Monte-Carlo event generation for the interaction of x-ray laser fields and hot electrons

Polish-German WE-Heraeus Seminar & Max Born Symposium

December 6th, 2023 // Uwe Hernandez Acosta

CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

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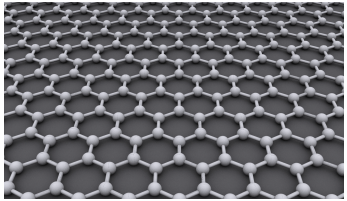
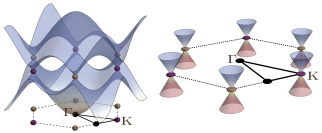
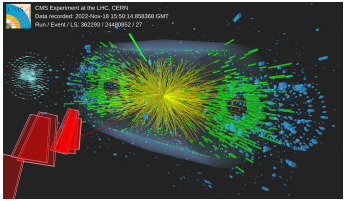
Neutron stars

Dirac-/Weyl materials



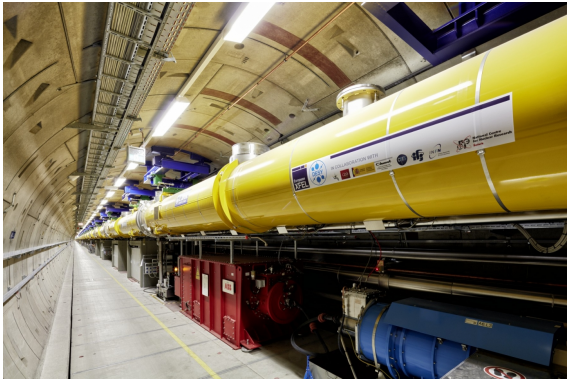


Particle colliders

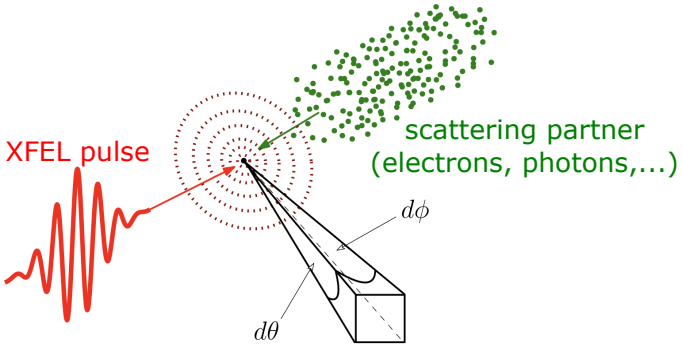


Quantum Electrodynamics!

EuropeanXFEL



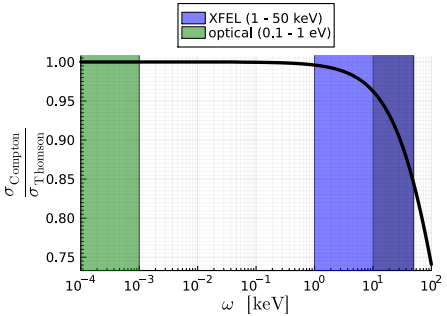
XFEL pulse as a driver



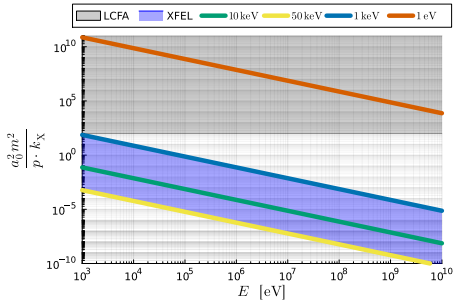
The parameter space: EuropeanXFEL

ω_X [keV]	λ_X [nm]	I [$\frac{\mathrm{W}}{\mathrm{cm}^2}$]	a_0	τ [fs]	N_{cycles}
~ 10	0.12	10^{21}	$\sim 10^{-3}$	20	$\sim 10^5$

Thomson scattering?



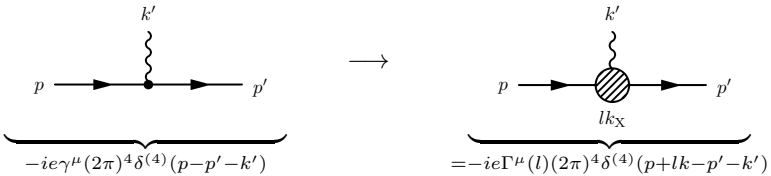
locally-constant field approximation?



→ we need a more QED-like description & new tools!

Model: strong-field quantum electrodynamics

- Feynman-rule: vertex



- vertex function

$$\Gamma^\mu(l,p,p',k) = \Gamma_0^\mu B_0(l) + \Gamma_1^{\mu\nu} B_{1\nu}(l) + \Gamma_2^\mu B_2(l)$$

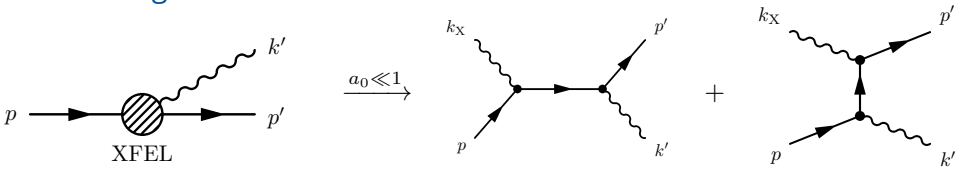
- Phase integrals

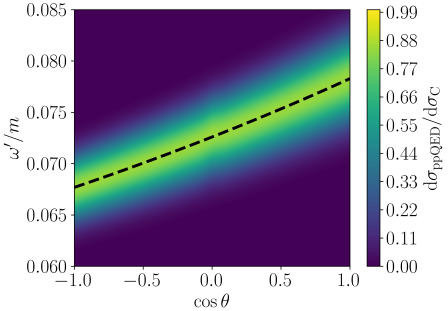
$$\left.\begin{matrix} B_0(l) \\ B_1^\mu(l) \\ B_2(l) \end{matrix}\right\} = \int_{-\infty}^{\infty} \mathrm{d}\phi \, \exp(il\phi + iG(\phi)) \begin{cases} 1 \\ A^\mu(\phi) \\ A^\mu(\phi)A_\mu(\phi) \end{cases}$$

[UHA, Kämpfer. Phys.Rev.D 108 (2023) 1, 016013][UHA. PhD thesis (2021)]

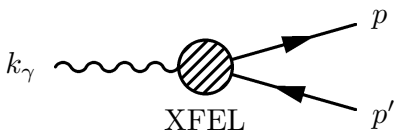
[Meuren,Keitel,Di Piazza. Phys. Rev. D 88, 013007 (2013)] [Mitter. Acta Phys. Austriaca Suppl. 14, 397–498 (1975)]

First-order processes I
Compton scattering

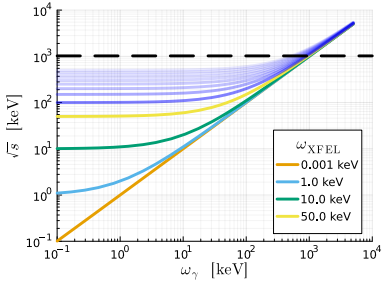




First-order processes II
Breit-Wheeler pair production



threshold: $\sqrt{s} = 2m_e \approx 1022\,\mathrm{keV}$

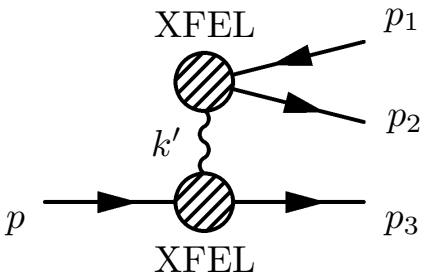


- positron in the final state
  → "easy" to detect
- investigated in optical setups

  [DiPiazza et al. Rev. Mod. Phys. 84 (2012), Fedotov et al. arXiv:2203.00019 [hep-ph]]
  - seminal experiment: E-144@SLAC
  - upcoming: LUXE@Desy, E-320@FACET-II

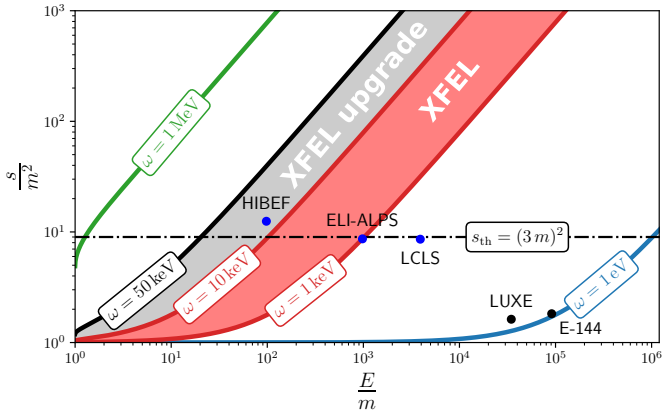
→ no **direct** observation yet

Second order process
Trident pair production



- positron in the final state
  $\rightarrow$ "easy" to detect
- threshold process
  - impact of spectral structure
- two vertex process
  - interesting physics
- no MeV partner photon needed
  - enabled by e^- beam

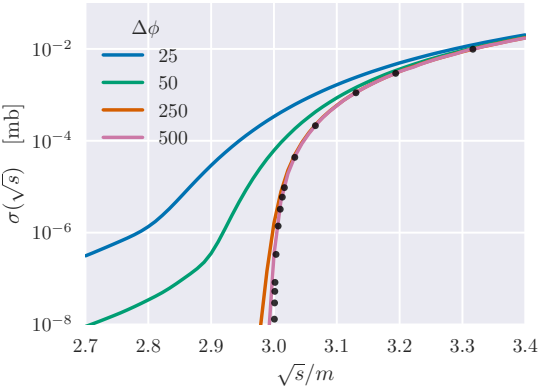
Trident process
kinematically reachable



- $\sim 10 - 50\,\mathrm{MeV}$ electron energy is sufficient
- conceivable electron sources
  - e^- guns
  - stable kHz+mJ laser wake field accelerator

    [J Faure et al 2019 Plasma Phys. Control. Fusion 61]
  - laser-driven e^- in thin targets @ HED/HIBEF

Trident process
previous insights are promising

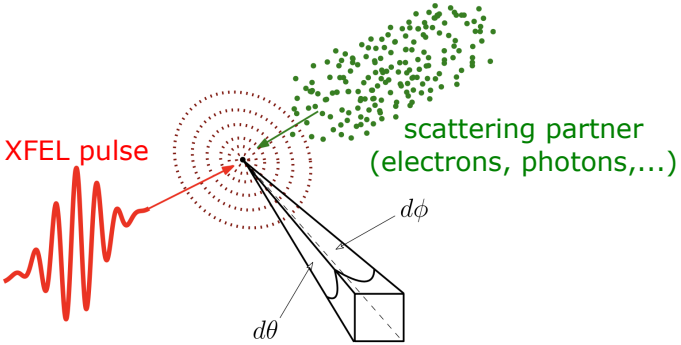


- Subthreshold effects for $\sqrt{s} < 3m_e$!
- raw estimate:
  - $\sigma_{\text{trident}} \sim 10^{-5}\,\text{mb}$
  - $1\,\text{nC}$ electron beam
  - XFEL focused on 1 micron

  $\Rightarrow \sim 6000$ positrons

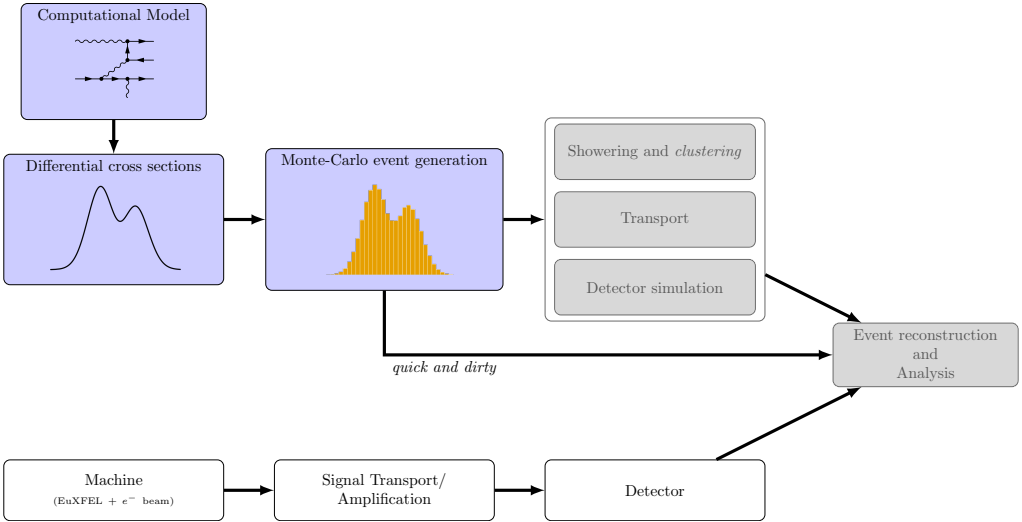
[UHA et al. Plasma Phys.Control.Fusion 61 (2019) 8, Titov et al. PRA 104 (2021) 6]

XFEL pulse as a driver



How many "ticks" will be in the pixel?

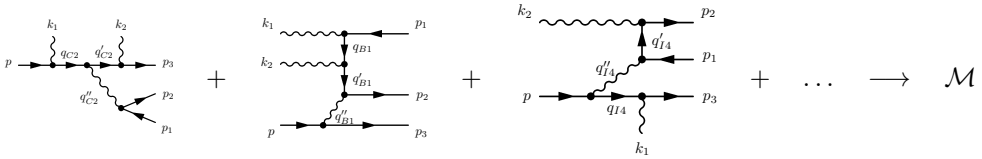
Particle-physics-like simulation workflow



[Stefan Gieseke - MCnet Vietnam summer school (2019)]

Differential Cross Sections: $k_1, \ldots, k_M \to p_1, \ldots, p_N$

- Scattering Matrix Element



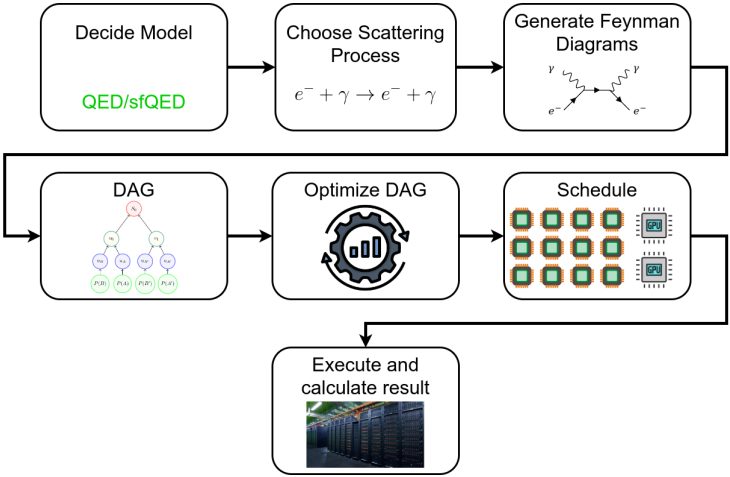
- Golden Rule

$$\mathrm{d}\sigma = \underbrace{\frac{1}{4\mathcal{I}}}_{\text{incident flux}} \times \underbrace{\sum_{\sigma_1 \ldots, \lambda_1 \ldots} |\mathcal{M}|^2}_{\text{squared matrix element}} \times \underbrace{\prod_{i=1}^{N} \frac{\mathrm{d}^3 p_i}{(2\pi)^3 2p_i^0} (2\pi)^4 H(k_1, \ldots, k_M, p_1, \ldots, p_N)}_{\text{phase space measure}}$$

$$H_{\mathrm{QED}}(k_1, \ldots, k_M, p_1, \ldots, p_N) = \delta^{(4)}(k_1 + \cdots + k_M - (p_1 + \cdots + p_N)) \times \Theta(\mathrm{cuts})$$

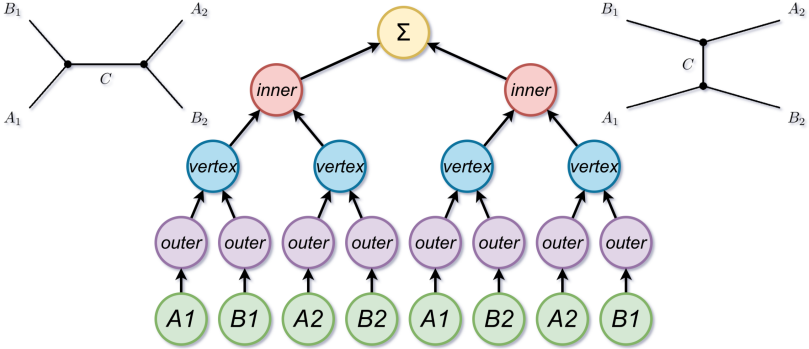
$$H_{\mathrm{sfQED}}(K, k_1, \ldots, p_1, \ldots; l, r, \ldots) = \delta^{(4)}((l + r + \ldots)K + k_1 + \cdots - (p_1 + \ldots)) \times \Theta(\mathrm{cuts})$$

Differential Cross-Section: get your hands dirty

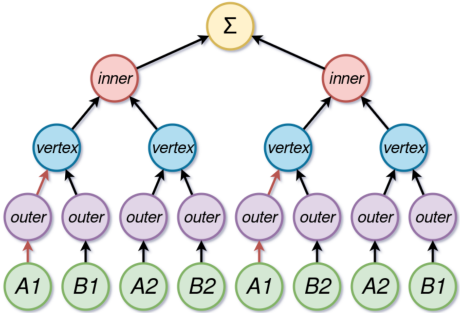


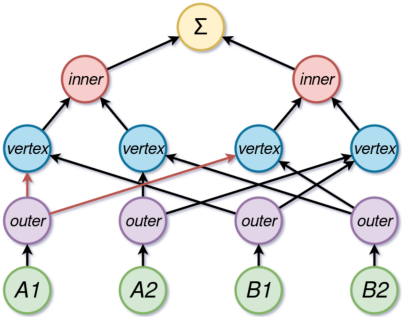
[WIP: Anton Reinhard]

Directed acyclic graphs - simplified



Optimization for target architecture

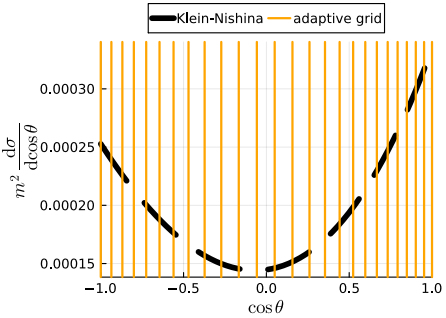




How to generate events

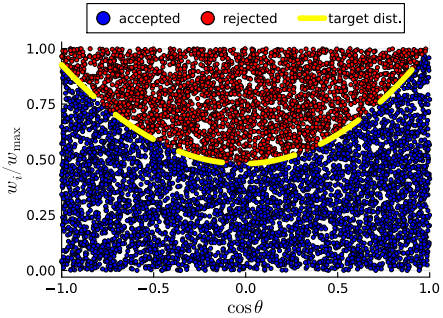
total cross section

$$\sigma \approx \frac{1}{N} \sum_{u \in \mathcal{R}[g]} \underbrace{\frac{\mathrm{d}\sigma/\mathrm{d}\cos\theta(u)}{g(u)}}_{\sim w_u}$$



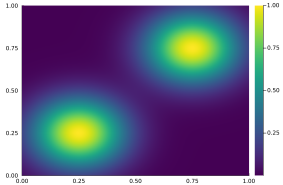
sample drawing (unweighting)

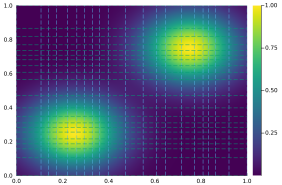
$$(u, w_u) \to (\tilde{u}, 1)$$

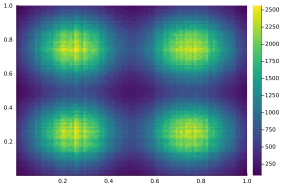


NN-Enhanced sampling [WIP: Tom Jungnickel]

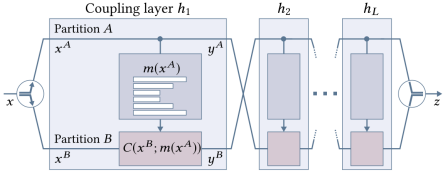
- VEGAS (standard) [Lepage. J.Comput.Phys. 27 (1978), 192]



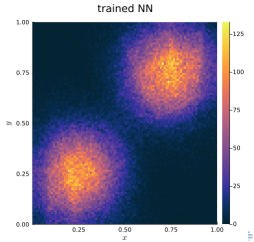




- Neural importance-sampling [Bothmann et al. SciPost Physics, 8(4):069, 2020]

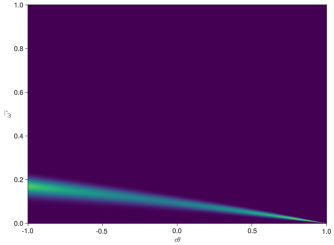


borrowed from [Müller, et al. ACM Transactions on Graphics (ToG) 38.5 (2019)]

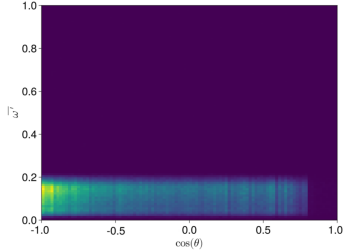


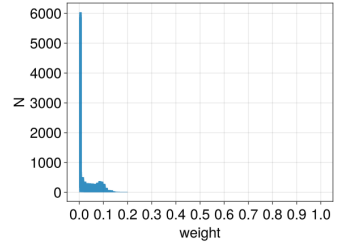
Neural importance-sampling: Pulsed-perturbative Compton

groundtruth

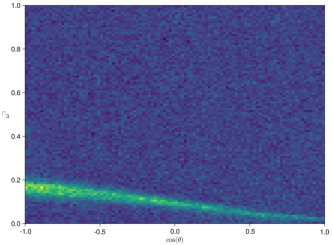


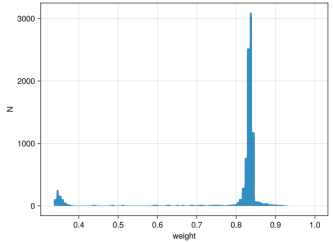
VEGAS sample





NIS sample



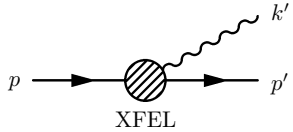


$$\overline{\omega}' := \frac{\omega'}{\omega'_{\max}(\cos\theta)}$$

$$\Delta\phi = 20$$

preliminary results!

Pulsed-perturbative Compton events - preliminary results



- LO pulsed-perturbative QED
- $\omega_X = 40\,\mathrm{keV}$ on electron at rest
- pulse profile: $\cos^2(\frac{\pi\phi}{2\Delta\phi})\sqcap_{2\Delta\phi}(\phi)$

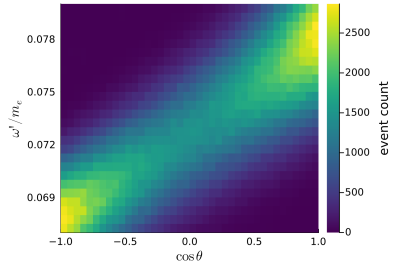
1000000×17 DataFrame

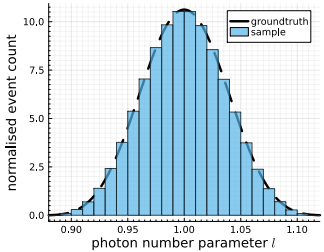
Row	pnum	i_photon_p0	i_photon_p1	i_photon_p2	i_photon_p3	i_elec_p0	i_elec_p1	i_elec_p2	i_elec_p3	o_photon_p0	o_photon_p1	o_photon_p2	o_photon_p3	o_elec_p0	o_elec_p1	o_elec_p2	o_elec_p3
	Float64	Float64	Float64	Float64	Float64	Float64	Float64	Float64	Float64	Float64	Float64	Float64	Float64	Float64	Float64	Float64	Float64
1	1.03299	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0777125	0.0305309	-0.0600246	0.0387833	1.00057	-0.0305309	0.0600246	0.0394948
2	1.05571	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0753346	0.0675228	0.0307501	-0.0130537	1.00294	-0.0675228	-0.0307501	0.0913318
3	1.02622	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.079136	-0.0156972	-0.0426269	0.0648538	0.99989	0.0156972	0.0426269	0.0134543
4	1.0084	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0693306	0.034683	0.0293837	-0.0523491	1.00895	-0.034683	-0.0293837	0.130627
5	0.988468	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.073214	0.0672119	-0.0215691	0.0194324	1.00586	-0.0672119	0.0215691	0.0588457
6	0.97474	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0664333	0.0182999	0.0111097	-0.0628894	1.01184	-0.0182999	-0.0111097	0.141167
7	0.963371	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.067178	-0.0498587	-0.0162319	-0.0419944	1.0111	0.0498587	0.0162319	0.120272
8	0.959015	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0691533	-0.0574692	-0.037231	-0.00966031	1.00912	0.0574692	0.037231	0.0879384
9	1.03851	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0780784	0.0629793	0.00371275	0.0450047	1.0002	-0.0629793	-0.00371275	0.0322774
10	1.0279	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0695265	0.00560484	-0.0198914	-0.0663841	1.00875	-0.00560484	0.0198914	0.144662
11	1.07726	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0729856	0.0379429	-0.0102991	-0.0614912	1.00529	-0.0379429	0.0102991	0.139769
12	1.0179	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0745428	0.0731398	0.0102775	0.0100701	1.00374	-0.0731398	-0.0102775	0.0682001
13	0.982411	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0712574	0.0254992	-0.0665046	-0.0021324	1.00702	-0.0254992	0.0665046	0.0804104
14	1.05344	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0716858	0.00557886	-0.040349	-0.0589889	1.00659	-0.00557886	0.040349	0.137267
15	1.01337	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0706587	-0.0103051	0.0502852	-0.0385913	1.00762	0.0103051	-0.0502852	0.116869
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
999986	0.993865	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0756503	-0.0541247	-0.0220227	0.0480467	1.00263	0.0541247	0.0220227	0.0302313
999987	1.0159	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0794708	-0.0100127	0.00157875	0.0788218	0.998807	0.0100127	-0.00157875	-0.000543702
999988	0.946853	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.072449	-0.0577775	0.0235338	0.0734161	1.00583	0.0577775	-0.0235338	0.0283441
999989	1.00806	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0690182	0.0150056	0.0369607	-0.0563227	1.00926	-0.0150056	-0.0369607	0.134601
999990	1.05844	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0749693	0.0706619	-0.0148392	-0.0201764	1.00331	-0.0706619	0.0148392	0.0984545
999991	0.958313	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0720688	-0.0513603	-0.0237413	0.0488839	1.00621	0.0513603	0.0237413	0.0373942
999992	1.05614	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.080803	-0.0560486	0.00147259	0.0581851	0.997475	0.0560486	-0.00147259	0.020093
999993	0.924985	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0636467	0.0237841	-0.0140955	-0.0573283	1.01463	-0.0237841	0.0140955	0.135606
999994	1.00732	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0729507	-0.00276008	-0.0728743	-0.00187523	1.00533	0.00276008	0.0728743	0.0818533
999995	1.02406	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0797067	-0.0245916	0.0163606	0.0740321	0.998571	0.0245916	-0.0163606	0.00424597
999996	1.01809	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0769205	0.0436517	-0.0473042	0.0421143	1.00136	-0.0436517	0.0473042	0.0361637
999997	1.01691	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0791456	-0.0077222	0.0285338	0.0734161	0.999132	0.0077222	-0.0285338	0.0225996
999998	1.00992	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0726986	-0.0692727	-0.0206647	-0.00770396	1.00558	0.0692727	0.0206647	0.085982
999999	1.01483	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0756504	-0.0242247	0.0656648	0.0287103	1.00263	0.0242247	-0.0656648	0.0495678
1000000	1.05075	0.0782781	0.0	0.0	0.0782781	1.0	0.0	0.0	0.0	0.0744422	-0.0713618	-0.00539393	-0.0204947	1.00384	0.0713618	0.00539393	0.0987728

999970 rows omitted

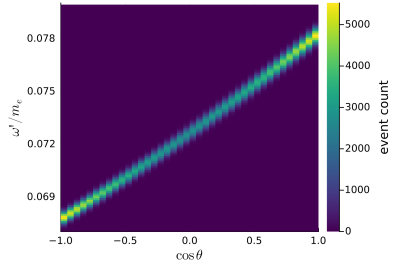
Pulsed-perturbative Compton events - preliminary results

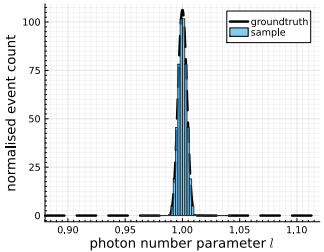
$\Delta\phi = 50$



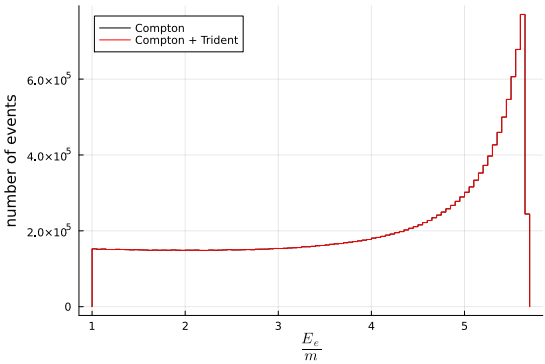


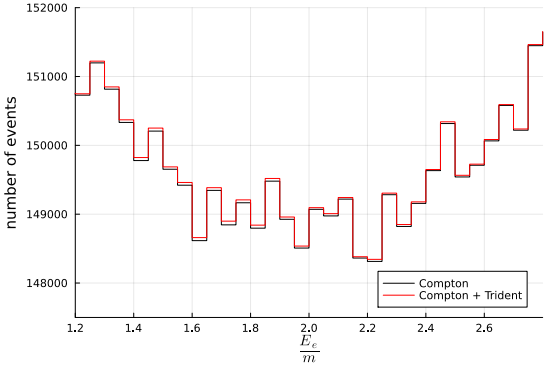
$\Delta\phi = 500$



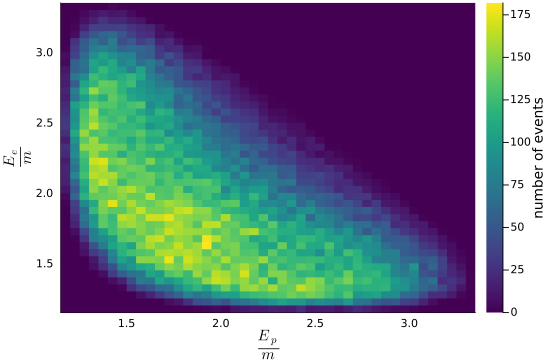


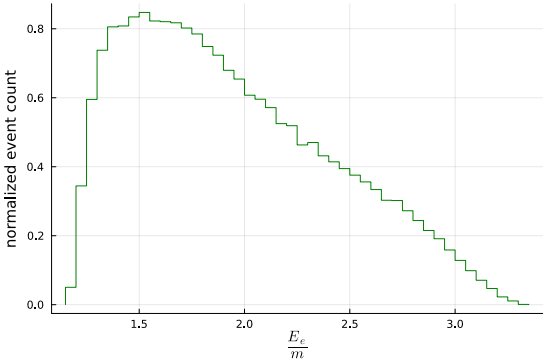
Trident + Compton (perturbative): preliminary results
includsive electron distribution





Trident process: preliminary results
exclusive electron distribution



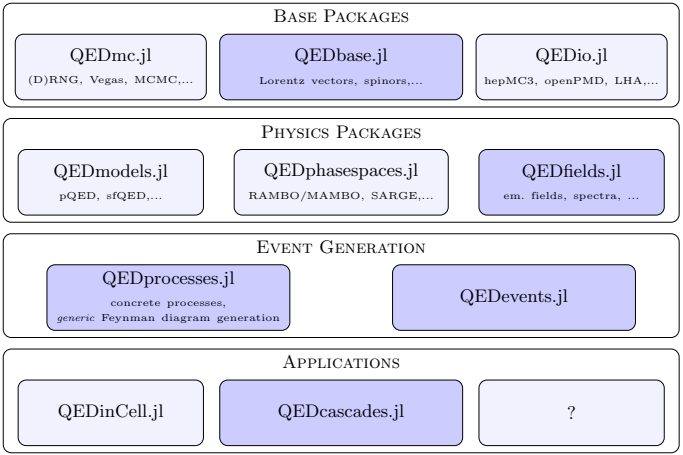


QED.jl - Strong-field particle physics code

[https://github.com/QEDjl-project]

Requirements

- open source
- written in Julia
- user-friendly
- modularised
- extensible
- performant
- CPU + GPU



`QED.jl` - Strong-field particle physics code

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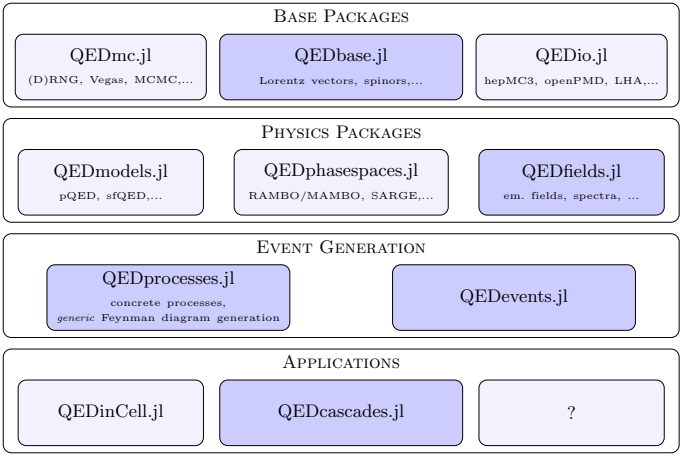

⟶ Proof-of-concept release: soon!

- Collaborators

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HiBEF

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- Acknowledgements:

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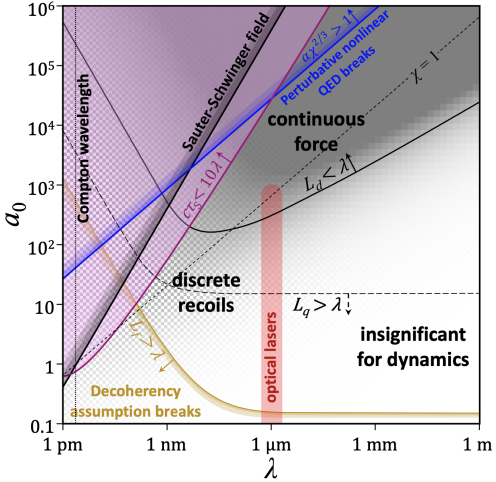
Janina Schreiber
Sachin K. Thekke Veettil

BACKUP

Parameter space
Where are we?



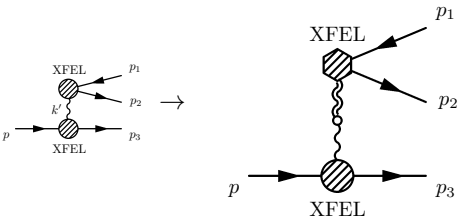
[Gonoskov, et al. Reviews of Modern Physics 94.4 (2022)]

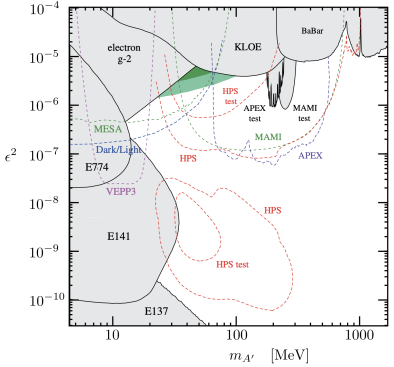
ω_X [keV]	λ_X [nm]	I [$\frac{\mathrm{W}}{\mathrm{cm}^2}$]	a_0	τ [fs]	N_{cycles}
~ 10	0.03	10^{21}	$\sim 10^{-3}$	20	$\sim 10^5$

- decoherence assumption breaks
  - → interactions accumulate over several XFEL wave-cycles
  - → modeled with higher order processes and spectral extensions
- almost monochromatic
  - $K \sim 1.5 - 9 \Rightarrow$ higher harmonics?
- high-precision description available
  - → pulsed-perturbative QED

EuXFEL pulse as a driver
Trident for dark matter exclusion

[Gakh et al. PRD 101 (2020) 7]





[Endo et al. PRD 86 (2012), Graham el al. Ann.Rev.Nucl.Part.Sci. 71 (2021)]

- Dark photon
  - $\rightarrow$ hypothetical dark matter candidate
  - $\rightarrow$ massive photon-like particle kinematically mixing with photons

  [Holdom. PLB 166 (1986)]

- sensitive for lower pair energy
- full control over the pure-QED background