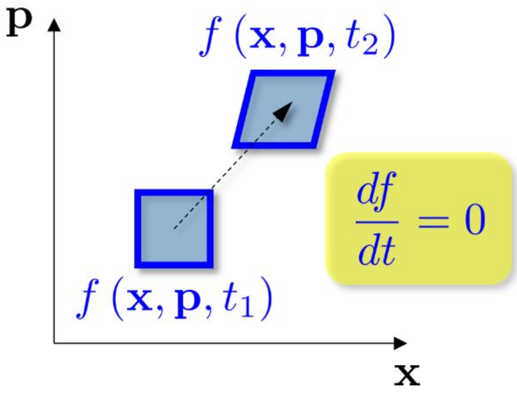


- **Vlasov** eqn. (Boltzmann eqn. w/o collisions)
  - describes the time evolution of collisionless plasmas as

$$\frac{df\left(\mathbf{x}, \mathbf{p}, t\right)}{dt} = 0 \quad \Rightarrow \quad \frac{\partial f}{\partial t} + \frac{d\mathbf{x}}{dt} \cdot \nabla_{\mathbf{x}} f + \frac{d\mathbf{p}}{dt} \cdot \nabla_{\mathbf{p}} f = 0$$

  - Particles are **uncorrelated** and **collectively interact** through long-range electromagnetic (Coulomb) forces.
  - Collisionless plasmas are **hot** (very fast) and **dilute**.

characteristic time		collisional time
characteristic length		mean free path



Coarse-Grained $f(\mathrm{x}, \mathrm{v}, t)$: “Super-Particle”

- **The phase space volume is preserved** (incompressible) over time due to ‘**collisionless**’ feature.

$$f = \sum_{s}^{e,i} f_s \qquad f_s = \sum_{p=1}^{N_p} f_p$$

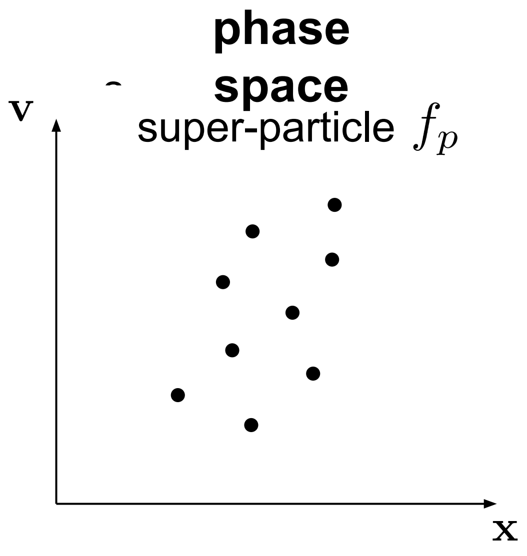
by species

segmented

shape function

$$f_p = q_s C_p \underbrace{S\left(\mathbf{x} - \mathbf{x}_p\right)}_{\text{space}} \underbrace{S\left(\mathbf{v} - \mathbf{v}_p\right)}_{\text{velocity}}$$

$$\boxed{f_p \approx q_s C_p \delta\left(\mathbf{x} - \mathbf{x}_p\right) \delta\left(\mathbf{v} - \mathbf{v}_p\right)}$$



- another option is with B-spline:

$$f_p = q_s C_p B_l\left(\mathbf{x} - \mathbf{x}_p\right) \delta\left(\mathbf{v} - \mathbf{v}_p\right)$$

- Each superparticle usually represents millions of actual electrons or ions.
- It results in a large reduction of the computational load.

Maxwell-Vlasov System (Multiphysics)

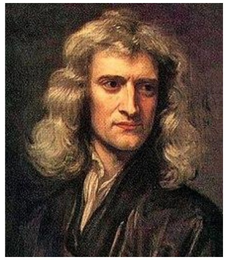
- Derivation of equations of motion coupled to EM fields
  - Applying 'Moment 0, $1_{\mathbf{x}}$, $1_{\mathbf{v}}$' into Vlasov equation,

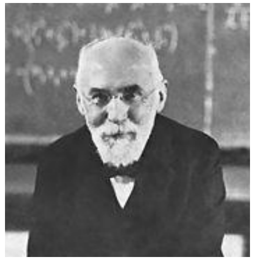
$$\iiint_{\mathbb{R}^3_{\mathbf{v}}} \iiint_{\mathbb{R}^3_{\mathbf{x}}} (\dots)\, d\mathbf{x} d\mathbf{v} \qquad \iiint_{\mathbb{R}^3_{\mathbf{v}}} \iiint_{\mathbb{R}^3_{\mathbf{x}}} (\dots) \cdot \mathbf{x} d\mathbf{x} d\mathbf{v} \qquad \iiint_{\mathbb{R}^3_{\mathbf{v}}} \iiint_{\mathbb{R}^3_{\mathbf{x}}} (\dots) \cdot \mathbf{v} d\mathbf{x} d\mathbf{v}$$

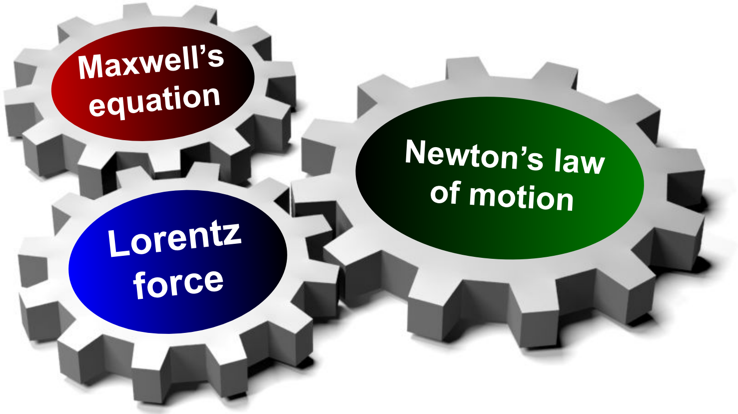
1 $$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p$$

2 [redacted]

3 $$\begin{cases} \nabla \times \mathbf{E} = -\dfrac{\partial \mathbf{B}}{\partial t} \\ \nabla \times \mathbf{H} = \dfrac{\partial \mathbf{D}}{\partial t} + \mathbf{J} \end{cases}$$

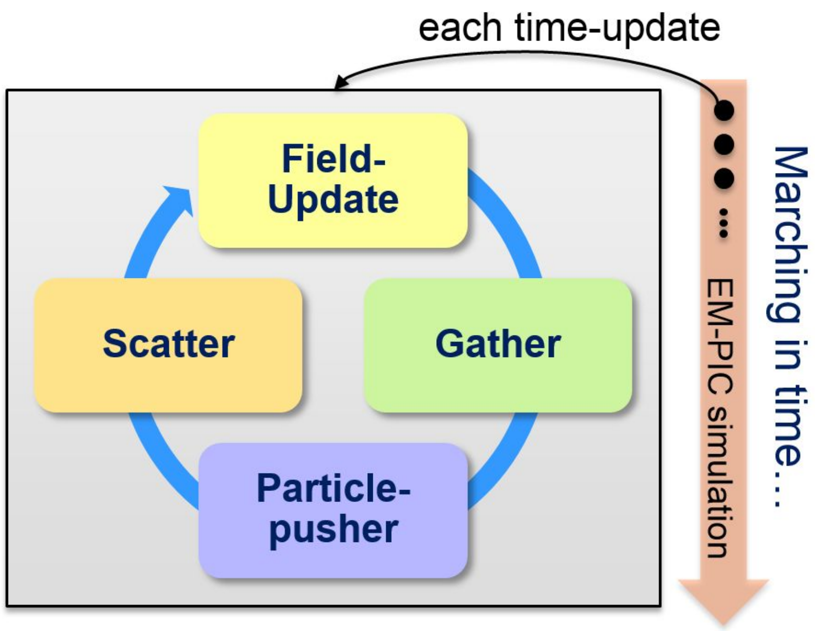




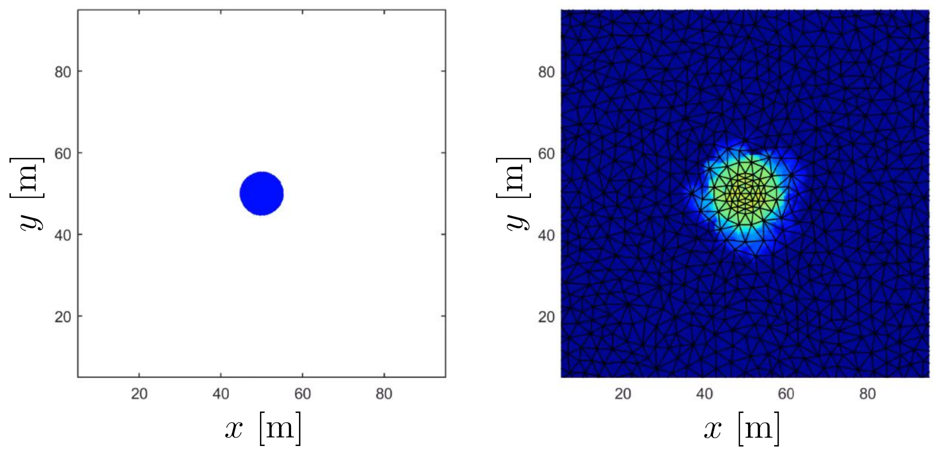


Electromagnetic Particle-in-Cell (EM-PIC)

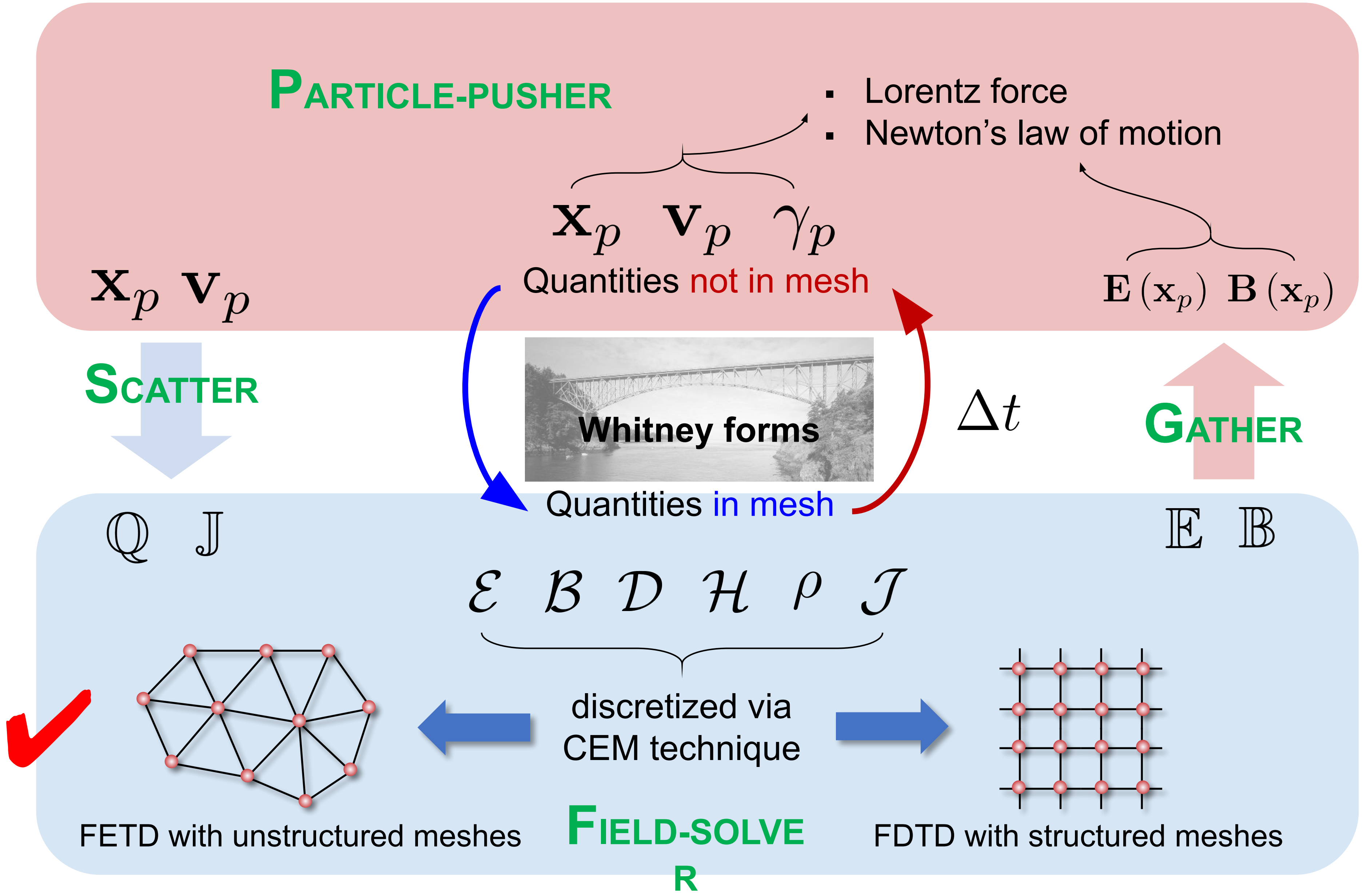
- Numerical technique to solve Maxwell-Vlasov system
- Updating (i) Maxwell's fields and
  (ii) Superparticle's kinetic parameters marching on time
- Origin of the name 'Particle-in-Cell' (Particle-Mesh)
- 4 fundamental steps at each time update :



Example of PIC for Plasma ball expansion



Coarse-Grained $f(x, v, t)$: "Super-Particle"



How to Model High Energy Plasmas?

Maxwell-Vlasov equations

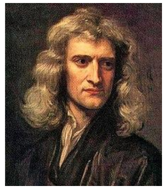
1 $$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p$$

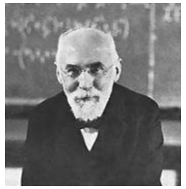
2 $$\frac{d(\gamma_p \mathbf{v}_p)}{dt} = \frac{q}{m_0}\left(\mathbf{E}_p + \mathbf{v}_p \times \mathbf{B}_p\right)$$

3 $$\begin{cases} \nabla \times \mathbf{E} = -\dfrac{\partial \mathbf{B}}{\partial t} \\ \nabla \times \mathbf{H} = \dfrac{\partial \mathbf{D}}{\partial t} + \mathbf{J} \end{cases}$$

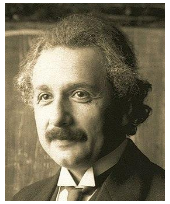
The **linear theory is no longer available** (e.g., Lorentz-Drude model and gyroscopic description)

Full description on kinematics of charged particles in reaction to electromagnetic fields is needed (**via Maxwell-Vlasov systems**).

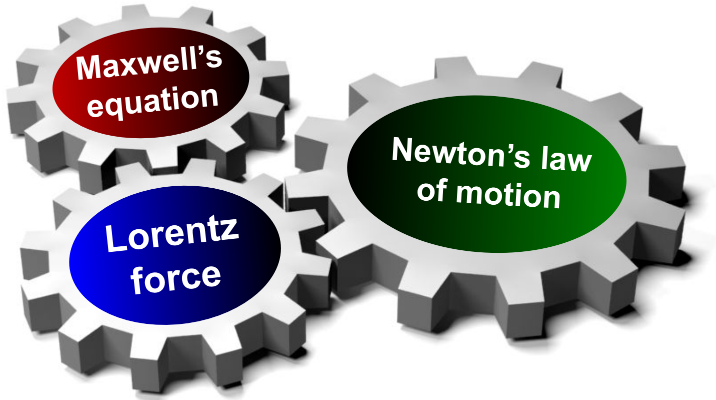




+

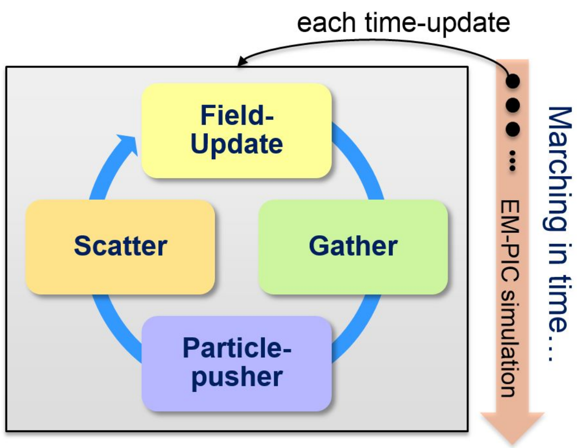


Special relativity

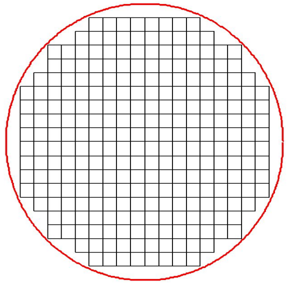


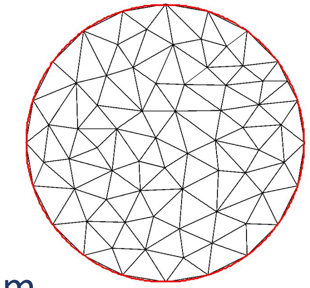
Multiphysics Involved

Utility and Limitations of Particle-in-Cell (PIC) Algorithms



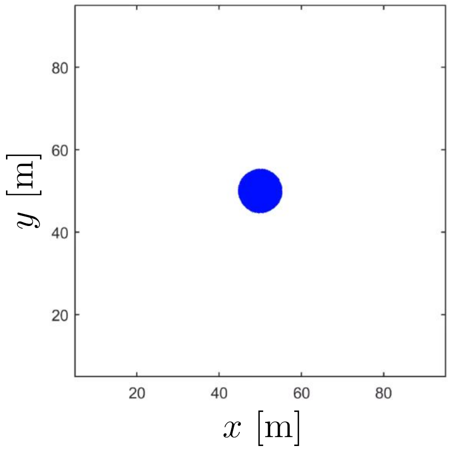
- **Particle-in-Cell (PIC) algorithms**
  - ✔ Superparticles (each particle representing few millions of actual charged particles)
  - ✔ Field-solver □ Gather □ Particle push □ Scatter

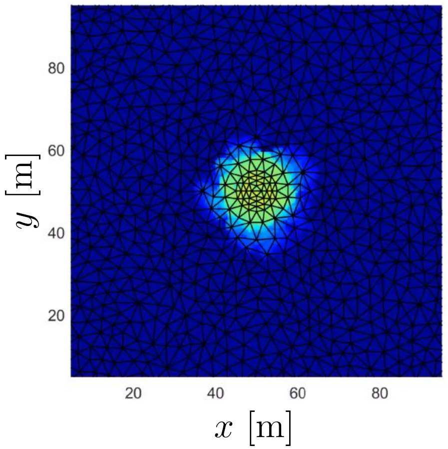




- **Issues in existing PIC algorithms**
  - ✔ Most of them have relied on **finite-difference time-domain methods** on structure meshes (low geometric fidelity).
  - ✔ The unstructured-mesh-based PIC has suffered from the **violation of charge conservation**

Example of PIC for Plasma ball expansion





- **Novelty of this work:**
  - ✔ Uses discrete exterior calculus (DEC) for consistent discretization
  - ✔ Obtains exact charge conservation on unstructured mesh from the first principle.

Maxwell’s Equations in Differential Forms

Exterior derivative

$$\boxed{d}\mathcal{E} = -\frac{\partial \mathcal{B}}{\partial t} \qquad \boxed{d}\mathcal{H} = \frac{\partial \mathcal{D}}{\partial t} + \mathcal{J} \qquad \mathcal{D} = \boxed{\star_\epsilon}\mathcal{E} \qquad \mathcal{B} = \boxed{\star_\mu}\mathcal{H}$$

Hodge star operator

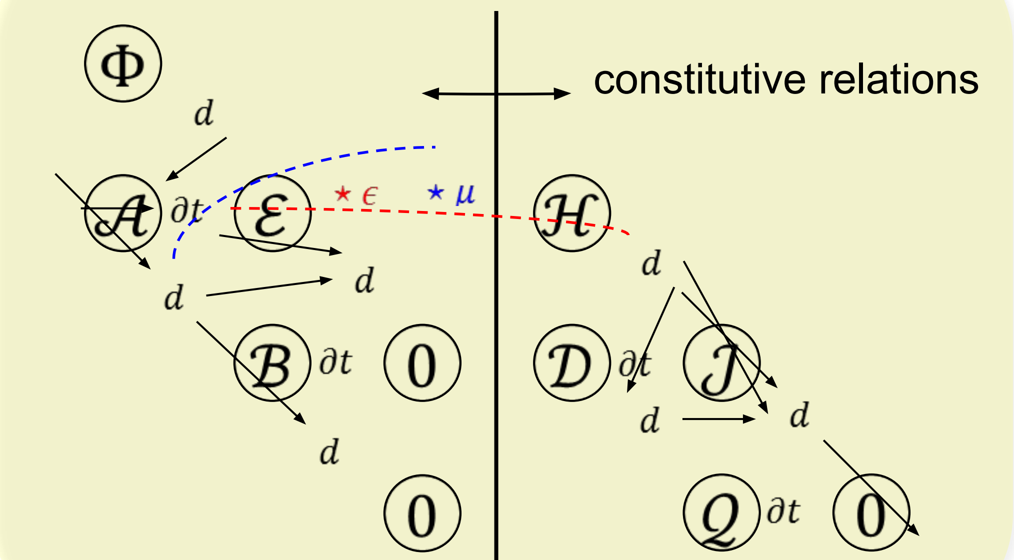
$$\mathcal{E} = E_x dx + E_y dy + E_z dz \qquad \mathcal{B} = B_x dy \wedge dz + B_y dz \wedge dx + B_z dx \wedge dy$$

dual

$$\mathbf{E} = E_x \mathbf{x} + E_y \mathbf{y} + E_z \mathbf{z} \qquad \mathbf{B} = B_x \mathbf{x} + B_y \mathbf{y} + B_z \mathbf{z}$$

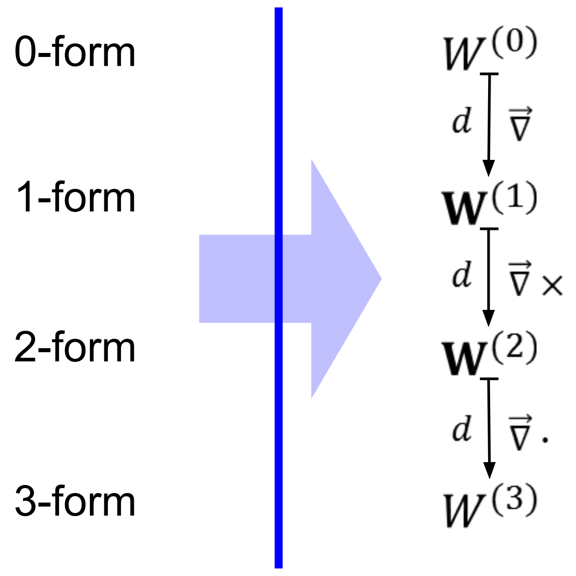
(easily translatable)

Tonti diagrams



Orientation: Original form | Twisted form

Whitney forms



consistent discretization

Maxwell’s Equations in Differential Forms

in primal mesh

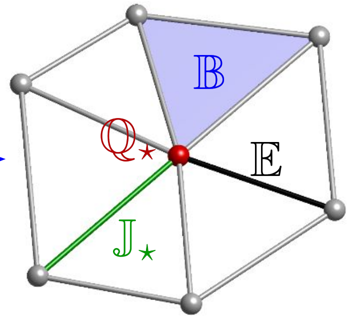
$$\mathbf{E}(\mathbf{r},t) \approx \sum_{j=1}^{N_1} \mathbb{E}_j(t)\, \mathbf{W}_j^{(1)}(\mathbf{r})$$

$$\mathbf{B}(\mathbf{r},t) \approx \sum_{k=1}^{N_2} \mathbb{B}_k(t)\, \mathbf{W}_k^{(2)}(\mathbf{r})$$

$$\mathbf{J}_\star(\mathbf{r},t) \approx \sum_{j=1}^{N_1} \mathbb{J}_{\star j}(t)\, \mathbf{W}_j^{(1)}(\mathbf{r})$$

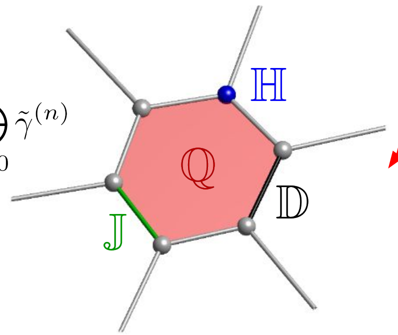
$$\mathbf{Q}_\star(\mathbf{r},t) \approx \sum_{i=1}^{N_0} \mathbb{Q}_{\star i}(t)\, W_i^{(0)}(\mathbf{r})$$

Degrees of freedom (DoF)



$$\mathcal{T} = \bigoplus_{n=0}^{3} \gamma^{(n)}$$

$$\tilde{\mathcal{T}} = \bigoplus_{n=0}^{3} \tilde{\gamma}^{(n)}$$



in dual mesh

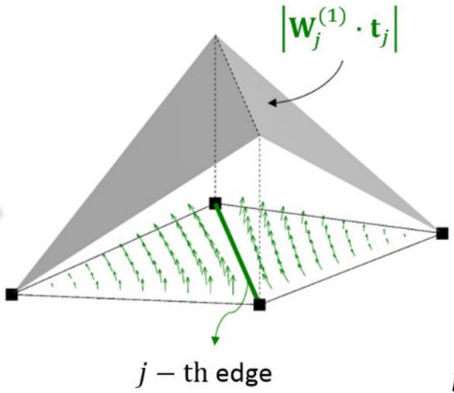
$$\mathbf{D}(\mathbf{r},t) \approx \sum_{\tilde{j}=1}^{\tilde{N}_2} \mathbb{D}_{\tilde{j}}(t)\, \tilde{\mathbf{W}}_{\tilde{j}}^{(2)}(\mathbf{r})$$

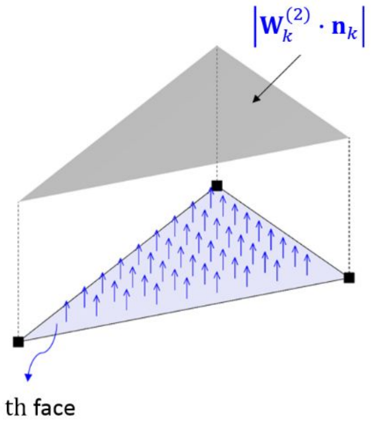
$$\mathbf{H}(\mathbf{r},t) \approx \sum_{\tilde{j}=1}^{\tilde{N}_1} \mathbb{H}_{\tilde{j}}(t)\, \tilde{\mathbf{W}}_{\tilde{j}}^{(1)}(\mathbf{r})$$

$$\mathbf{J}(\mathbf{r},t) \approx \sum_{\tilde{k}=1}^{\tilde{N}_2} \mathbb{J}_{\tilde{k}}(t)\, \tilde{\mathbf{W}}_{\tilde{k}}^{(2)}(\mathbf{r})$$

$$\mathbf{Q}(\mathbf{r},t) \approx \sum_{\tilde{l}=1}^{\tilde{N}_3} \mathbb{Q}_{\tilde{l}}(t)\, \tilde{W}_{\tilde{l}}^{(3)}(\mathbf{r})$$

Whitney forms (WF)





Discrete Exterior Calculus (DEC)

Cell complex in unstructured grids (in 3-D space)

$$\mathcal{T} = \bigoplus_{n=0}^{3} \gamma^{(n)} \qquad \gamma^{(0)} = \sum_{i=1}^{N_0} \sigma_i^{(0)} \qquad \gamma^{(1)} = \sum_{j=1}^{N_1} \sigma_j^{(1)} \qquad \gamma^{(2)} = \sum_{k=1}^{N_2} \sigma_k^{(2)} \qquad \gamma^{(3)} = \sum_{l=1}^{N_3} \sigma_l^{(3)}$$

$$d\mathcal{E} = -\frac{\partial \mathcal{B}}{\partial t}$$

Field expansions

$$d\mathcal{H} = \frac{\partial \mathcal{D}}{\partial t} + \mathcal{J}$$

space discretization

Leapfrog time integration

time discretization

Linear systems for DoFs
(discrete counterparts of Maxwell's eqn.)

$$\left\langle \sigma_i^{(p)}, w_j^{(p)} \right\rangle = \delta_{i,j}$$ (pairing □ contraction)

$$\left\langle \sigma_i^{(p)}, dw_j^{(p-1)} \right\rangle = \left\langle \partial\sigma_i^{(p)}, w_j^{(p-1)} \right\rangle$$ (generalized Stokes' theorem)

Coarse-Grained $f(\mathrm{x}, \mathrm{v}, t)$: "Super-Particle"

- Discrete representations of Maxwell's equations

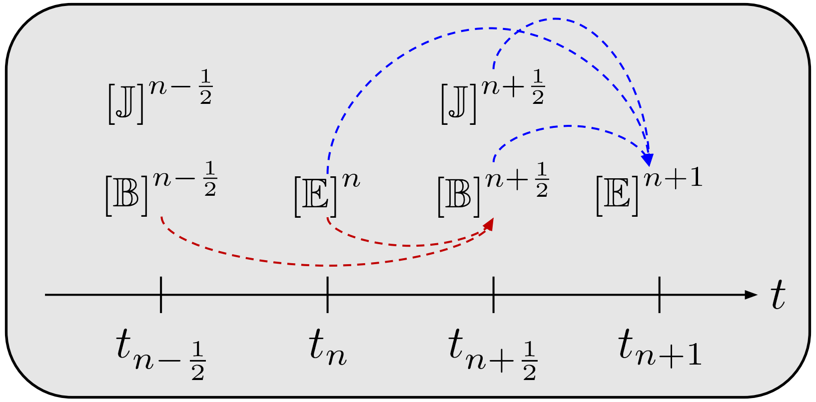
$$[\mathbb{B}]^{n+\frac{1}{2}} = [\mathbb{B}]^{n-\frac{1}{2}} - \Delta t \, [\mathcal{D}_{\text{curl}}] \cdot [\mathbb{E}]^{n}$$

[redacted]

implicit

$[\mathcal{D}_{\text{curl}}]$ is incidence matrix.
(topological and metric-free)

Leapfrog time integration



- Discrete constitutive relations

$$[\mathbb{D}] = [\star_{\epsilon}] \cdot [\mathbb{E}], \quad [\mathbb{H}] = [\star_{\mu}^{-1}] \cdot [\mathbb{B}]$$

$$\left.\begin{aligned} [\star_{\epsilon}]_{J,j} &= \epsilon \int_{\Omega} \mathbf{W}_{J}^{(1)} \cdot \mathbf{W}_{j}^{(1)} dV \\ [\star_{\mu}^{-1}]_{K,k} &= \mu^{-1} \int_{\Omega} \mathbf{W}_{K}^{(2)} \cdot \mathbf{W}_{k}^{(2)} dV \end{aligned}\right\}$$

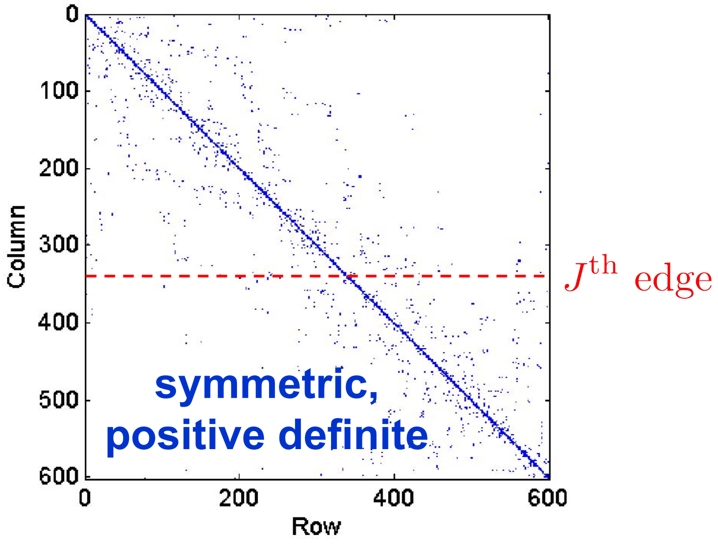
are discrete Hodge matrices.
(constitutive relations and all metric info.)

symmetric / positive-definite / symplectic
□ Conditionally stable, energy-conserving

Coarse-Grained $f(\mathrm{x}, \mathrm{v}, t)$: “Super-Particle”

$$[\star_\epsilon]_{J,j} = \epsilon \int_\Omega \mathbf{W}_J^{(1)} \cdot \mathbf{W}_j^{(1)} dV$$

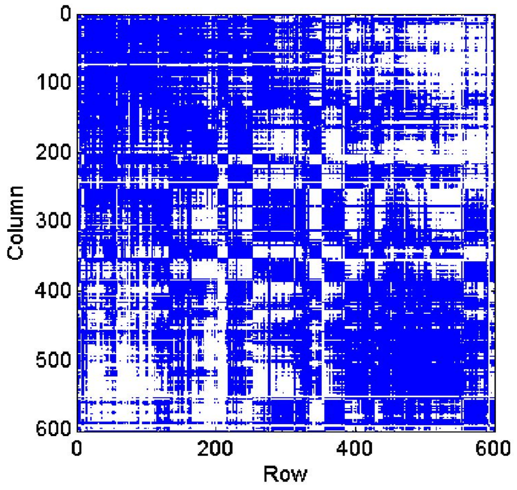
dominantly-diagonal and sparse



- Why $[\star_\epsilon]$ is sparse?
  1. their supports are compact.
  2. some pairs are overlapping.

$$[\star_\epsilon]^{-1}$$

LU decomposition

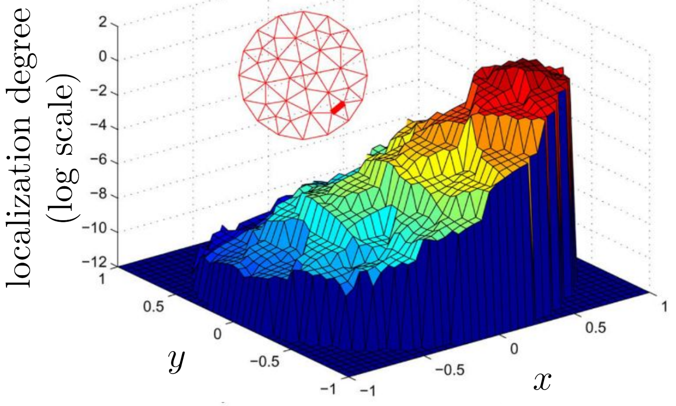


Inversion is costly and **Full !**

- **Mass lumping** (diagonalization) :
  It destroys positive definiteness leading to unconditionally unstable.

Coarse-Grained $f(\mathrm{x}, \mathrm{v}, t)$: "Super-Particle"

$[\star_\epsilon]^{-1}$ is strongly localized [1]



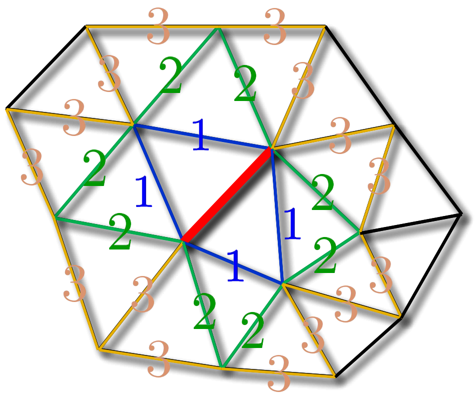
$[\star_\epsilon]_a^{-1}$ → sparse approximate inverse

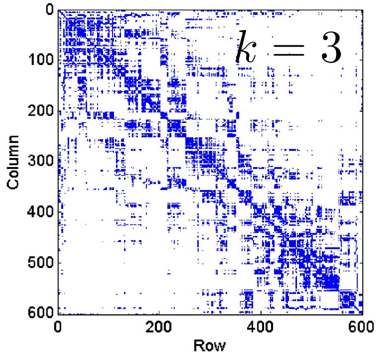
$$\boxed{[\star_\epsilon]^{-1}} \cdot \mathbb{D} = \mathbb{E} \qquad \mathbb{E} = \boxed{[\star_{\epsilon^{-1}}]} \cdot \mathbb{D}$$

$$[\star_\epsilon^{-1}]_{K,k} = \iiint_{\mathbb{R}^3} \tilde{\mathbf{W}}_K^{(2)} \cdot \tilde{\mathbf{W}}_k^{(2)} dV$$

[1] **B. He and F. L. Teixeira,** ***IEEE Trans. Antennas Propag.*****, vol. 55, pp. 1359-1368 (2007).**

- Algebraic thresholding
- Topological thresholding
  - Level of neighbor edges : k



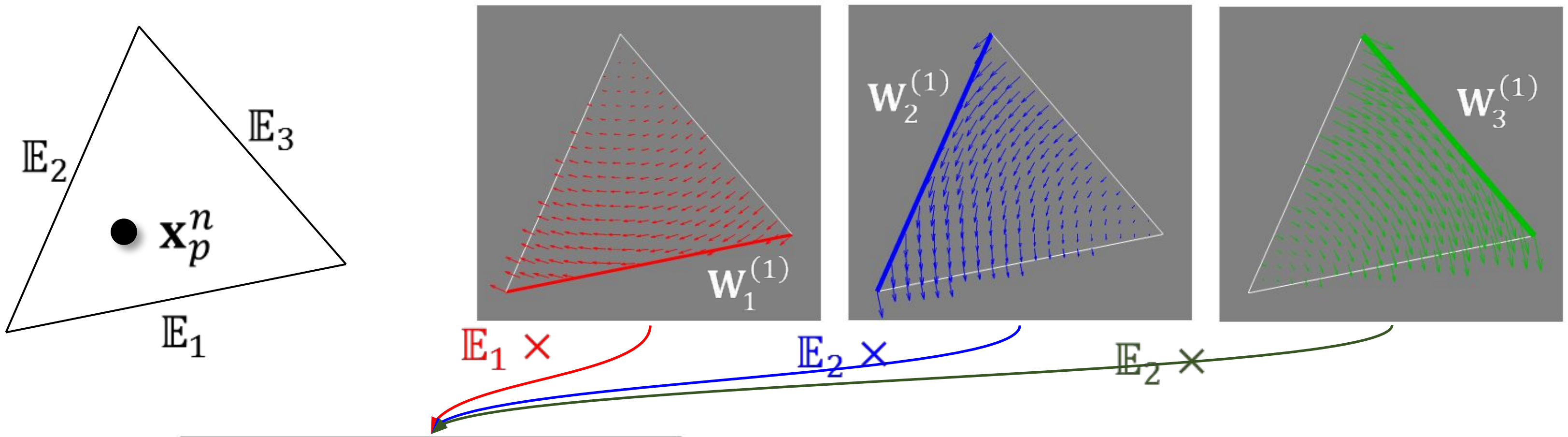


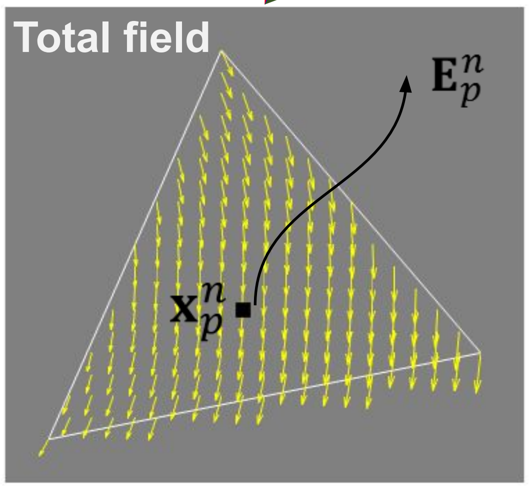
- $\text{Sparsity}\left([\star_\epsilon]_a^{-1}\right) = \text{Sparsity}\left([\star_\epsilon]^k\right)$
- Least square method for
  $$[\star_\epsilon]_a^{-1} \cdot [\star_\epsilon] - [I]$$

symmetric, positive definite, easily parallelizable

Coarse-Grained $f(\mathrm{x}, \mathrm{v}, t)$: "Super-Particle"

- Interpolation of electric field at particle's position via Whitney 1-forms:





$$\mathbf{E}(\mathbf{x}_p^n, t_n) = \mathbf{E}_p^n = \sum_{j=1}^{N_1} \mathbb{E}_j^n \mathbf{W}_j^{(1)}(\mathbf{x}_p^n)$$

Similarly, $\mathbf{B}_p^n$ can be evaluated with Whitney 2-forms.

Coarse-Grained $f(\mathrm{x}, \mathrm{v}, t)$: "Super-Particle"

- Plasma kinetic simulations are Nonlinear & Long-time evolution.

Hamiltonian dynamical systems ➡ **Numerical integrator** ➡ **1. Explicit** → Computational efficiency; **2. Symplectic** → Stringent condition for energy conservation (desirable for long time evolution)

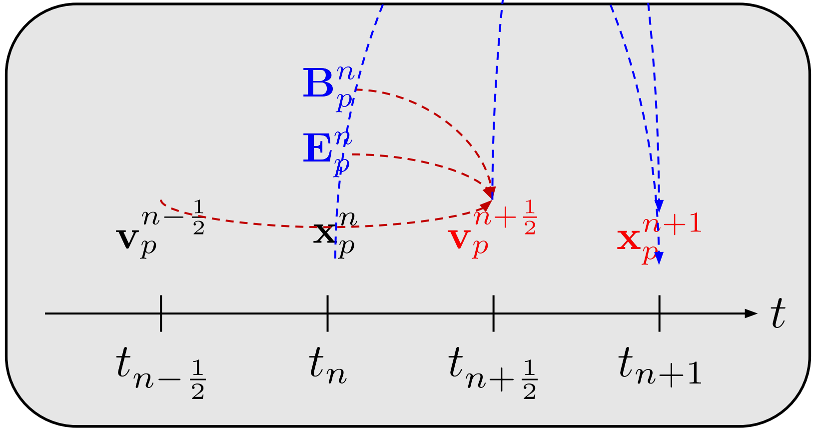
for arbitrary field distribution

Phase space volume preserving $\leftarrow$ / $\not\rightarrow$ **Symplectic**

(relaxed condition for energy conservation)

- Time derivatives are discretized through central difference method as
  - $\mathbf{v}_p^{n+\frac{1}{2}} = \mathbf{v}_p^{n-\frac{1}{2}} + \Delta t \dfrac{q_p}{m_p} \left(\mathbf{E}_p^n + \bar{\mathbf{v}}_p \times \mathbf{B}_p^n \right),$
  - $\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \Delta t \mathbf{v}_p^{n+\frac{1}{2}}$

average velocity



- Implicit (expensive, accurate)
- **Boris algorithm**
  (explicit, phase-volume-preserving)

Coarse-Grained $f(\mathrm{x}, \mathrm{v}, t)$: “Super-Particle”

- Decomposition of **irrotational** and **rotational** forces (1970)

[redacted]

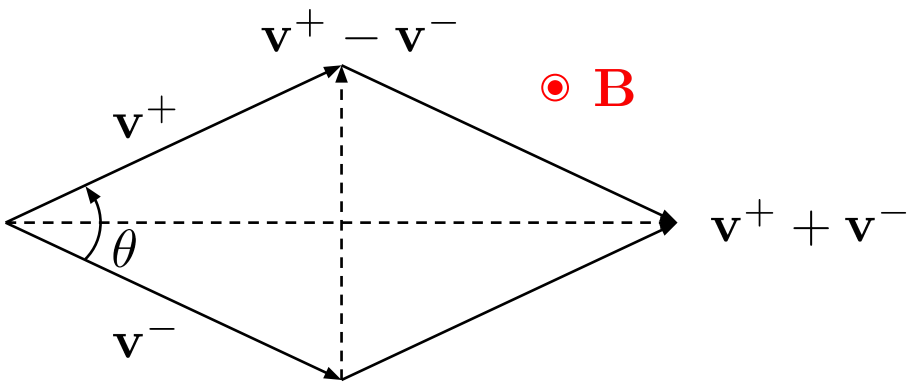
$$\epsilon = \frac{q\mathbf{E}}{2m_0}\Delta t \qquad \beta = \frac{q\,|B|}{m_0}\Delta t/2 = \omega_c \Delta t/2$$

$$\mathbf{v}^{n-\frac{1}{2}} = \mathbf{v}^{-} - \boldsymbol{\epsilon}$$

$$\mathbf{v}^{n+\frac{1}{2}} = \mathbf{v}^{+} + \boldsymbol{\epsilon}$$

$$\frac{\mathbf{v}^{+} - \mathbf{v}^{-}}{\Delta t} = \frac{q}{2m_0}\frac{\mathbf{v}^{+} + \mathbf{v}^{-}}{2} \times \mathbf{B}^{n}$$

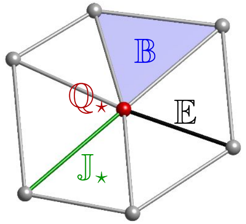
$$\left|\tan\frac{\theta}{2}\right| = \frac{|\mathbf{v}^{+} - \mathbf{v}^{-}|}{|\mathbf{v}^{+} + \mathbf{v}^{-}|} = \beta$$



- Rotation θ is product of cyclotron angular frequency ω_c and Δt

Explicit and **Phase space (PSV) volume preserving**

Finite-Element Time-Domain & Exact Charge Conservation



Finite-element time-domain scheme based on Whitney forms and DEC

$$\mathbf{E}(\mathbf{r},t) \approx \sum_{j=1}^{N_1} \mathbb{E}_j(t)\,\mathbf{W}_j^{(1)}(\mathbf{r})$$

$$\mathbf{B}(\mathbf{r},t) \approx \sum_{k=1}^{N_2} \mathbb{B}_k(t)\,\mathbf{W}_k^{(2)}(\mathbf{r})$$

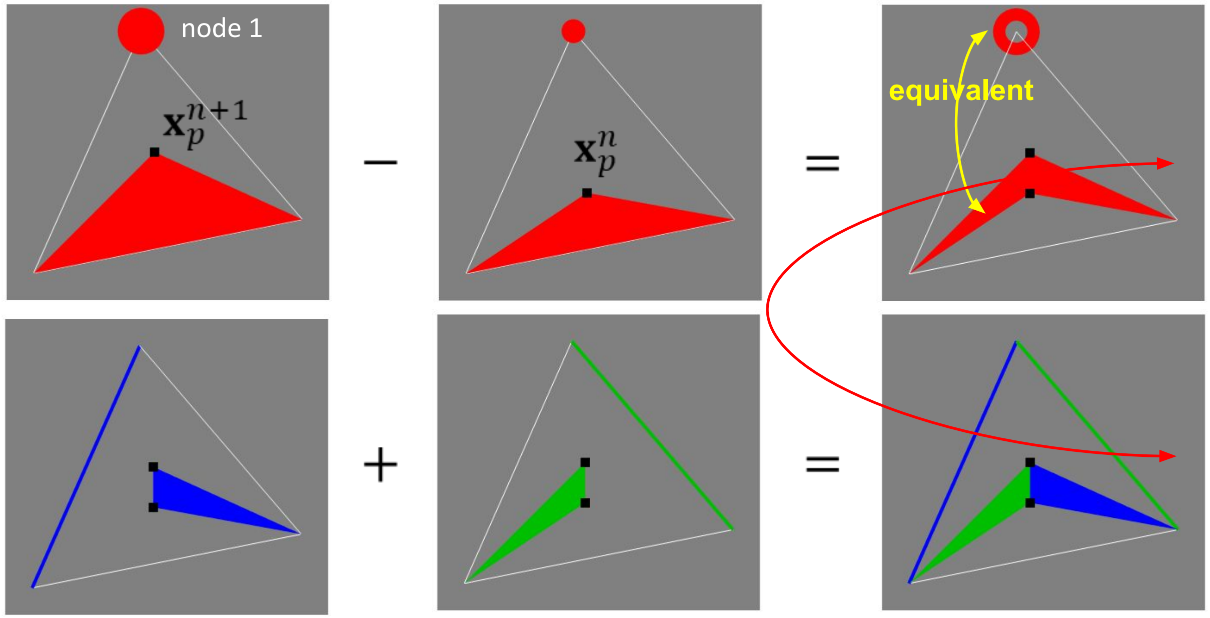
$$\mathbf{J}_{\star}(\mathbf{r},t) \approx \sum_{\tilde{k}=1}^{\tilde{N}_2} \mathbb{J}_{\star j}(t)\,\mathbf{W}_j^{(1)}(\mathbf{r})$$

$$\mathbf{Q}_{\star}(\mathbf{r},t) \approx \sum_{i=1}^{N_0} \mathbb{Q}_{\star i}(t)\,W_i^{(0)}(\mathbf{r})$$

$$[\mathbb{B}]^{n+\frac{1}{2}} = [\mathbb{B}]^{n-\frac{1}{2}} - \Delta t\,[\mathcal{D}_{\mathrm{curl}}]\cdot[\mathbb{E}]^{n}$$

[redacted]

Exact charge conservation inspired from differential geometry (geometric aspect)

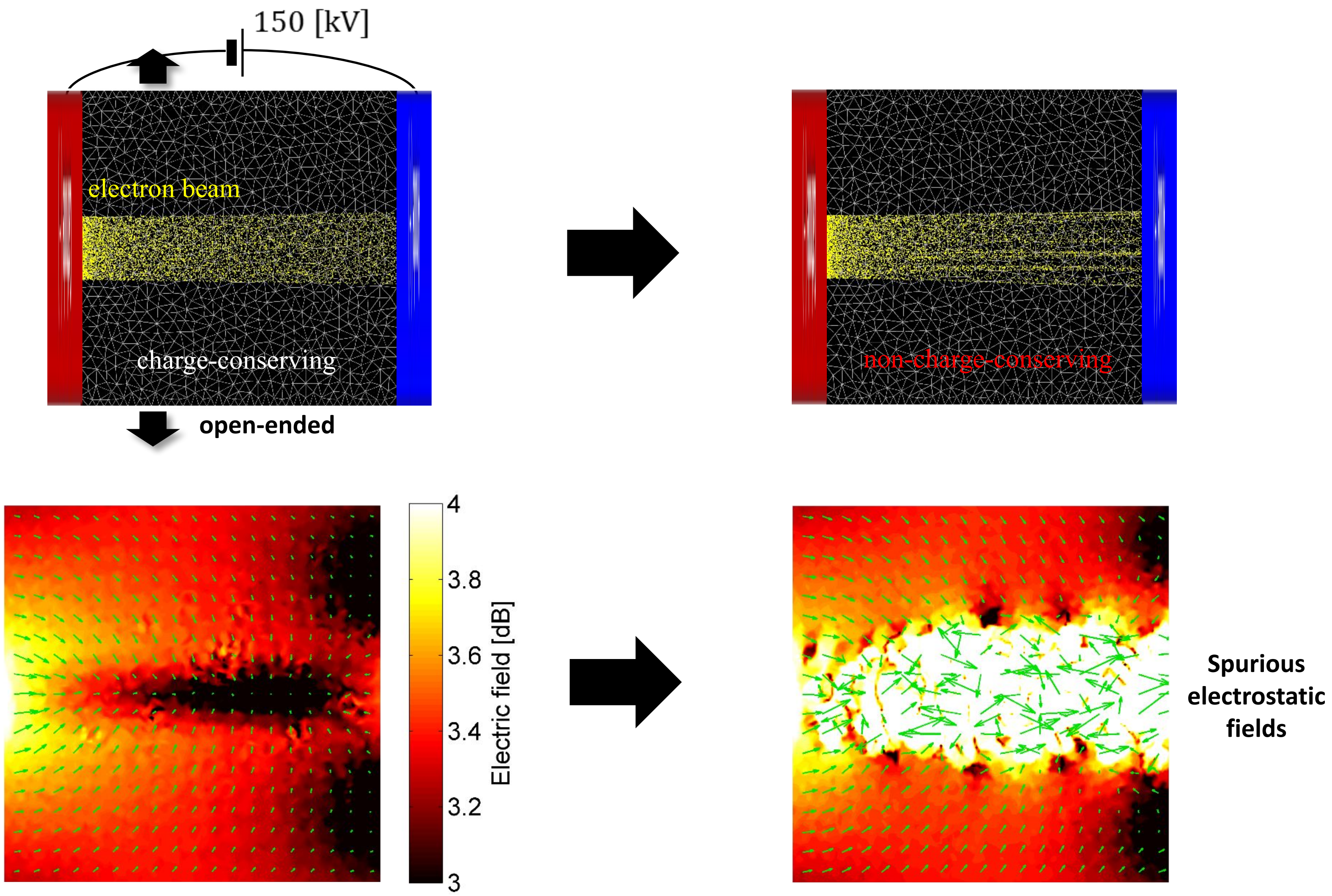


Identical!

$$\frac{[\mathbb{Q}]^{n+1} - [\mathbb{Q}]^{n}}{\Delta t} + \left([\mathcal{D}_{\mathrm{div}}]^{T}\cdot[\mathbb{J}]^{n+\frac{1}{2}}\right) = 0$$

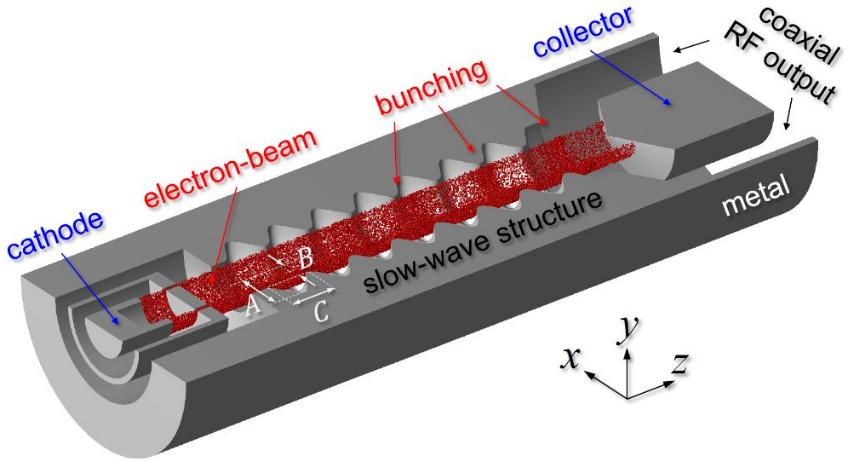
D.-Y. Na, H. Moon, Y. A. Omelchenko, and F. L. Teixeira, *IEEE Transactions on Plasma Science*, vol. 44, pp. 1353-1362 (2016)

Effects of Violation of Charge Conservation

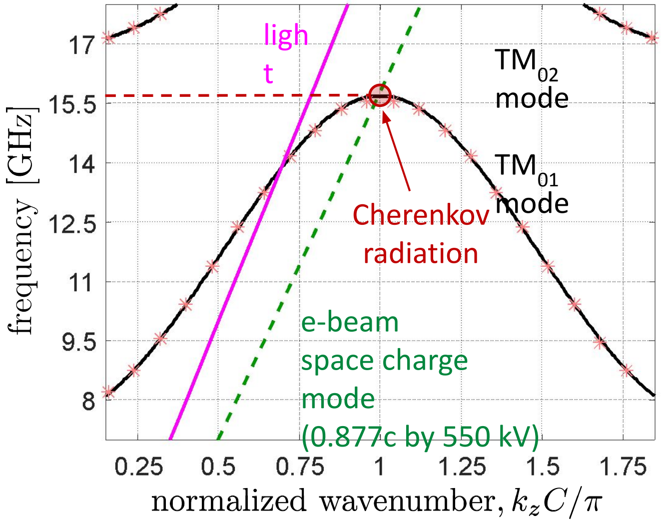


D.-Y. Na, H. Moon, Y. A. Omelchenko, and F. L. Teixeira, *IEEE Transactions on Plasma Science*, vol. 44, pp. 1353-1362 (2016)

Simulations of Backward-Wave Oscillators



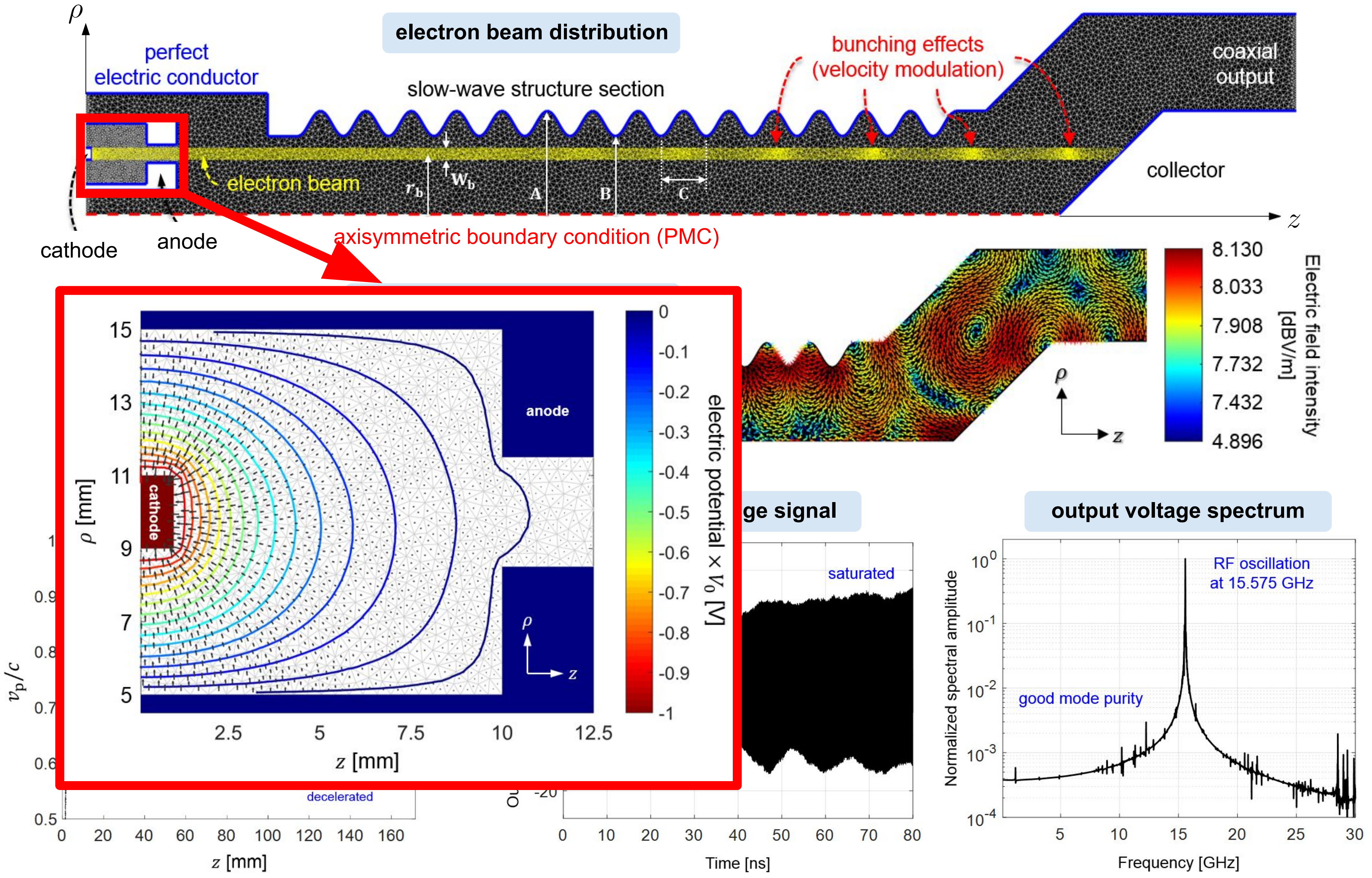
- Power converter from DC to radio frequency
- Non-linear oscillation from beam-structure interaction via *Cherenkov* radiation
- Beam bunching and velocity modulation



- Design procedure of slow-wave structures:
  1. Specification of output radio frequency
  2. Speed of electron beam (DC voltage),
  3. Designing slow wave structure
  4. Dispersion matching

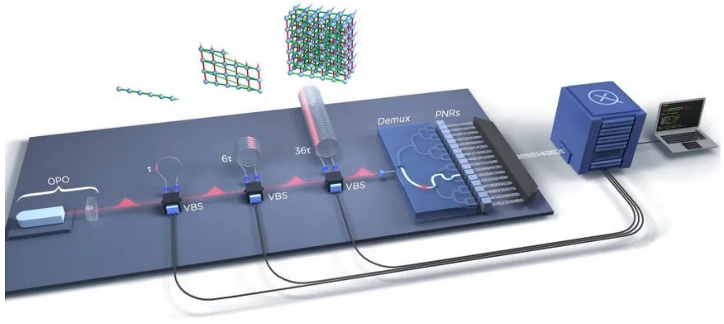
D.-Y. Na, Y. A. Omelchenko, H. Moon, B. H. V. Borges, and F. L. Teixeira, *Journal of Computational Physics*, vol. 346, pp. 295-317 (2017)

Simulations of Backward-Wave Oscillators (cont.)



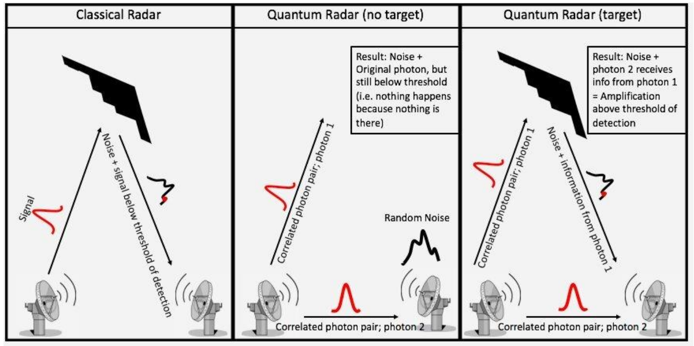
Quantum Optics/Electromagnetics

Photonic Quantum Computer



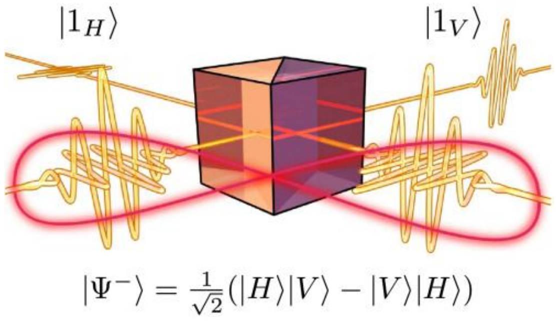
Retrieved from [6]

Quantum Radar Technology



Retrieved from [7]

Entangled Photons



Retrieved from [8]

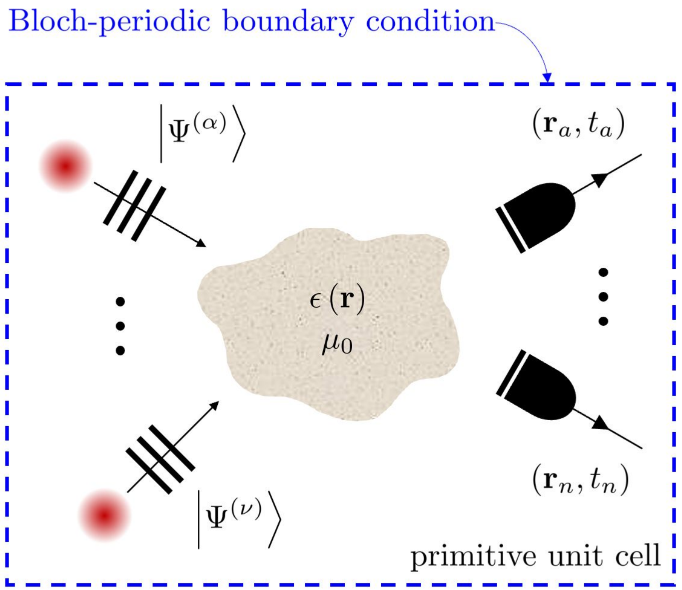
- **Quantum theory of electromagnetic fields** (randomness, second quantization)
- **Photonic QC, quantum imaging/radar technology** (superposition and entanglement of photons)
- **Enhanced performance against classical counterparts** (super-resolution and beating noises)

- **Two main challenges**:
  - Hardware needs to be matured much more.
  (e.g., single-photon sources, detections, storing, & producing microwave photons)
  - Lack of numerical/theoretical frameworks to study scattering and propagation properties of non-classical EM fields, which needs
  (1) building an appropriate math-physics model, and
  (2) applying optimized CEM methods.

[6] L. S. Madsen et al., *Nature*, vol. 606, pp. 75-81 (2022).
[7] https://www.aeropolaris.com/quantum-science-technology
[8] M. Rezai et al., *Optica*, vol. 6, pp. 34-40 (2019).

Quantization of Electromagnetic Fields via Numerical Mode Decomposition

- **Quantum theory of electromagnetic fields in the free space (Hermitian) has been well-grounded.**
  - Hamiltonian framework, finding eigenmodes (diagonalization), and subsequent quantization
- **How to describe the scattering of (entangled) photons in the presence of dielectric objects?**
  - Via numerical eigenmodes encoding all the scattering and mode-conversion process



[redacted]

$$\nabla \times \frac{1}{\mu_0} \nabla \times \tilde{\mathbf{E}}_{\omega,\lambda}(\mathbf{r}) - \omega^2 \epsilon(\mathbf{r}) \tilde{\mathbf{E}}_{\omega,\lambda}(\mathbf{r}) = 0$$

CEM methods

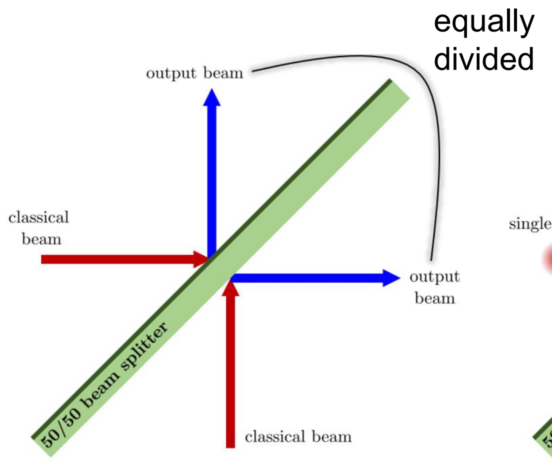
$$\bar{\mathbf{S}} \cdot \bar{\mathbf{e}} = \bar{\mathbf{M}} \cdot \bar{\mathbf{e}} \cdot \bar{\boldsymbol{\omega}}^2$$

Generalized Hermitian eigenvalue problem

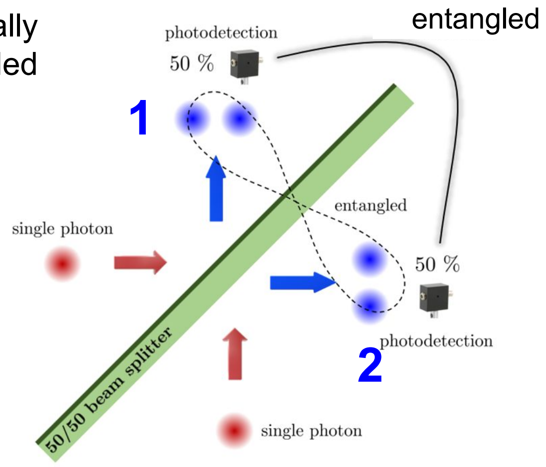
$$\hat{H} = \sum_{\lambda} \int_0^{\infty} \hbar\omega \left(\hat{a}^{\dagger}(\omega,\lambda)\hat{a}(\omega,\lambda) + \frac{1}{2}\hat{I} \right)$$

D.-Y. Na, J. Zhu, W. C. Chew, and F. L. Teixeira, *Physical Review A*, vol. 103, p. 013711 (2020)

Hong-Ou-Mandel (HOM) Effect

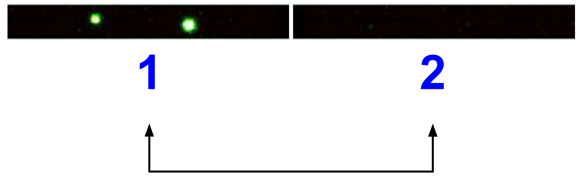


classical



quantum

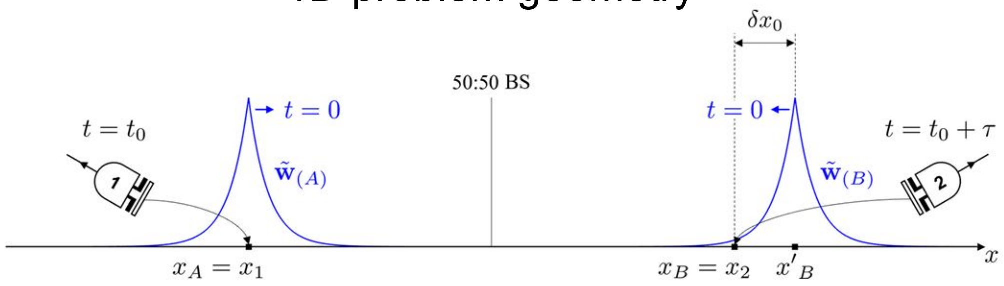
photodetection

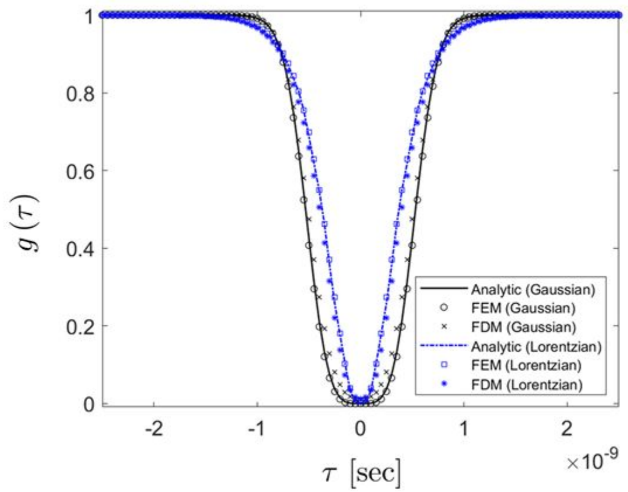


Coincidence: $g(\tau)$

τ is a time delay b/w the two input photons.

1D problem geometry





- Underlying principle of Hadamard (H) gate

D.-Y. Na, J. Zhu, W. C. Chew, and F. L. Teixeira, *Physical Review A*, vol. 103, p. 013711 (2020)

Extension into Cases Involving Dispersive Media

- Implicit eigenvalue problem: [redacted]

- Diagonalization of an explicit model where EM fields interact with auxiliary polarization fields.

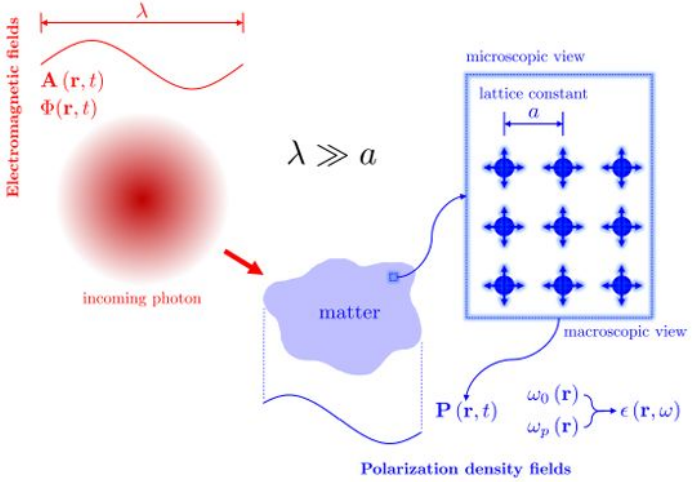
Hamilton equations of motion

$$
\begin{aligned}
\frac{\partial \mathbf{A}}{\partial t} &= \frac{\delta H}{\delta \mathbf{\Pi}_A} = \frac{1}{\epsilon_0}\left(\mathbf{\Pi}_A + \mathbf{P}\right), \\
\frac{\partial \mathbf{\Pi}_A}{\partial t} &= -\frac{\delta H}{\delta \mathbf{A}} = -\nabla \times \frac{1}{\mu_0}\nabla \times \mathbf{A}, \\
\frac{\partial \mathbf{P}}{\partial t} &= \frac{\delta H}{\delta \mathbf{\Pi}_P} = \frac{\epsilon_0}{\beta(\mathbf{r})}\mathbf{\Pi}_P, \\
\frac{\partial \mathbf{\Pi}_P}{\partial t} &= -\frac{\delta H}{\delta \mathbf{P}} = -\frac{1}{\epsilon_0}\mathbf{\Pi}_A - \frac{f(\mathbf{r})+1}{\epsilon_0}\mathbf{P}
\end{aligned}
$$

$$
\frac{\partial}{\partial t}\begin{bmatrix}\mathbf{q}\\ \mathbf{p}\end{bmatrix} = \begin{bmatrix}\overline{\mathbf{0}} & \overline{\mathbf{M}} \\ -\overline{\mathbf{K}} & \overline{\mathbf{0}}\end{bmatrix}\cdot\begin{bmatrix}\mathbf{q}\\ \mathbf{p}\end{bmatrix}
$$

$$
\boxed{\overline{\mathbf{K}}\cdot\tilde{\mathbf{q}}_{\omega,\lambda}(\mathbf{r}) = \omega^2\overline{\mathbf{M}}^{-1}\cdot\tilde{\mathbf{q}}_{\omega,\lambda}(\mathbf{r})}
$$

Generalized Hermitian eigenvalue problem

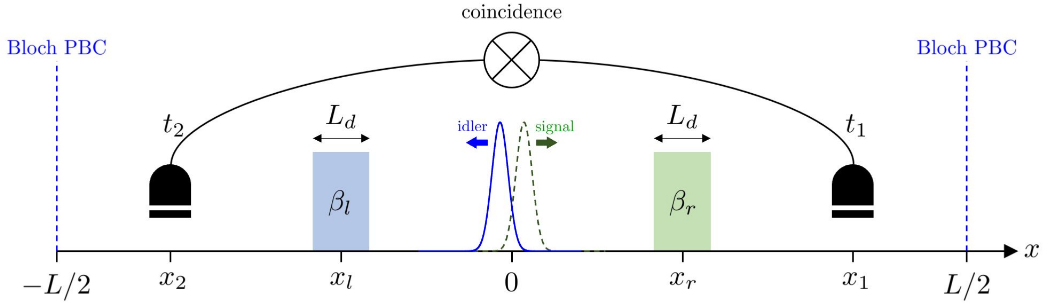


New canonical transformation

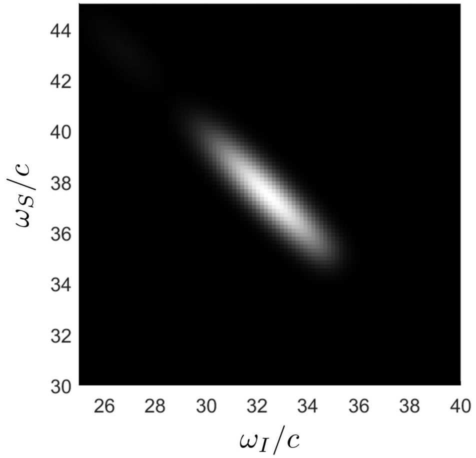
$$
\mathbf{q} \triangleq \left[\mathbf{A},\ \mathbf{\Pi}_P\right]^T, \quad \mathbf{p} \triangleq \left[\mathbf{\Pi}_{AP}, -\mathbf{P}\right]^T,
$$

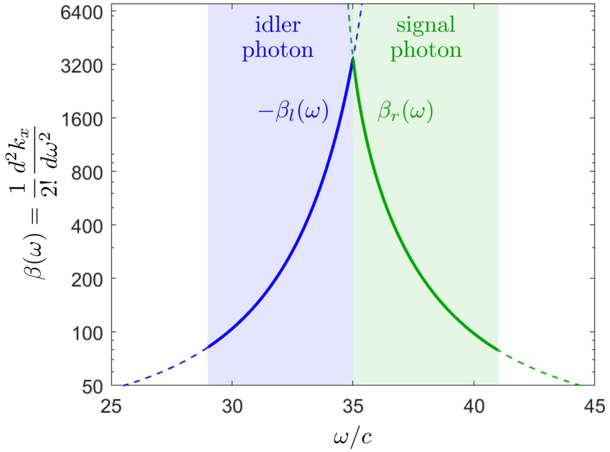
D.-Y. Na, J. Zhu, and W. C. Chew, *Physical Review A*, vol. 103, p. 063707 (2021)

Non-Local Dispersion Cancellation

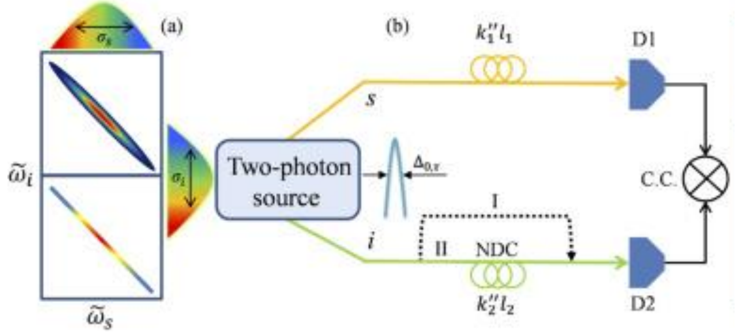


Frequency-entangled photons (signal/idler)
Opposite signs of the second-order dispersions

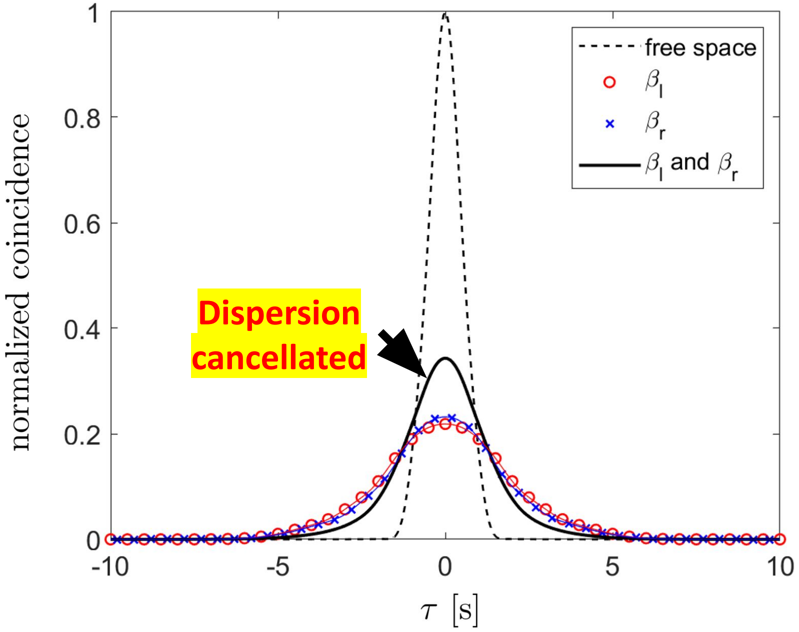




Long-distance quantum communication



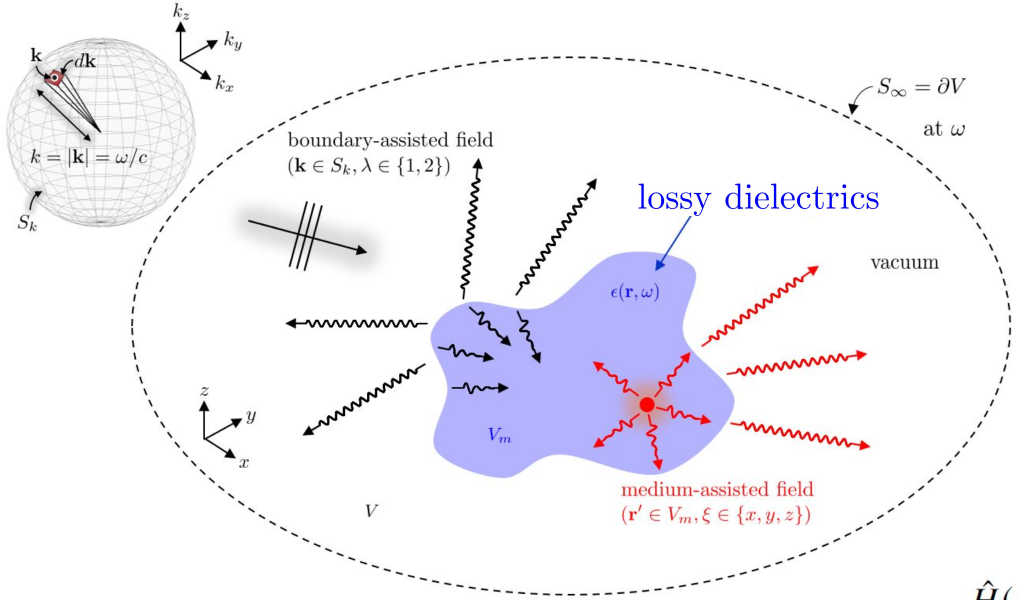
X. Xiang et al., Optics Express, vol. 28, pp. 17697-17707 (2020)



D.-Y. Na, J. Zhu, and W. C. Chew, *Physical Review A*, vol. 103, p. 063707 (2021)

Numerical Framework for New Langevin Noise (LN) Formalism

Non-Hermitian EM systems cannot be quantized through the traditional procedure.



- **Fluctuation-dissipation theorem**
  - Quasi-Hermiticity (in an ensemble sense)
  - Losses can be compensated by fluctuations
- **New Langevin noise formulation**
- **Finite-element method modeling**

$$\boxed{\textbf{New LN formalism:}\quad \hat{\mathbf{E}}^{(+)}(\mathbf{r},\omega) = \hat{\mathbf{E}}^{(+)}_{(\mathrm{BA})}(\mathbf{r},\omega) + \hat{\mathbf{E}}^{(+)}_{(\mathrm{MA})}(\mathbf{r},\omega)}$$

$$\hat{\mathbf{E}}^{(+)}_{(\mathrm{BA})}(\mathbf{r},\omega) = i\left(\sqrt{2\pi}\right)^{-3}\int_{S_k} d\mathbf{k} \sum_{\lambda\in\{1,2\}} \mathbf{\Phi}_{(\mathrm{tot})}(\mathbf{r},\mathbf{k},\lambda,\omega)\sqrt{\frac{\hbar\omega}{2}}\hat{a}(\mathbf{k},\lambda,\omega),$$

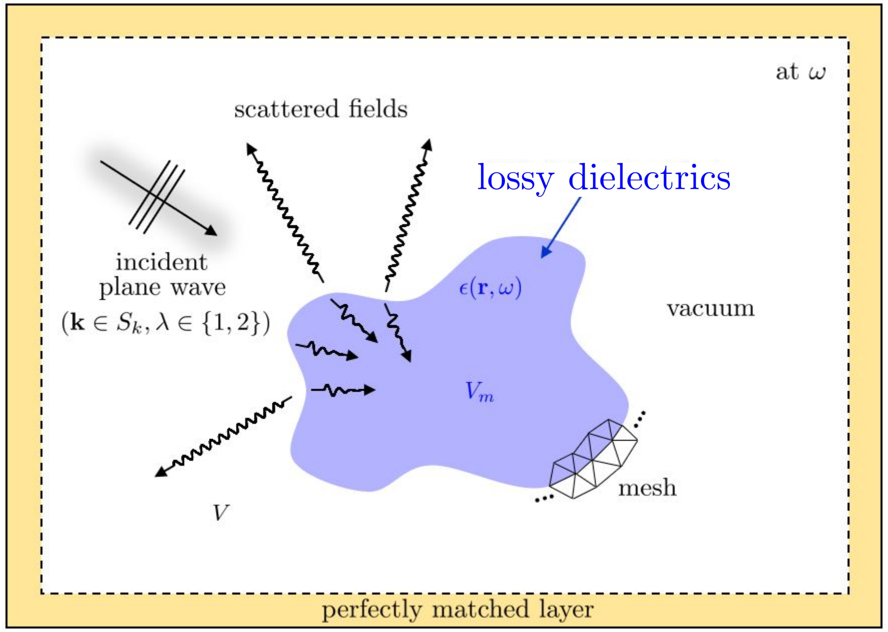
$$\hat{\mathbf{E}}^{(+)}_{(\mathrm{MA})}(\mathbf{r},\omega) = i\frac{\omega^2}{c^2}\int_{V_m} d\mathbf{r}' \sum_{\xi\in\{x,y,z\}} \left(\overline{\mathbf{G}}(\mathbf{r},\mathbf{r}',\omega)\cdot\hat{\xi}\right)\sqrt{\frac{\hbar}{\pi\epsilon_0}\epsilon_I(\mathbf{r}',\omega)}\hat{f}(\mathbf{r}',\xi,\omega),$$

$$\hat{H}(\omega) = \int_{S_k} d\mathbf{k} \sum_{\lambda\in\{1,2\}} \hbar\omega\hat{a}^\dagger(\mathbf{k},\lambda,\omega)\hat{a}(\mathbf{k},\lambda,\omega) + \int_{V_m} d\mathbf{r}' \sum_{\xi\in\{x,y,z\}} \hbar\omega\hat{f}^\dagger(\mathbf{r}',\xi,\omega)\hat{f}(\mathbf{r}',\xi,\omega).$$

D. Y. Na, T. E. Roth, J. Zhu, W. C. Chew, and C. J. Ryu, "Numerical Framework for Modeling Quantum Electromagnetic Systems Involving Finite-Sized Lossy Dielectric Objects in Free Space," *Preprint (10.48550/arXiv.2205.03388)*, 2023.

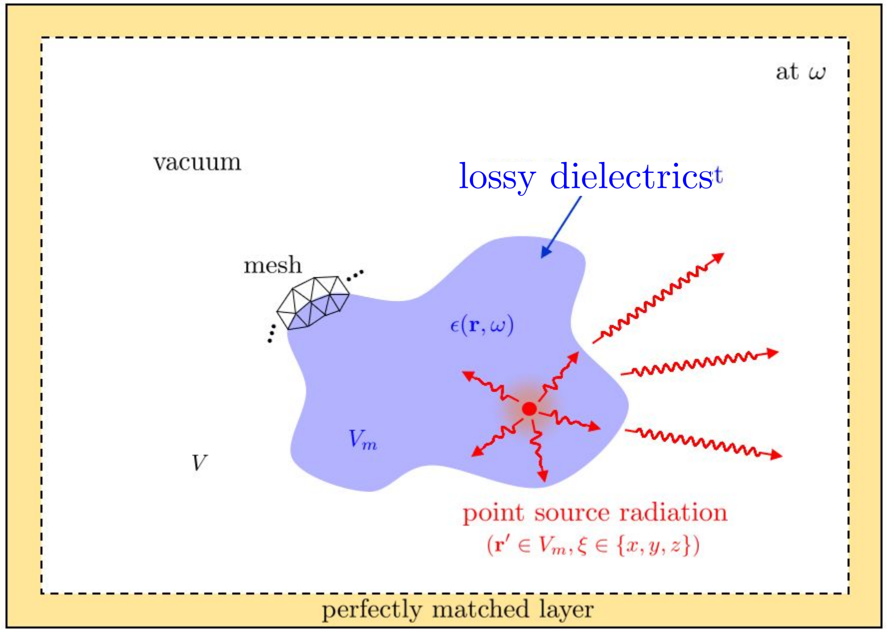
FEM Modeling of Plane-Wave-Scattering & Point-Source-Radiation Problems

- **Plane-wave-scattering problem**



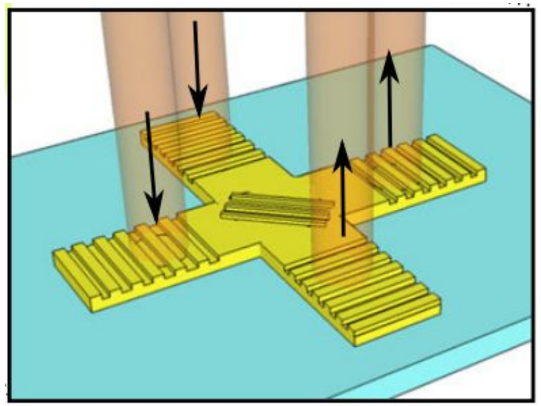
$$\mathbf{\Phi}_{(\text{tot})}(\mathbf{r}, \mathbf{k}, \lambda, \omega)$$

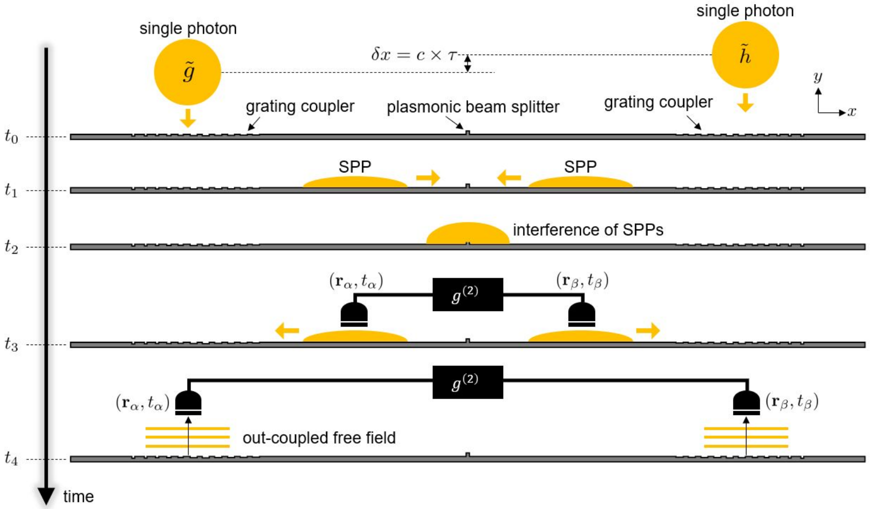
- **Point-source-radiation problem**



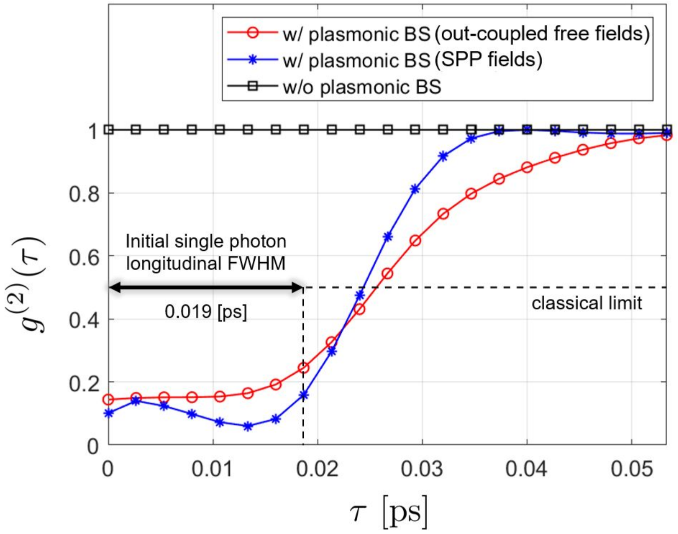
$$\overline{\mathbf{G}}(\mathbf{r}, \mathbf{r}', \omega)$$

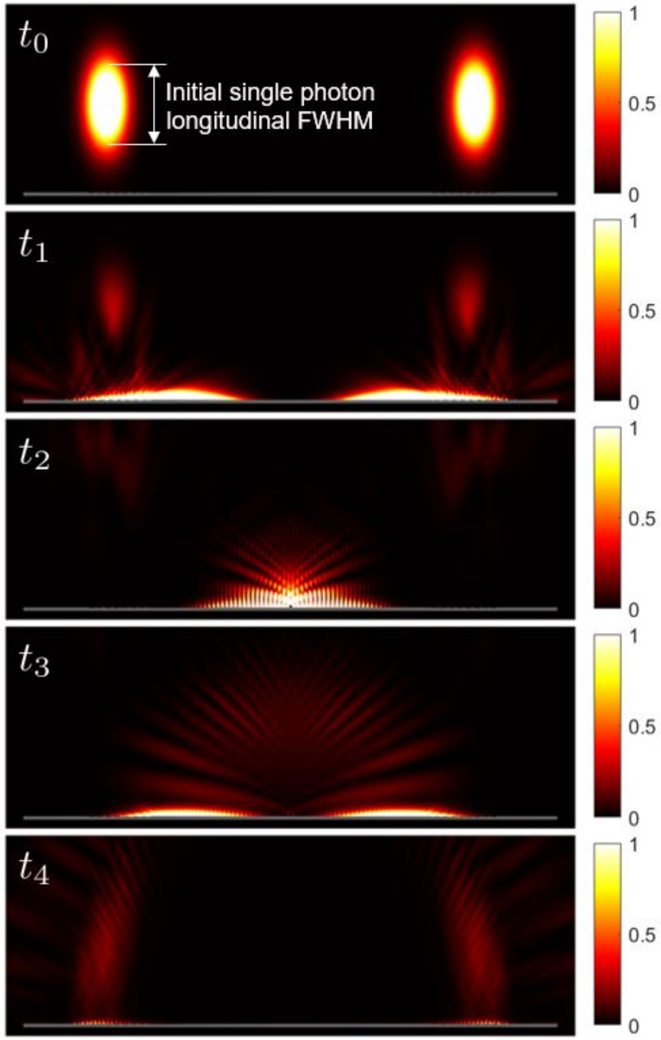
Quantum Plasmonic Hong-Ou-Mandel Effects





Plasmonic HOM effect





D. Y. Na, T. E. Roth, J. Zhu, and W. C. Chew, "Numerical Framework for New Langevin Noise Model: Applications to Plasmonic Hong-Ou-Mandel Effects," *Preprint, (10.48550/arXiv.2205.03388)*, 2022

Concluding Remarks

- **‘Multiphysics’ Electromagnetics (Modeling High Energy Plasma Systems)**
  - Charge-conserving electromagnetic Particle-in-Cell algorithms on irregular grids (differential geometry)
  - Finite-Element Time-Domain Scheme (geometric fidelity)
  - Proof-of-principle simulations (vacuum diode and backward wave oscillator)

- **Quantum Electromagnetics/Optics**
  - Canonical quantization via numerical mode decomposition / Langevin noise formalism
  - Numerical verifications of (plasmonic) Hong-Ou-Mandel effects

Thank You,

Q & A