DE LA RECHERCHE À L'INDUSTRIE

Examples of PIC code limit and potential for the simulation of wakefield acceleration and accelerator applications.

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EuroNNAc4, Elba, 2022

Task: Present the mitigation strategy of NCR/NCI in PIC code
Discuss the modeling of wakefield-driven light sources.

Warning: PIC simulation of wakefield are subject to errors!
But, broader PIC code potential: toward the modeling of applications.

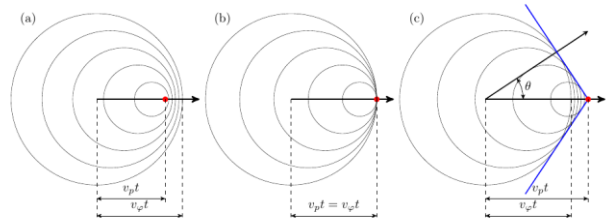
- Example of PIC code limits: Numerical Cerenkov Radiation / Instability (NCR/NCI)

- PIC code developments help to foster accelerator applications
  - radiation sources
  - Beam interactionwith EM fields or target/plasma
  - Needs for code developments

Numerical Cerenkov Radiation[1] (NCR): Principle

- (Physical) Cerenkov Radiation

  It appears when an charged particle is faster than the speed of light in a medium ($v_p > v_\phi$)



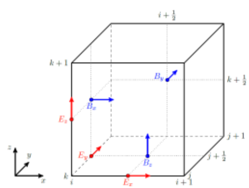
$$\cos(\theta) = \frac{c}{v_p n(\omega)} \qquad \omega = \boldsymbol{v_p} \cdot \boldsymbol{k}$$

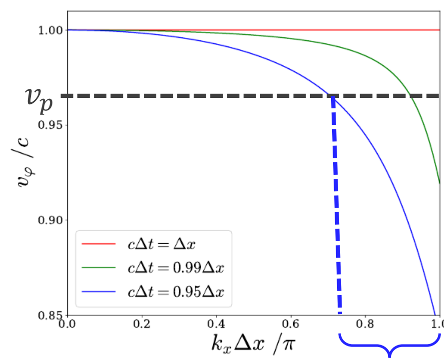
- Origin of Numerical Cerenkov Radiation (NCR) in PIC code

$$v_\varphi^{num} = \frac{2}{k\Delta t} \arcsin\left(c\Delta t \sqrt{\frac{1}{\Delta x^2}\sin^2\left(\frac{k_x \Delta x}{2}\right) + \frac{1}{\Delta y^2}\sin^2\left(\frac{k_y \Delta y}{2}\right) + \frac{1}{\Delta z^2}\sin^2\left(\frac{k_z \Delta z}{2}\right)}\right)$$

In plasma, light phase velocity $v_\phi \geq c \Rightarrow$ no CR.

In a PIC code with the standard Yee[2] scheme, we have $v_\phi^{num} < c$ in vacuum $\Rightarrow$ NCR...

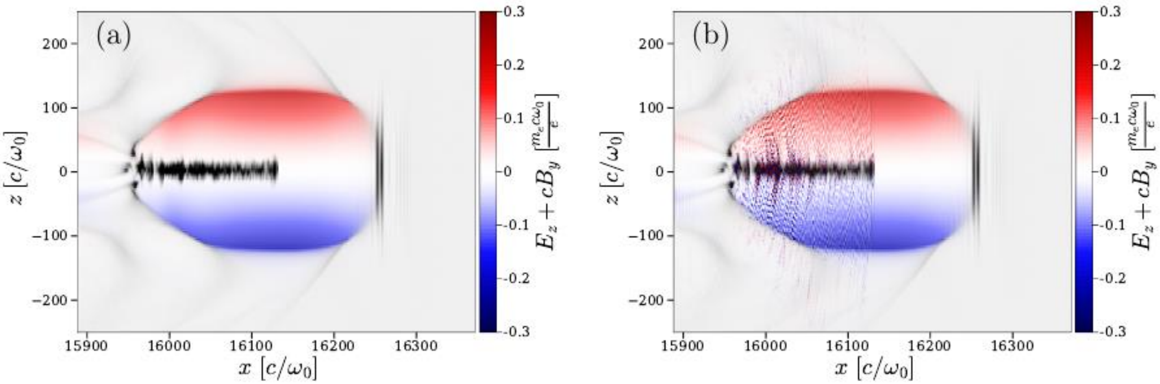




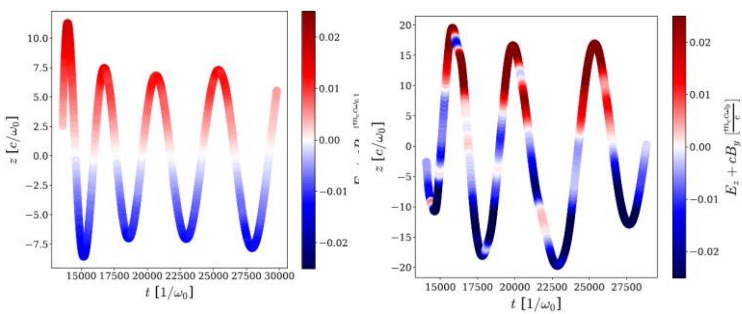
Emission of NCR in the high frequency domain

[1] B.B. Godfrey, JCP 15(4) 504–521 (1974).
[2] K. Yee, IEEE Trans. Antennas Propag. **14**, 302 (1966)

- Consequences: emission of spurious and high frequency radiation, which can affect the beam/plasma dynamic



Depending on the beam charge: wrong beam divergence, transverse size, transverse emittance…

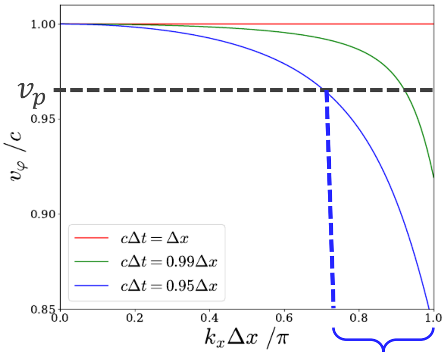


P.-L. Bourgeois, PhD, IP Paris (2020)
P.-L. Bourgeois *et al*., JCP **413** 109426 (2020)

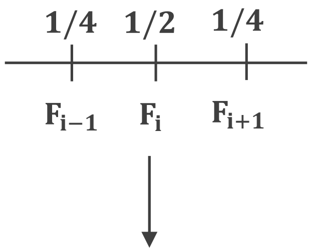
Numerical Cerenkov Radiation (NCR): Mitigation technics

- “Standard” spatial filtering.
- Higher resolution.
- Modified Maxwell solver.
- Modified field interpolation.
- **Combination of different technics.**
  - Needs to give the details in the reports/papers

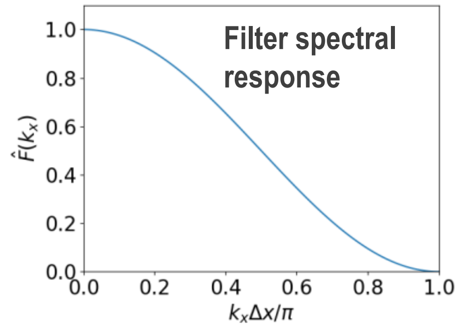
- "Standard" spatial filtering[1]
  - Low path filters such as Binomial Filters + Compensator



Emission of NCR in the high frequency domain



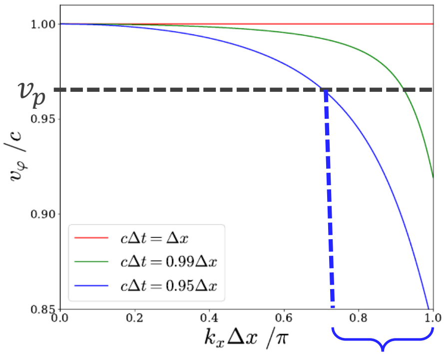
$$\widehat{F_i} = \frac{1}{4} F_{i-1} + \frac{1}{2} F_i + \frac{1}{4} F_{i+1}$$



  - Number of paths N per time step Δt? $\frac{N}{\Delta t} > 1$ or < 1 ?
  - Usually aggressive filtering of the currents can be used.
  - Filtering of the fields: be carful with LWFA, the laser field should not be damped too much!

[1] J.-L. Vay *et al.*, JCP **230** 5908–5929 (2011)

- Higher resolution
  - Costly, not a good idea alone (NCR still exist with high resolution), but can help to use more aggressive filtering



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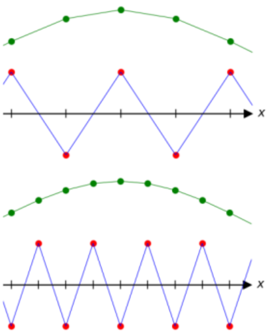
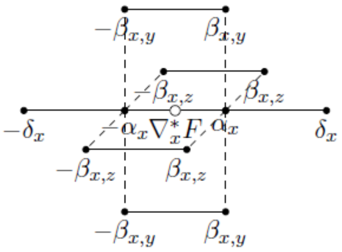


  - The use of $\Delta z, \Delta y \gg \Delta x$ can help to get cΔt $\sim \Delta x$ if Yee[1] scheme is used.
  - Dispersion free schemes allow cΔt $= \Delta x$ [2-4].

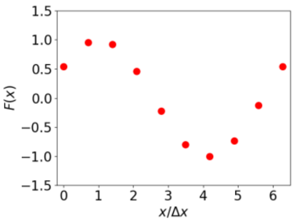
[1] K. Yee, IEEE Trans. Antennas Propag. **14**, 302 (1966)
[2] A. Pukhov, JPP **61**(3) 425 (1999)
[3] M. Kärkkäinen, Proceedings of ICAP (2006)
[4] B. M. Cowan, PRSTAB **16** 041303 (2013)

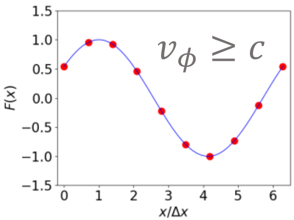
- Modified Maxwell solver (FTDT)
  - Main idea: modification of the Maxwell solver to modify the numerical dispersion relation and avoid $v_\phi < c$ in vacuum.
  - A new stencil is often used to compute the derivative in the Maxwell equations:



[1] A. Pukhov, JPP **61**(3) 425 (1999)
[2] A.D. Greenwood, *et al.*, JCP. **201**(2) 665–684 (2004).
[3] M. Kärkkäinen, Proceedings of ICAP (2006)
[4] J.-L. Vay *et al.*, JCP **230** 5908–5929 (2011)
[5] R. Lehe, *et al.*, PRSTAB **16** 021301 (2013).
[6] B. M. Cowan, PRSTAB **16** 041303 (2013)
[7] R. Nuter *et al.*, JCP **305** 664–676 (2016).
[8] F. Li *et al.*, CPC **214** 6–17 (2017)
[9] A. Blinne *et al.*, CPC **224** 273–281 (2018)
[10] X. Xu *et al.*, JCP **413** 109451 (2020)
[11] A. Pukhov, JCP **418** 109622 (2020)

  - Limitations:
    - Can produced EM waves with $v_\phi \geq c$ or other spurious results
    - Difficulties to tackle aliasing modes.





Numerical Cerenkov Radiation (NCR): Mitigation technics

- Modified Maxwell solver (FTDT)
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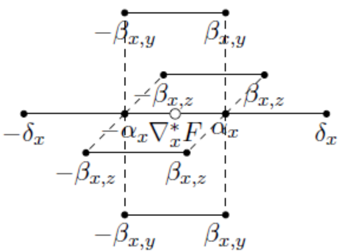

[1] A. Pukhov, JPP **61**(3) 425 (1999)
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[4] J.-L. Vay *et al.*, JCP **230** 5908–5929 (2011)
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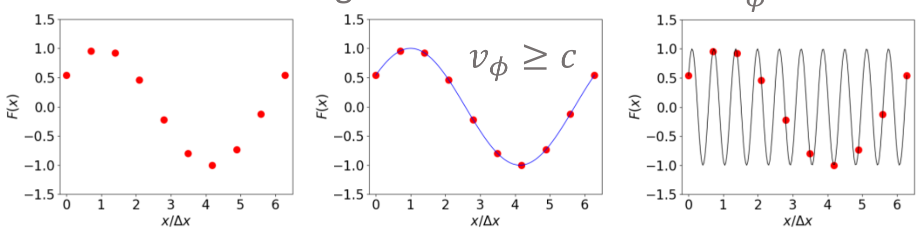

Numerical Cerenkov Radiation (NCR): Mitigation technics

- Modified Maxwell solver (FDTD) **+ spectral solvers (NCI)**
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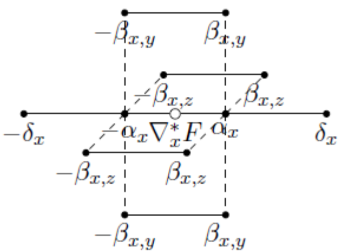
  - A new stencil is often used to compute the derivative in the Maxwell equations:



[1] A. Pukhov, JPP **61**(3) 425 (1999)
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[4] J.-L. Vay *et al.*, JCP **230** 5908–5929 (2011)
[5] R. Lehe, *et al.*, PRSTAB **16** 021301 (2013).
[6] B. M. Cowan, PRSTAB **16** 041303 (2013)
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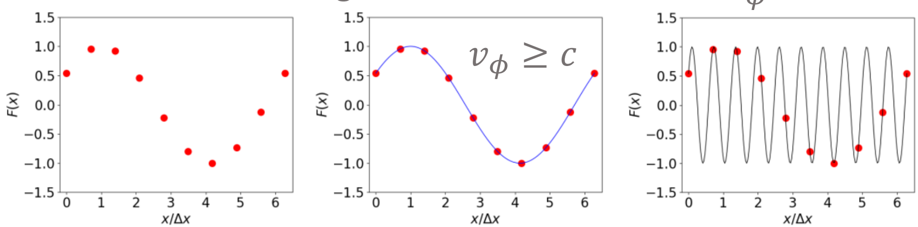
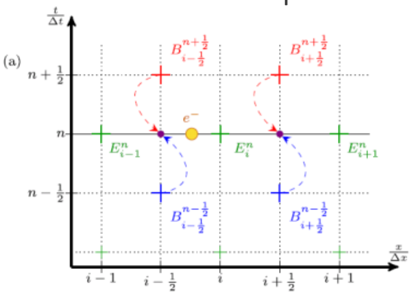
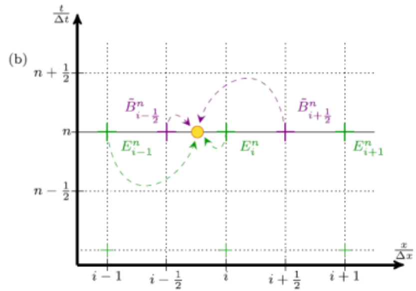


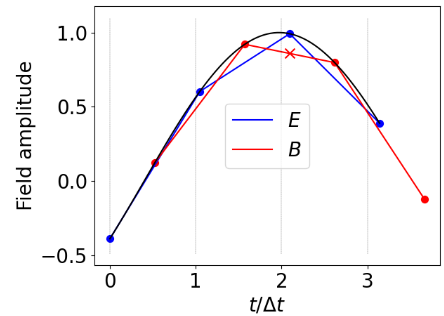
Numerical Cerenkov Radiation (NCR): Mitigation technics

- Modified field interpolation.
  - Field filters used only to push the particles **(NCI)** [1,2].
  - BTIS scheme [3-5] : NCR propagates with the beam: E and B force compensate => no transverse force on the beam. Easy to implement!

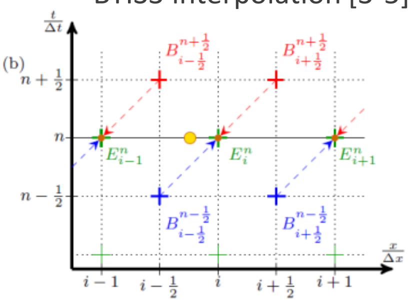
Standard interpolation

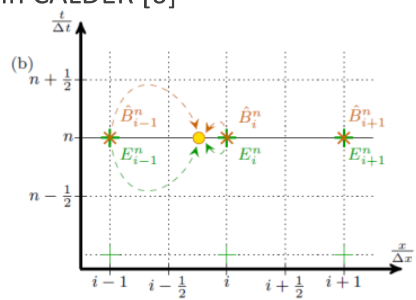






BTIS3 interpolation [3-5] in CALDER [6]





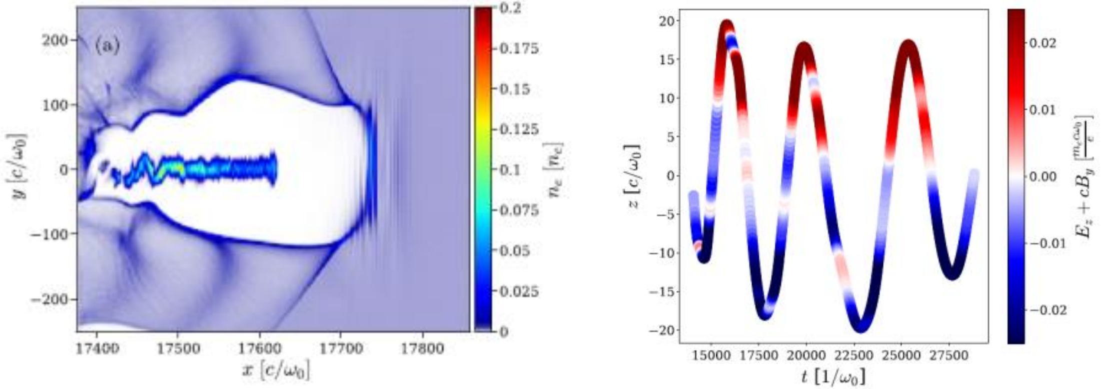
[1] B. B. Godfrey *et al.*, JCP **267** 1–6 (2014)
[2] Y. Lu *et al.*, JCP **413** 109388 (2020)

[3] P.-L. Bourgeois, PhD, IP Paris (2020)
[4] P.-L. Bourgeois, JCP **413** 109426 (2020)
[5] P.-L. Bourgeois, to be published

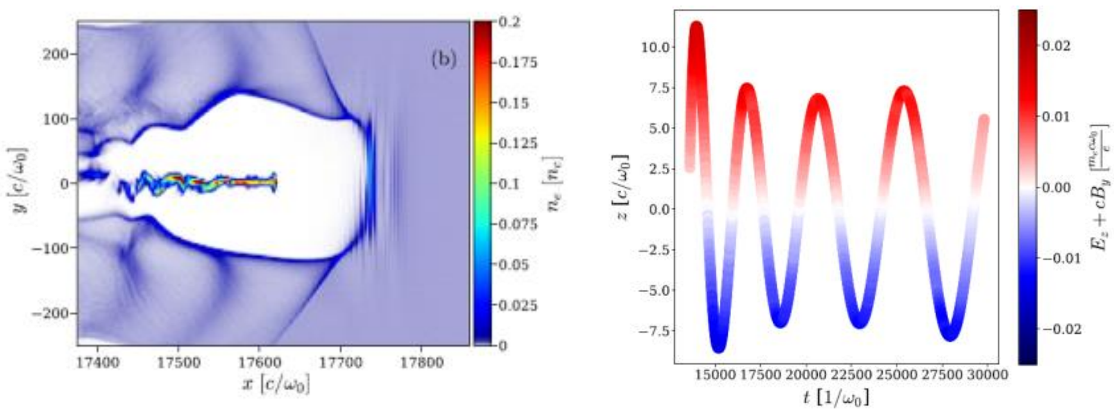
[6] E. Lefebvre et al., Nuc. Fus. 43 629 (2003)

Numerical Cerenkov Radiation (NCR): Mitigation technics

Standard interpolation



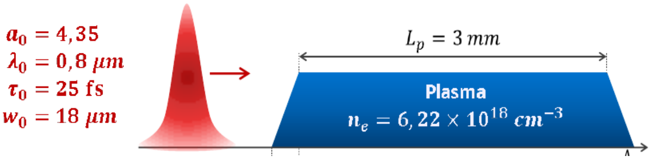
BTIS interpolation [1-3]



Numerical Cerenkov Radiation (NCR): Effect on a betatron source

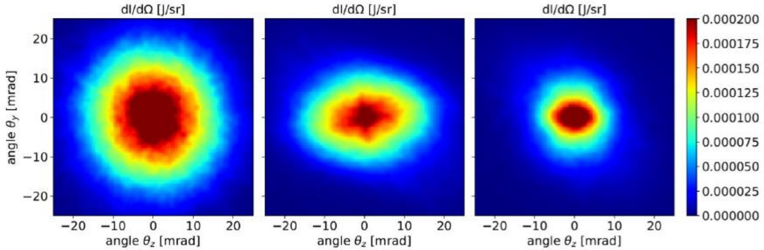
- Benchmark between Yee[1], a modified Maxwell solver[2], and BTIS scheme[3,4]

[1] K. Yee, IEEE Trans. Antennas Propag. **14**, 302 (1966)
[2] R. Lehe, *et al.*, PRSTAB **16** 021301 (2013).
[3] P.-L. Bourgeois, PhD, IP Paris (2020)
[4] P.-L. Bourgeois, JCP **413** 109426 (2020)

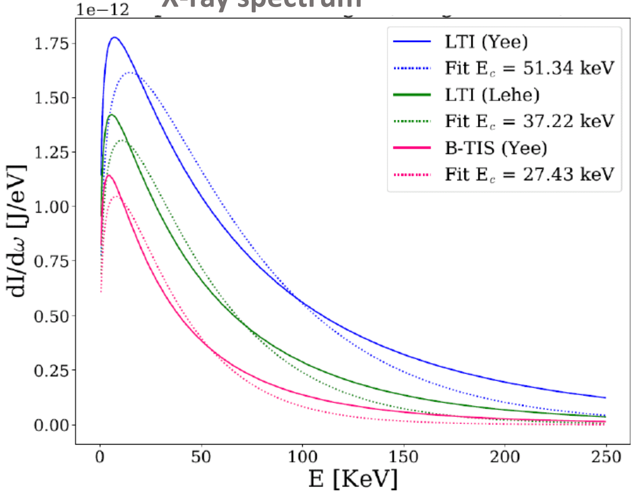


X-ray spot

LTI (Yee) LTI (Lehe) B-TIS (Yee)



X-ray spectrum



Numerical Cerenkov Instability (NCI): Principle

- NCR: "spontaneous" and incoherent emission
- **NCI: coupling between NCR and plasma**
  - The beam is "bunched" by the NCR and produced more coherent and amplified radiation
  - **Numerical instability: exponential growth** of the radiation and beam response
- Main goal: suppressing NCI is very difficult due to the aliasing. Instead the growth rate is often kept as low as possible to avoid significant effect of NCI during the simulation time.
- It is mainly observed when a "large" plasma/beam is drifting, like in
  - **boosted frame simulation** (used to speed up wakefield simulation)
  - **simulation of beam propagation** (applications)

Numerical Cerenkov Instability (NCI): Mitigation technics

- Solutions: same as before, but usually not enough. Other specific scheme have been developed.
  - Spatial filters,
  - Temporal filter: Friedman filter [1,2]. To be used carefully. Physical frequency can also be damped.
  - Adapted field filters/interpolation technics [3,4]
  - Modified Maxwell solvers (FDTD) ([5-7] and others)
  - **Spectral solvers** ($\partial_x \rightarrow ik_x \Rightarrow$ no error in the derivative $\Rightarrow v_\phi = c$.)
    - **Pseudo-spectra**l time domain (PSTD)
    - Pseudo-spectral analytic time domain (PSATD).
    - Still not enough, **specific solution to solve NCI are developed [8-16]**

[1] J.-L. Vay *et al.*, JCP **230** 5908–5929 (2011)
[2] A. Friedman, J. Comput. Phys. **90** 292312 (1990)
[3] B.B. Godfrey, J. Comput. Phys. **267** 1–6 (2014).
[4] Y. Lu *et al.*, JCP **413** 109388 (2020)
[5] F. Li *et al.*, CPC **214** 6–17 (2017)
[6] X. Xu *et al.*, JCP **413** 109451 (2020)
[7] A. Pukhov, JCP **418** 109622 (2020)
[8] X. Xu, *et al.*, CPC **184**(11) 2503–2514 (2013).
[9] B. B. Godfrey *et al.*, CPC **196** 221–225 (2015).
[10] P. Yu *et al.*, CPC **192** 32–47 (2015).
[11] R. Lehe *et al.*, PRE **94**, 053305 (2016)
[12] M. Kirchen *et al.*, POP **23**, 100704 (2016)
[13] S. Jalas *et al.*, POP **24** 033115 (2017).
[14] M. Kirchen *et al.*, PRE **102**, 013202 (2020)
[15] O. Shapoval *et al.*, PRE **104**, 055311 (2021)
[16] E. Zoni *et al.*, CPC **279** 108457 (2022)

- Example of PIC code limits: Numerical Cerenkov Radiation / Instability (NCR/NCI)
  - Solutions are diverse, they should be known, used, mention in publications

- PIC code developments help to foster accelerator applications
  - radiation sources
  - Beam interaction with EM fields or target/plasma
  - Needs for code developments

Applications to photons sources

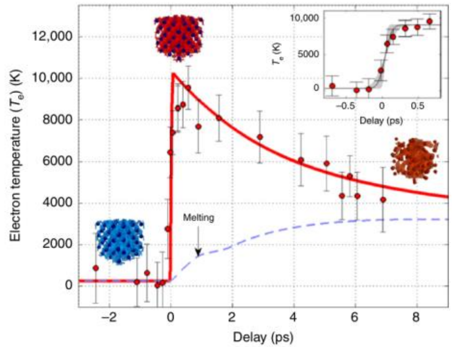
- X/γ-ray sources
  - Betatron sources (X-ray) particles tracking and use of Liénard-Wiechert potential (or not [1,2]) + NCR should be limited!
    - See the talk of S. Mangles on Thursday

Warm dense matter probing:

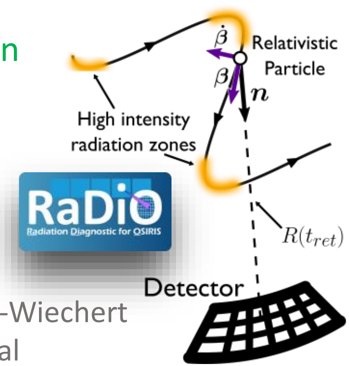
[1] B. Mahieu *et al.*, Nat. Comm. **9** 3276 (2018)

[2] A. Grolleau *et al.*, PRL **127** 275901 (2021)

For this application, LWFA can already be considered as a beamline used by external users!



- Bremsstrahlung (γ-ray)
- Compton sources ("peaked" γ-ray) Synchrotron radiation
- Others... (e.g. "Boosted" betatron producing γ-ray [3])



Liénard-Wiechert potential

- THz sources [4,5]

[1] R. Pausch *et al.*, NIMA **740** 250–25 (2014)

[2] M. Pardal, J. Vieira, RaDiO, to be published

[3] J. Ferri *et al.*, PRL **120** 254802 (2018)

[4] J. Dechard *et al.*, PRL **120** 144801 (2018)

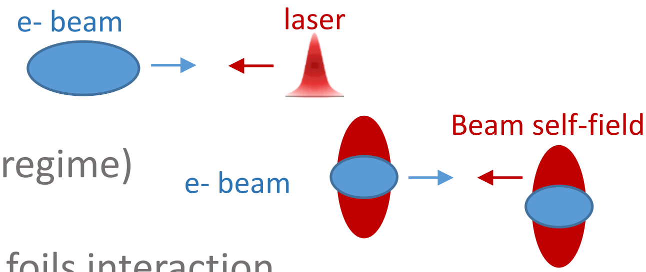
[5] J. Dechard *et al.*, PRL **123** 264801 (2019)

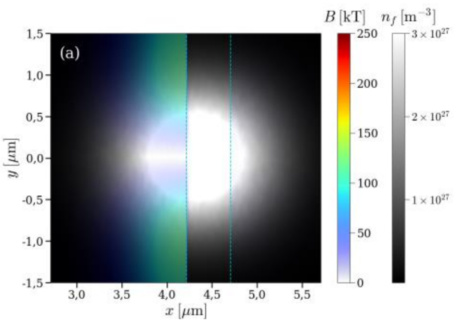
- Example of PIC code limits: Numerical Cerenkov Radiation / Instability (NCR/NCI)
    - Solutions are diverse, they should be known, used, mention in publications

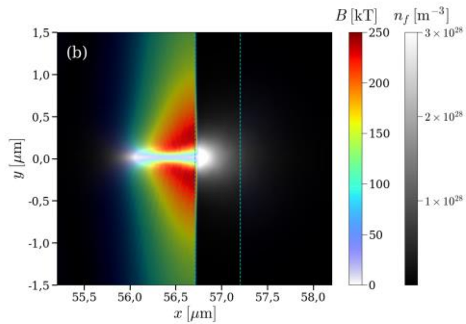
- PIC code developments help to foster accelerator applications
    - radiation sources
    - **Beam interaction with EM fields or target/plasma. (beams from conventional accelerators, PWFA, LWFA)**
    - Needs for code developments

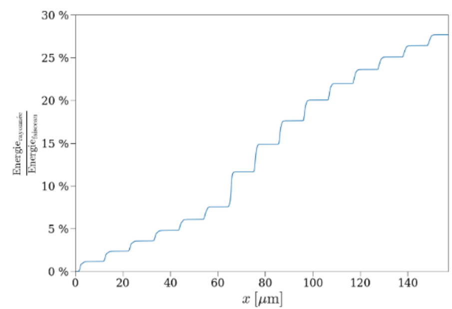
Study of the Strong-Field QED regime (SF-QED)
Production of intense γ ray sources, e+e- pairs

- Laser-Beam interaction
  M. Lobet et al., PRAB 20 043401 (2017), …
- Beam-Beam collision (beamstrahlung regime)
  V. Yakimenko *et al*., PRL **122**, 190404 (2019)
- Beam-foil interaction and beam-multi foils interaction









10 GeV, 2 nC, 0.55 μm
0.5 μm Al foil

A. Sampath *et al*., PRL 126, 064801 (2021)
Collaborators of the SLAC E332 experiment

PHYSICAL REVIEW LETTERS **126**, 064801 (2021)

Extremely Dense Gamma-Ray Pulses in Electron Beam-Multifoil Collisions

Archana Sampath,[1] Xavier Davoine,[2,3] Sébastien Corde,[4] Laurent Gremillet,[2,3] Max Gilljohann,[4] Maitreyi Sangal,[1] Christoph H. Keitel,[1] Robert Ariniello,[5] John Cary,[5] Henrik Ekerfelt,[6] Claudio Emma,[6] Frederico Fiuza,[6] Hiroki Fujii,[7] Mark Hogan,[6] Chan Joshi,[7] Alexander Knetsch,[4] Olena Kononenko,[4] Valentina Lee,[5] Mike Litos,[5] Kenneth Marsh,[7] Zan Nie,[7] Brendan O'Shea,[6] J. Ryan Peterson,[6,8] Pablo San Miguel Claveria,[4] Doug Storey,[6] Yipeng Wu,[7] Xinlu Xu,[6] Chaojie Zhang,[7] and Matteo Tamburini[1,*]
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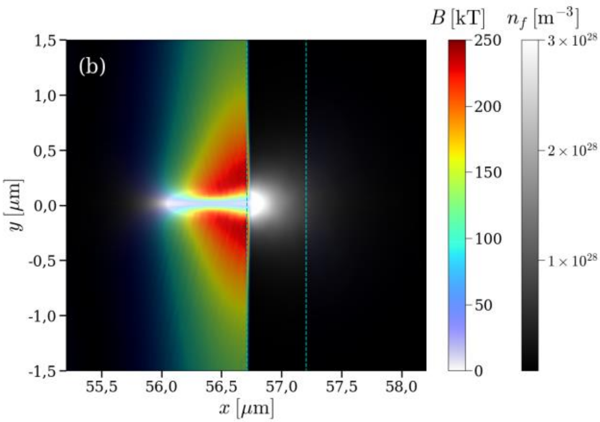
[4]*LOA, ENSTA Paris, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, 91762 Palaiseau, France*
[5]*University of Colorado Boulder, Department of Physics, Center for Integrated Plasma Studies, Boulder, Colorado 80309, USA*
[6]*SLAC National Accelerator Laboratory, Menlo Park, California 94025, USA*
[7]*University of California Los Angeles, Los Angeles, California 90095, USA*
[8]*Stanford University, Physics Department, Stanford, California 94305, USA*

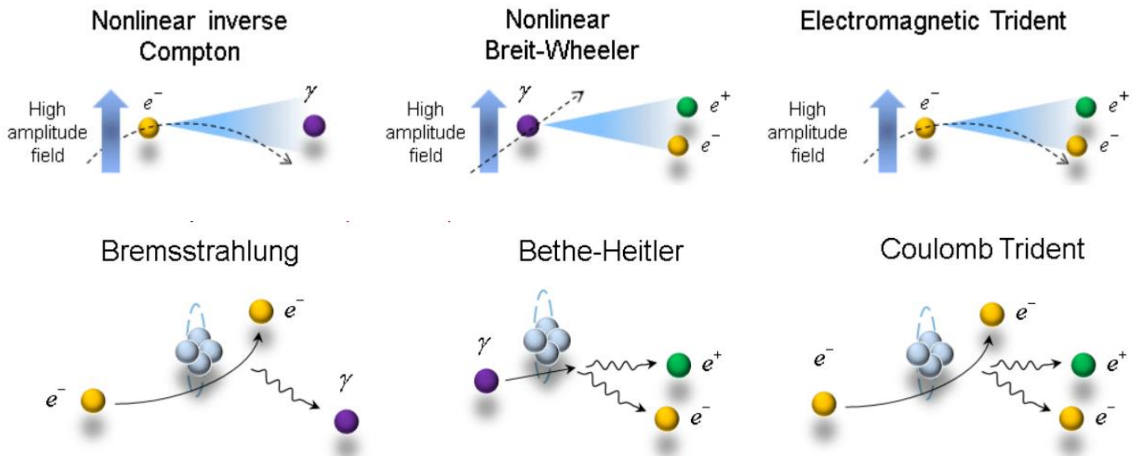
Study of the Strong-Field QED regime (SF-QED)
Production of intense γ ray sources, e+e- pairs



Implemented in CALDER [1-4]:

- Filed ionization
- Collisions (elastic + ionization)
- SF-QED processes
- Coulomb processes

[1] M. Lobet *et al.*, J. Phys.: Conf. Ser. **688**, 012058 (2016).
[2] B. Martinez *et al.*, POP **26**, 103109 (2019).
[3] M. Lobet, PhD, Université de Bordeaux (2015)
[4] B. Martinez, PhD, Université de Bordeaux (2018)



Study of relativistic beam-plasma instabilities

- Probing Current Filament Instability (CFI) on short time-scale
  - CFI in laser-solid target interaction
  - Probing CFI with LWFA e- beam

PHYSICAL REVIEW RESEARCH **2**, 023123 (2020)

Editors' Suggestion

Probing ultrafast magnetic-field generation by current filamentation instability in femtosecond relativistic laser-matter interactions

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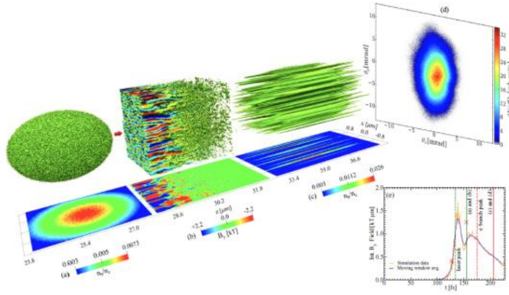

- Competition between CFI and Oblique Two Stream Instability (OTSI).

PHYSICAL REVIEW RESEARCH **4**, 023085 (2022)

Spatiotemporal dynamics of ultrarelativistic beam-plasma instabilities

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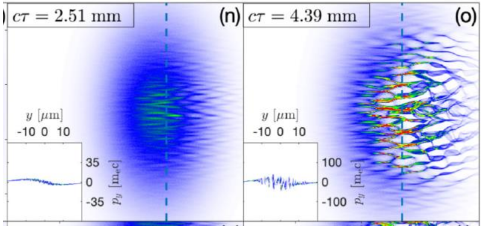
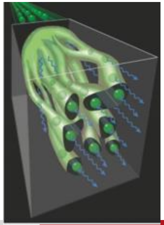
E305 SLAC experiment



- Fundamental studies relevant to beam propagation, laser-plasma interaction, astrophysics, γ ray emission.

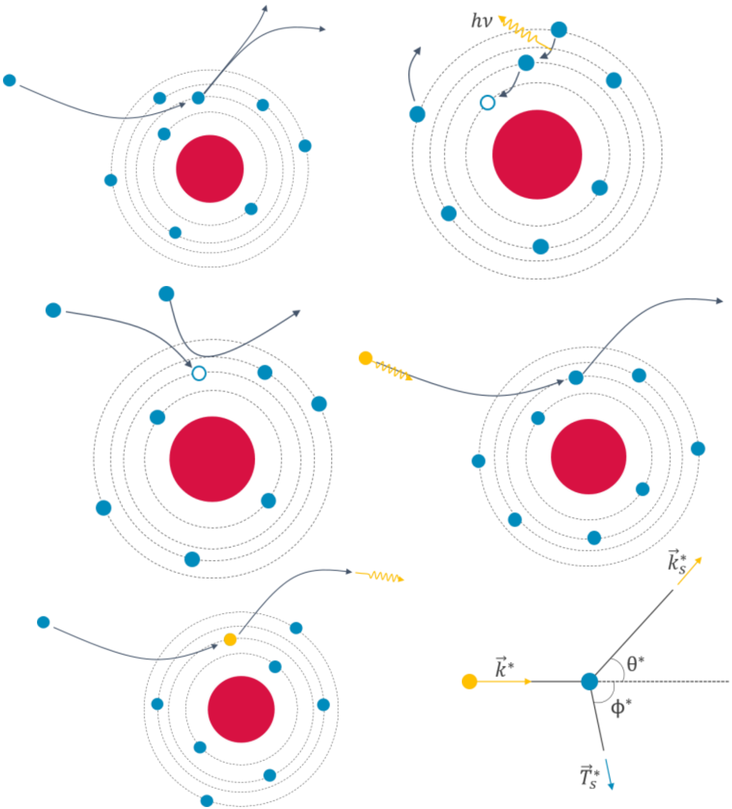
Validity of the collisional algorithm in beam-solid interaction?

A. Benedetti et al., Nat. Phot. **12** 319–323 (2018)

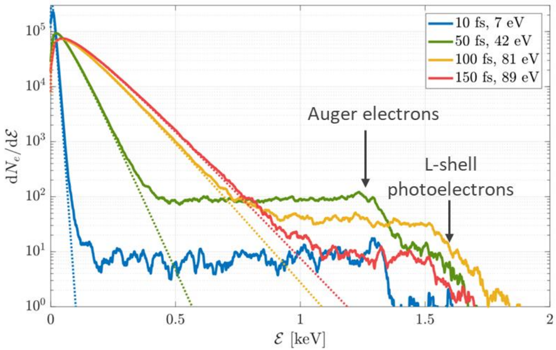


XFEL pulse interaction with matter
implementation of “simple” atomic model

- Implemented in CALDER:
  - Collisional ionization
  - Atomic deexcitation
  - Three-body recombination
  - Photoionization (from X-ray)
  - Radiative recombination
  - Compton scattering
  - Ionization potential depression



Self-consistent simulation of XFEL pulse interacting with Al target



D. Tordeux, PhD, Université Paris-Saclay (2022)
R. Royle *et al.*, Phys. Rev. E **95**, 063203 (2017).

Conclusion

- Numerical errors limiting PIC code prediction should be understood and reduced, e.g.:
  - NCR can impact the beam divergence, emittance, betatron source in standard wakefield simulation.
  - Reducing NCI is crucial in propagating beam or boosted frame simulation.
  - Solutions now exist to reduce NCR/NCI impact, but these solutions should be known and used by the community when needed.

- PIC code is a good tool to study some accelerator applications
  - Can foster the collaboration between the accelerator, plasma and laser communities
  - Dedicated developments are needed (physical modules, numerical schemes, …)

1) Future developments needed and planned as seen from the speakers and their groups

2) Do the planned activities address the requirements from funded projects (AWAKE, EuPRAXIA, …) and from various roadmaps for plasma accelerators? Are there urgent holes?

3) Does simulations and theory require its own roadmap or is work adequately driven/supported through funded projects and through overall plasma accelerator roadmaps?