Simulations of the Microbunching Instability in FEL Beam Delivery Systems

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The setting: beam delivery system of a free electron laser (FEL)

The problem under study: the growth of the microbunching instability driven by longitudinal space charge (LSC) and coherent synchrotron radiation (CSR), and the efficacy of a “laser heater” as a means of suppressing it

The challenge: to distinguish effects due to physical microstructure from purely numerical (“sampling noise”) effects

Computational tools: IMPACT-Z and Impact-T beam dynamics codes

Simulations: focus on the growth of the uncorrelated (slice) energy spread in simulations, varying the number of macroparticles and the initial slice energy spread

Assessment of simulation results

Summary
• Recent work: modeling FERMI@Elettra FEL at Sincrotrone Trieste (Italy) [LBNL-Sincrotrone Trieste collaboration]

Beam energy at the entrance of laser heater $\sim$100 MeV (peak current $\sim$70A); at the exit of Linac4, $E \sim 1.2$ GeV (peak current 500A or 800A depending on configuration)

• Medium bunch (0.7 ps) and long bunch (1.4 ps) options
• 2 bunch compressors, 4 linacs (a total of 15 RF cavities), followed by a spreader used to direct the beam into one of two undulator lines
• In the case of the FERMI FEL, high peak current, low emittance, and low energy spread are required; preservation of the beam quality during bunch compression and acceleration is challenging
• Slice energy spread is small in the beam exiting the injector, but grows down the linac due to the LSC- and/or CSR-driven microbunching instability
• A fundamental instability with its roots in the discreteness/sampling noise, the entire machine acting as an amplifier of the initial noise
• A laser heater was proposed to facilitate the suppression of the instability by increasing the uncorrelated rms energy spread
• In simulations, not easy to separate effects due to numerical noise from those due to the discrete nature of the physical system
• High-resolution numerical simulations are needed to correctly model the instability
Microbunching Instability

- At a scale much smaller than the bunch length, LSC and CSR effects become significant; together, they give rise to the microbunching instability.
- A fundamental instability with its roots in the discreteness/sampling noise, the entire machine acting as an amplifier of the initial noise.
- Shot noise/discrete nature of the system are responsible for the initial microstructure in the beam.
- These microstructures induce LSC forces that over time produce energy modulation within the bunch.
- When the bunch propagates through the magnets of the bunch compressor, energy modulation is transformed into spatial modulation with increased magnitude of microbunching, which gives rise to increased intensity of CSR, resulting in even more energy modulation and more microbunching.
- At the end, the electron beam with significant fragmentation in the longitudinal phase space.
Modeling Collective Instabilities

- Correct modeling the instability is crucial in this setting

  *Left*: Longitudinal phase space of the bunch at the end of the beam delivery linac: LSC-driven microbunching instability as seen in simulations with 2M particles (green) and 100M particles (blue), with CSR turned off, compared with the no-space-charge, no-CSR result (red); the same initial uncorrelated energy spread in all three simulations.

- Approximately 4.5 B electrons in the actual bunch
- Low sample particle count results in exaggerating the initially-present microstructure, hence greatly overestimating the final slice energy spread
- As the number of simulation particles is increased, does one see an asymptotic behavior that can be used to extrapolate the results to the actual number of electrons in the beam?
Gain Function

- The simulations must resolve the relevant spatial frequencies where most gain occurs.

Spectral gain function of the microbunching instability calculated after BC1 (left) and at the end of the linac (right) as predicted by linear theory.

- Linear theory will likely eventually fail at the high frequency end of the noise spectrum; the evolution of the distribution has to be modeled using particle-based codes or (nonlinear) Vlasov solvers.

- In PIC simulations, choose grid to reliably resolve spatial scales in the 10-30 µm range (used 64x64x2048 grid for 100M-particle simulations).
Modeling Tools: IMPACT Suite of Codes

- Capabilities of IMPACT relevant to modeling FELs:
  - Two parallel particle-in-cell (PIC) codes: IMPACT-T, a time-based code, and IMPACT-Z, a z-coordinate based code
  - Fully self-consistent, 3D space charge with six types of boundary conditions
  - Extensive library of beamline elements, with arbitrary overlap of external fields allowed
  - 1D CSR wake
  - Short-range longitudinal and transverse wakes (computed using FFT)
  - Realistic fields in forward and backward travelling wave RF cavities
  - Integrated Green’s function algorithm for high aspect ratio beams
  - Multiple slices/bins to handle the beam with large energy spread (in IMPACT-T)
Modeling CSR

- A free-space, 1D (zero transverse emittance), steady state (short bunch, no transition regions) model [Saldin et al., NIM A 490, 1(2002)]
- (Ultra)relativistic beam; renormalized Coulomb term
- The rate of energy change of reference particle with coordinate $s$ is:

$$\frac{dE}{cdt} = \frac{2e^2}{R^2} \gamma^4 \int_{-\infty}^{s} \frac{\theta^6 + 2\theta^4 - \theta^2 - 6}{(\theta^2 + 1)^3(\theta^2 + 3)^2} \lambda(s') ds'$$

where \( \frac{1}{3} \theta^3 + \theta = \frac{\gamma^3}{R}(s - s') \)

- An approximate expression for the above 1D CSR wake:

$$\frac{dE}{cdt} = -\frac{2e^2}{3^{1/3} R^{2/3}} \int_{-\infty}^{s} \frac{1}{(s - st)^{1/3}} \frac{d\lambda(st)}{dst} dst$$

- Numerical evaluation requires due care: a weakly singular kernel and a noisy charge density $\lambda(s)$
Modeling CSR (cont-d)

- Numerical evaluation involved handling separately regions near and far from the singularity, as well as use of filters that conserve total charge, preserve the positivity of density, and have transfer functions that uniformly approach zero as $\omega \rightarrow \omega_N$
- Must be able to resolve the range of spatial frequencies where most of the gain occurs
- Two tests shown here: a flat-top density (top), and a flat-top with sinusoidal modulation (bottom); 2M particles, single bend magnet, no initial energy spread in both cases
- A recent improvement: added transition regions
Modeling CSR (cont-d)

• An alternative to the filter-based approach: piecewise polynomial approximation of the charge density convolved with the CSR wake kernel

• Finding parameters of approximation requires solving an ill-conditioned linear system by SVD

• Advantages:
  -- arguably easier to make adaptive, hence more accurate at modeling localized features/spikes
  -- functional form analytically known, $C^n$ if necessary
  -- approach can be extended to higher dimensions
  -- combined with multiscale techniques, can be the basis for efficient and accurate 3D CSR modeling algorithms

Bunch current profile after the 3rd bend in the ILC TA chicane ($\sigma_z \sim 0.5\text{ps}$)
Simulations: Initial Distribution

The uncorrelated part of the longitudinal phase space distribution at the entrance to the laser heater, before a smooth approximation is constructed which will be used for sampling the longitudinal phase space with up to 100M particles.

- A 200k - particle distribution produced in a separate simulation (from the injector to the laser heater) was used as a “template” for upsampling.
- A smooth approximation to the longitudinal phase space distribution was constructed as the direct product of the denoised bunch current and smoothed projected “energy profile”; it was then sampled by the rejection method with up to 100M macroparticles.
- Transverse distribution is produced by replicating the “template” transverse distribution (correlation between z and local transverse distribution is lost).
Simulations: Results of Parametric Studies

- To study the suppression of the instability, increased the initial rms slice energy spread to \( \sigma_{E_0} = 7.7 \text{ keV}, 15.3 \text{ keV}, \text{ and } 22.1 \text{ keV} \)
- Used \( N = 2, 6, 20, 60, \text{ and } 100M \) particles
- Extrapolation to the actual number of particles (~4.5B) was found to be speculative at best; in particular, no \( N^{1/2} \) dependence seen for “numerical” contribution to the \( \sigma_E \)
- As expected, weaker/slower instability growth seen at higher \( \sigma_{E_0} \)
• Simulations with 1B particles (but using a different upsampling scheme) placed $\sigma_E$ within design specifications:
  - $\sigma_E \sim 210$ keV for $\sigma_{E0} = 7$ keV; $\sigma_E \sim 190$ keV for $\sigma_{E0} = 15$ keV

• Upsampling has to be done in parallel, the speed of random number generators matters

• A new approach to domain decomposition to distribute evenly the particles and computational domain among processors

• Major next step: start-to-end simulations

Longitudinal phase space at the end of the spreader section of the FERMI FEL linac: 10M, 1B, and no SC or CSR results
The growth of the microbunching instability in the beam delivery system of a free electron laser is modeled using PIC codes IMPACT-Z and IMPACT-T with the number of macroparticles ranging up to 1B. Distinguishing effects due to low sample-particle count from those due to physical microstructure is exceedingly difficult, with no robust schemes available for extrapolating results to the actual number of electrons in the bunch. Simulation results support using a laser heater to suppress the onset of the instability and bring down the slice energy spread. One outcome of the project is that simulations with the actual number of particles are now within reach! Work still in progress: enabling start-to-end simulations, 2D and 3D CSR modeling, and detailed comparisons with the direct Vlasov solver simulations.
1D: Filtering-Based and SVD-Based Piecewise-Polynomial-Approximation Approaches

- A free-space, 1D (zero transverse emittance, constant radius trajectory), ultrarelativistic model [Saldin et al., NIMA 398, 373]
- Developed and implemented a filter-based algorithm and a new, SVD-based adaptive analytic (piecewise-polynomial) density approximation algorithm
- New algorithms can resolve the range of spatial frequencies where most of the gain occurs, as well as sharp, highly localized spikes in the distribution
- New algorithms have been used in simulations of FERMI@Elettra Linac and ILC TA

Top: A test of the filter-based algorithm (longitudinal phase space shown): a flat-top charge density with a sinusoidal modulation before (green) and after (red) a single bend magnet, compared with analytic result (blue). 2M particles, no initial energy spread. Bottom: Approximation of the spike in the bunch current profile from ILC TA simulations
Advantages of the filter-based approach:
- Computationally efficient
- Filters can be custom-designed

Example:

\[ y_n = \frac{1}{96}[7u_{n-2} + 24u_{n-1} + 34u_n + 24u_{n+1} + 7u_{n+2}] \]

\[ u(t) = \sum_{m=1}^{M} C_m e^{i\omega_m t} \rightarrow y_n = \sum_{k=-N}^{N} c_k u_{n-k} \rightarrow y(t) = \sum_{m=1}^{M} C_m H(\omega_m) e^{i\omega_m t} \]

\[ H(\omega) = \frac{1}{96}[7e^{-2i\omega} + 24e^{-i\omega} + 34 + 24e^{i\omega} + 7e^{2i\omega}] = \frac{34 + 48 \cos \omega + 14 \cos 2\omega}{96} \]

Advantages of the piecewise-polynomial approximation approach:
- better than filter-based algorithms at capturing sharply localized spikes in the distribution
- approximation is known analytically,--useful for testing (new and old) algorithms
- unlike the filtering-based approach, can be extended to higher dimensions
- can be used in a multiscale framework if, e.g., the approximation is done with multiwavelets
Ideas for Efficient Multiscale Algorithms for Modeling CSR in 2D and 3D

• The need for efficient 2D/3D CSR algorithms
  • significant differences in computed transverse emittance growth have been found between 1D and 2D/3D simulations
  • in the final bend magnet of a chicane, the bunch can be almost at right angle to the reference trajectory: a 1D approximation can be difficult to justify
  • the trade-offs between resolution and speed/memory efficiency are often drastic

• Within the logic of integrating over the bunch history, low separation rank (LSR) sparse separable representations of the bunch density and the wake function integral operator kernel promise a solution to the speed and memory requirements in multiple dimensions

• Multidimensional convolution operations are effectively reduced to one-dimensional convolutions → increase in the speed of simulations

• Working in a multiscale basis (e.g., multiwavelets):
  • compact storage in memory of the distribution history
  • Green’s function can likely have a sparse representation
  • adaptive algorithms for integration (over the bunch history) in the time domain can be constructed such that old(er) history data is discarded scale-by-scale without recomputing

• These ideas are the subject of a recently submitted CSR modeling Phase I SBIR proposal
\[ \delta = \frac{\Delta E}{E} \]

\[ V = V_0 \cos(\kappa z) \]

\[ \Delta z = R_{56} \delta + T_{566} \delta^2 \]

Graph showing rms \( \Delta E \) past BC2 (KeV) vs. initial rms \( \Delta E \) (KeV):