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3-D Simulation of KeV-photon laser operation using GeV ultra-short laser-generated electron bunches*

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Abstract

The recent discovery of electron bunch acceleration to GeV energies using ultra-short laser pulses propagating through centimeter-scale plasmas¹ has stimulated interest in the use of these “mono-energetic” electron bunches to drive Self-Amplified Spontaneous Emission (SASE) free-electron lasers (FELs). Theoretically, one can generate 0.1-1 KeV coherent FEL photon pulses provided an electron bunch having high peak current, concomitant with low emittance and energy spread, can be achieved and successfully injected into the FEL wiggler. We have simulated the bubble acceleration of electrons using the 3-D particle-in-cell (PIC) code VPIC². The VPIC code has recently been optimized for the Roadrunner computer platform³ facilitating simulation of the entire acceleration process in the laboratory frame in 3-D. The electron distribution from these VPIC simulations is used as input for the 3-D FEL code FELEX⁴ to calculate the self-consistent growth from spontaneous emission of the 0.1-1 KeV photon pulse produced in the wiggler. FELEX models the interaction of the electron pulse with the optical pulse including the transverse dependences of the wiggler field (including wiggler field errors, if desired), and the transverse fall off of the electron density and optical field intensity. Examples of these simulation will be shown including the effects of electron beam quality on FEL extraction efficiency. These calculations provide an initial estimate of the specifications for both the electron acceleration quality and the FEL wiggler design parameters.

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A table-top XFEL consists of three main subsystems

VPIC → PARMELA → FELEX

- The fundamental scientific challenge is to achieve needed beam quality
- Plasma acceleration stage is crucial to understand and optimize
- Integrated modeling effort needed as metric for beam quality “improvements”
- Experimental validation of model optimization provides “reality check”

3D VPIC Simulations of electron acceleration have begun

VPIC is the world fastest PIC code running on the world's fastest computer (Roadrunner) at up to ~400 Tflops

Example: Bubble acceleration, $I = 4 \times 10^{21}$ W/cm², 5 fs pulse

3D VPIC simulation yields “mono-energetic” e⁻-bunch

- Initial simulation produced 30 nC of charge at 410 MeV!

- How do the e⁻ bunch characteristics change as the axial and transverse profile of either the plasma and laser pulse is modified?

VPIC output used as FELEX input

- Use “computational energy and emittance scraping” to generate a range of FEL beam conditions

- Detailed transport calculations are also being performed

electron-beam transport and phase-space conditioning investigated using PARMELA

emittance conditioning reveals correlation between longitudinal and transverse motions

energy selection performed at high dispersive region in the achromatic bend

before energy selection

after energy selection

energy spread leads to increase in transverse
emittance

- **Parmela simulations show large increase in emittance through the transport section**
- **This may be caused by the large energy spread generating an increase in the projected transverse**
- **phase space**
- **FELEX simulations using the Parmela electron distribution soon will be performed to address this issue**

FELEX: 3-D(t) Model for FEL System Physics

- Three-dimensional modeling code developed over 7 year span by modeling team
- FELEX was benchmarked against FRED (Ginger) for the GBFEL
- FELEX currently operational at LANL (updated FORTRAN code)
- Includes FEL interaction in wiggler and complex optical resonators
- Code results validated against Free-Electron Laser experiments (HIBAF, APEX, RAFEL, Stanford Mark III, Boeing ring resonator)
- Electron beam input and output links to PARMELA for INEX calculations

Example: Electric field profile versus time and transverse space at the wiggler exit after 120 passes around the resonator.

FEL optical pulse electric field profile

FELEX has Extensive Modeling Capabilities

- Single frequency, pulse and periodic options
- 3-D optical grid models complete pulse field
- 3-D source grid drives field on optical grid
 - Electron bunching drives source amplitudes
 - Grids have independent sizes
 - Internally-generated electron distributions
 - Parmela input/output distributions
- Extensive wiggler design capability
 - 1-D or 2-D wiggler focusing
 - Tapers:
 - Power law (Halbach) taper
 - $B_w, k_w, a_w, a_w/k_w = \text{constant}$ tapers
 - Resonant phase taper
 - External $B_w(z)$ and $k_w(z)$ taper
 - Wiggler B_w and k_w statistical errors routine
 - User-determined beam correction stations
 - Pre-buncher section

Energy balance tracked

Pulse transverse electric field profile monitored in wiggler and resonator

FEL Equations Modeled in FELEX

- FELEX tracks the electron's (macro-particle's) guiding-center trajectories
 - Actual wiggler deviations are 10's of microns or less
- FELEX integrates the optical frequency-averaged electric field equations
 - ADI integration provides accurate gain estimates
- FELEX can run on a PC and has been ported to the ASCI machines for extensive parametric studies

OPTICAL FIELD EQUATIONS

$$E_f(\vec{r}, t) = \text{Re}[E_f e^{if(k_o z - \omega t)}]$$

$$E_f = E_{of}(\vec{r}) \exp[i\theta_{of}(\vec{r})]$$

$$2ifk_o \frac{\partial E_f}{\partial z} + \frac{\partial^2 E_f}{\partial x^2} + \frac{\partial^2 E_f}{\partial y^2} = S_1(\vec{r}) + S_2(\vec{r})$$

Mono-pole source term

$$S_1(\vec{r}) = - \left\langle \frac{4\pi J f k_o a_w(\vec{r})}{c} \mathcal{K}_f^{(1)}(\xi, \sigma) \delta(\vec{r} - \vec{r}_i) \frac{e^{-if\psi}}{\gamma} \right\rangle_e$$

Di-pole source term

$$S_2(\vec{r}) = \left\langle \frac{i4\pi J f k_o a_w(\vec{r})}{c} \mathcal{K}_f^{(2)}(\xi, \sigma) \frac{1}{2} [\delta(\vec{r} - \vec{r}_i - \hat{x}\chi/2) - \delta(\vec{r} - \vec{r}_i + \hat{x}\chi/2)] \frac{e^{-if\psi}}{\gamma} \right\rangle_e$$

$$\mathcal{K}_f^{(m)}(\xi, \sigma) = (-1)^f \sum_{n=-\infty}^{\infty} J_n(f\xi) [(-1)^m J_{2n+f-m}(f\sigma) - J_{2n+f+m}(f\sigma)]$$

$$\xi = \frac{k_o a_w^2}{8\gamma^2 k_w} \quad \chi = \frac{a_w}{\gamma k_w} \quad \sigma = \frac{8\xi\gamma\beta_x}{a_w} \quad a_w(\vec{r}) = \frac{eB_y(\vec{r})}{mc^2 k_w} \quad a_{sf}(\vec{r}) = \frac{eE_{of}(\vec{r})}{mc^2 f k_o}$$

ELECTRON EQUATIONS OF MOTION

$$\frac{d\gamma}{d(ct)} = (-1)^f \frac{e}{mc^2} \frac{a_w(\vec{r})}{2\gamma} \sum_{f=1}^{\infty} \text{Re} \left\{ \mathcal{K}_f^{(1)}(\xi, \sigma) E_f e^{if\psi} + i \frac{\chi}{2} \mathcal{K}_f^{(2)}(\xi, \sigma) \frac{dE_f}{dy} e^{if\psi} \right\}$$

$$\frac{d\psi}{d(ct)} = k_w(z) - \frac{k_o}{2\gamma^2} \left[1 + \frac{a_w^2(\vec{r})}{2} + (\gamma\beta_x)^2 + (\gamma\beta_y)^2 \right]$$

$$- \sum_{f=1}^{\text{odd}} a_w a_{sf} \cos[f\psi + \theta_{of}] + \sum_{f=2}^{\text{even}} a_w a_{sf} \sin[f\psi + \theta_{of}]$$

$$\vec{B}_w = -\nabla \chi_m, \quad k_w^2 = k_{wx}^2 + k_{wy}^2$$

$$\chi_m = - \frac{B_w(z)}{k_{wy}} \cosh(k_{wx}x) \sinh(k_{wy}y) \sin \left[\int k_w(z) dz \right]$$

$$\frac{d(\gamma\beta_x)}{d(ct)} = - \frac{a_w^2 k_{wx}^2}{2\gamma} x - \frac{e}{mc^2} (\beta_y B_x^e - \beta_x B_y^e)$$

$$\frac{d(\gamma\beta_y)}{d(ct)} = - \frac{a_w^2 k_{wy}^2}{2\gamma} y - \frac{e}{mc^2} (\beta_x B_y^e - \beta_y B_x^e)$$

$$\frac{dx}{d(ct)} = \beta_x, \quad \frac{dy}{d(ct)} = \beta_y$$

FELEX Optical Propagation Tailored to FEL Problem

- Linear (FFT) and nonlinear ADI (Alternating Direction Implicit) propagation of electric field envelope employed
- E-field modeled on a set of transverse rectangular grids
- Grid has automated expansion/contraction (for propagation through foci and over large ranges)
- Multiple electric field phase fronts used to model pulse z-dependence

- Transform of E-field in z-direction gives frequency content of pulse

FELEX Electron-Optical Wave Coupling Methodology

- Parmela, 4-D ellipsoid or Gaussian electron distributions assumed in space, velocity and energy.
- Individual electrons are generated from these distribution functions
- Each electron from the $(x, y, \beta_x, \beta_y, \gamma)$ distribution is reproduced N_{ephase} times in its ponderomotive bucket
- Electron centroids are precisely tracked through the wiggler
- The electron distribution in each bucket is used to calculate an optical source function on the source grid
- The electron source is weighted by the charge at each location in the micropulse

The electron source grid drives the complex electric field on the optical grid.

FELEX Optics Package Facilitates Diverse FEL Concept Analysis

- Amplifier seeding sensitivity
- RAFEL resonator analysis
- Oscillator and SAMOPA optimization
- Stable resonators
 - Mirror tip, tilt, offset, jitter
 - Mirror imperfections (Zernike polynomials)
 - Mirror thermal distortion modeled
- Unstable resonators (negative branch)
 - Produces solid output beam
- SE and CSE harmonic generation
 - Mirror damage assessment
 - Harmonic lasing
- Side-band suppression schemes
 - Dielectric filter
 - Grating rhomb (temporal discrimination)
 - Littrow/Stepped Mirror (spatial discrimination)

Optical Elements in FELEX

Mirrors, Lens, Circular aperture, Square aperture, Rectangular aperture, Rhomb3D, Littrow, Filter, Transmissive coupler, Hole coupler, Circular scraper, Rectangular scraper, Detector, Magnify, Collimate

FELEX stable/unstable optical field profile †

FELEX has Wiggler Field Error and Field Correction Algorithms

- Random field error realizations generated for a user-defined rms error level
- Different geometries allowed for e-beam diagnostic stations and error corrector coils
- Sensitivity analysis gives efficiency degradation and beam loss through wiggler

FELEX e-beam envelope with field errors and corrector stations

FELEX sensitivity analysis* of wiggler field errors versus beam position monitor error

FELEX Models Harmonic Generation/Suppression Physics

Validation: Harmonics are sensitive diagnostics of the FEL interaction

FELEX models both even and odd harmonic sources[†]

Odd and even electron sources

Harmonic power benchmarked against Stanford Mark III FEL[†]

- Mark-III FEL:
 $\gamma = 86.11$, $\Delta\gamma/\gamma = 0.3\%$, $\epsilon_x = 0.087\pi$ mm mrad, $\epsilon_y = 0.032\pi$ mm mrad, $I = 30.0$ A, $\lambda_w = 2.3$ cm, $B_w = 6570.0$ G, $L_w = 108.0$ cm, $\lambda_s = 3.16$ μ m, $P_{\text{circ}} = 40$ MW, $z_r = 73.6$ cm, $G = 33\%$, $\eta = 0.98\%$;

Effects of misalignments compared with HIBAF[†]

- Los Alamos FEL:
 $\gamma = 46.0$, $\Delta\gamma/\gamma = 1.2\%$, $I = 400.0$ A, $\epsilon = 2.1\pi$ mm mrad, $\lambda_w = 2.73$ cm, $B_w = 3927.0$ G, $L_w = 100.0$ cm, $\lambda_s = 10.36$ μ m, $P_{\text{circ}} = 0.5$ GW, $z_r = 49.5$ cm, $G = 16\%$, $\eta = 0.84\%$.

FELEX Functions as a Parametric Study Tool

- Scanning wavelength to produce gain curves in an integral part of the code
- IVARSCAN iteration capability was added to the code to allow parametric evaluation of two input variables simultaneously
 - Current FELEX setup: γ , P_{input} , $\Delta\gamma$, ϵ , I_{peak} , z_f , z_R , ψ_1 , ψ_2
 - Used for conceptual design of the 10 kW HPO FEL[†]

HPO Resonator Layout

Efficiency vs Cavity Filter Bandwidth

FELEX has Extensive Mirror Capabilities

- Mirror aberrations
 - Zernike polynomial inputs
- Mirror de-space, tilt and temporal jitter
- Mirror thermal distortion options
 - Thermal bowing option (user input)
 - Flat heat exchanger
 - Gaussian heat exchanger
 - Rocketdyne heat exchanger (GBFEL)
- Automatic mirror mode matching
- Thermal bowing used for HPO analysis with distortions provided by heat transfer and static stress analyses (external codes).
- Cold mirror analysis required to ensure laser will start up and reach saturation
- Transient thermal mirror analysis required to assess degradation for high average power operation

Mirror Thermal Distortion for HPO Out-coupler

FELEX Predicted Extraction efficiency of HIBAF High-Extraction- η Expts.

- FELEX simulations using PARMELA electron distributions were compared to HIBAF oscillator experiments for tapered wigglers with (+) and without prebunchers*.

- Agreement with the experiment are good.

- Differences in results attributed to experimental error, slight changes in accelerator operating parameters and the use of PARMELA to model the *thermionic* gun.

FELEX Validated with HIBAF Mode-Media Experiments

- Refractive effects of optical gain in the electron beam focuses (aligned e-beam) and steers the optical beam (misaligned e-beam)
- Refractive effects dominate optical mode properties for high beam currents
- Results from HIBAF optical axis displacement experiments* compared to FELEX simulations using electron beam distributions from PARMELA (INEX)

Mode displacement at outcoupler

Mode displacement at back reflector

- FELEX accurately predicted the HIBAF experimental results.

Bunching of electrons as they propagate through the 5 meter wiggler

$z = 0.0000$

Obligatory electron phase space movie

Example Estimate of FEL Performance

3D VPIC Simulation

FELEX Calculations

- FEL radiations grows from shot noise at the beginning of the wiggler
- Optimal extraction efficiency of 0.3% with 7m wiggler gives:
- ~100 GW or $\sim 10^{14}$ photons at wavelength of 32 nm

Slope of gain curve during linear growth as a function of emittance

- Modest decrease in gain as ϵ increases for $\epsilon \lesssim \lambda$
- Rapid decrease in gain for $\epsilon > \lambda$

$$\gamma = 2400$$

$$\Delta\gamma = .001\%$$

$$\lambda \sim 3.5 \times 10^{-7} \text{ cm}$$

Slope of gain curve during linear growth as a function of $\Delta\gamma$

- Somewhat flat gain curve from .1 to 1 %
- For large current, little loss in gain over 2 orders of magnitude

$$\gamma = 2400$$

$$\varepsilon = 1.75 \times 10^{-7}$$

$$\lambda \sim 3.5 \times 10^{-7} \text{ cm}$$

Conclusions

- Integrated simulation capability now exists at LANL to understand and optimize the nonlinear dynamics crucial to the operation of XFELs
- VPIC simulation already show large charges can be accelerated
- Emittance growth through the transport section must be addressed
- FELEX simulations using the Parmela electron distribution soon will be performed to address this effects on X-ray extraction