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Publication Date

2009-03-20

Design Studies for a High-Repetition-Rate FEL Facility at LBNL*

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Introduction

Lawrence Berkeley National Laboratory (LBNL) is working to address the needs of the primary scientific Grand Challenges now being considered by the U.S. Department of Energy, Office of Basic Energy Sciences: we are exploring scientific discovery opportunities, and new areas of science, to be unlocked with the use of advanced photon sources. A partnership of several divisions at LBNL is working to define the science and instruments needed in the future. To meet these needs, we propose a seeded, high-repetition-rate, free-electron laser (FEL) facility. Temporally and spatially coherent photon pulses, of controlled duration ranging from picosecond to sub-femtosecond, are within reach in the vacuum ultraviolet (VUV) to soft X-ray regime, and LBNL is developing critical accelerator physics and technologies toward this goal. We envision a facility with an array of FELs, each independently configurable and tunable, providing a range of photon-beam properties with high average and peak flux and brightness.

The underlying theme of the Grand Challenges now being posed for physics, chemistry, biology, and materials science is to understand, predict, and ultimately control the properties of matter. The “emergent” properties of complex systems are of particular interest. Here, correlated interactions among charge carriers, and between charge carriers and constituent atoms, give rise to new properties and functionality with tremendous potential for practical applications. These same correlated interactions also challenge our understanding of complex systems in that they defy conventional paradigms based on the Born–Oppenheimer approximation, single-electron band structure models, Fermi liquid theory, etc. These problems call for tools that are sharper than those currently available.

To meet these challenges, we must answer fundamental questions about the coupling between the correlated motion of electrons and the motion of atoms. The intrinsic time scales of those motions differ by four orders of magnitude:

- ~picoseconds, characteristic of conformational relaxations in molecular systems and electron–lattice energy transfer times in crystalline solids.
- ~100 femtoseconds, characteristic of atomic vibrational periods in molecules and solids.
- ~10 femtoseconds, characteristic of electron–electron scattering times in solids.
- ~100 attoseconds, characteristic of electron–electron correlations and valence electron motion.

*This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

The need to directly probe electronic structure and dynamics demands a focus on the VUV and soft X-ray regions and the creation of experimental facilities that complement those being constructed with hard X-ray capabilities.

Direct quantitative measurements of electronic and atomic structural dynamics on the ultrafast time scale of the underlying correlations will be indispensable for achieving new insight into the physics of complex systems and novel properties emerging from correlated phenomena in atoms, molecules, and complex solids. Thus, there is a strong scientific need to be able to probe matter with atomic spatial resolution, elemental specificity, meV energy resolution, momentum resolution, *and* ultrafast time resolution, in order to separate correlated phenomena in the time domain. Time resolution, high average flux, high repetition rate, high resolving power, and soft X-ray tunability emerge as critical needs.

Scientific requirements for next-generation light sources

In order to have a major impact on the fundamental questions, scientific goals, and research objectives of the future, a new generation of light source is required. The necessary capabilities of such a source are substantially beyond those of both third-generation storage rings and the X-ray FELs that are now planned or under construction. The two most challenging performance requirements that must be met simultaneously are ultrafast temporal resolution (driven by the fundamental time scales of correlation phenomena in matter) and high average flux (driven by the required measurement precision/resolution). Table 1 specifies the various performance requirements and summarizes the research areas that are the primary drivers of each requirement (see for example Refs. 1–4 for scientific conferences and workshops motivating these requirements).

A high-repetition-rate FEL facility

Advanced FEL technology, exploiting a high-repetition-rate, low-emittance electron source, superconducting radiofrequency (rf) technology, and optical manipulations of the electron beam, provides the basis for a future multi-user facility to meet the scientific requirements outlined in Table 1. FELs offer an increase of ten orders of magnitude in flux per pulse compared with third-generation synchrotron light sources, and with the implementation of optical manipulations, in which a “seed” laser is used to control the distribution of electrons within a bunch, the following benefits are gained:

- Temporal coherence of the FEL output pulse
- Control of the time duration and bandwidth of the coherent FEL pulse
- Close to the transform limit, pulse provides excellent resolving power without monochromators
- Complete synchronization of the FEL pulse to the seed laser
- Very high peak flux and brightness (comparable to self-amplified spontaneous emission [SASE] FELs)
- Very high average flux and brightness (\gg third-generation rings, at 100-kHz repetition rates)
- Tunability of the FEL output wavelength

- Enhancement of peak current
- Reduction in undulator length needed to achieve saturation

To address the scientific requirements outlined above, we suggest a new user facility equipped with an array of task-designated FELs, wherein each FEL may be configured to operate in a different mode, independently of the other FELs. Each FEL will have independent control of wavelength and polarization, and optical manipulations of the electron beam will be used to produce seeded X-ray pulses with control of pulse duration, offering flexibility and versatility to many experiments simultaneously [5–10]. High repetition rate and high average photon flux are essential to many experimental techniques. To meet these needs, we envision a facility composed of a high-bunch-repetition-rate (\sim MHz), low-emittance, low-energy-spread rf photocathode electron gun and a low-energy (\sim 2 GeV) superconducting linac feeding an array of approximately ten FELs through a beam switchyard. Each FEL operates independently at a repetition rate of \sim 100 kHz. Photon energies would span approximately 10 eV to 1 keV, with the possibility of reaching higher photon energies at the expense of photon flux. A variety of seeded and SASE FELs provide the above-described output radiation with a peak power of a few hundred megawatts to a few gigawatts. The temporal coherence available in the seeded FELs allows close to transform-limited X-ray pulses, resulting in a narrow-bandwidth signal that could be utilized in experiments without a monochromator. Techniques have also been developed to use optical manipulations of the electron bunch to produce X-ray pulses of a few hundred attosecond duration [8–10].

Figure 1 shows a schematic of a multi-user FEL facility concept. The major components are (1) a low-emittance, low-energy-spread rf photocathode electron gun providing electron bunches at up to MHz repetition rates, (2) hardware for manipulating the electron-beam emittance in preparation for the FEL process, (3) a continuous-wave (CW) superconducting rf linac, (4) a beam-switching system, (5) multiple independent FELs and beamlines, and (6) lasers for the photocathode gun, FEL seeding, pump-probe experiments, and timing and synchronization. A low-energy linac is used to minimize costs. The electron beam is dumped at the end of each FEL as we do not currently believe the added cost and complexity of electron-beam recirculation and energy recovery is worthwhile for a machine of modest electron beam power.

Using advanced technologies, a wide range of FEL performance parameters are possible. For the wavelength range from 1 to 200 nm (1.2 keV to 6 eV), one can envision three general types of beamlines, and based on projected technology limitations, Table 2 suggests reasonable performance goals over a range of X-ray pulse durations from picosecond to sub-femtosecond regimes.

Accelerator research and development program

Unlike third-generation synchrotron radiation (SR) facilities, next-generation light sources will need extensive research and development (R&D) to define the final optimum configuration. By driving the development of advanced technologies (for example, high-repetition-rate [\sim MHz], low-emittance electron injectors; CW superconducting rf linacs; and optical manipulations), a next-generation FEL facility will be able to open up new areas of research, complementing the SR facilities currently being built or planned, as well as enhancing the

technology base for other accelerator-based light sources. Efficient radiation at wavelengths down to 1 nm, with a low-cost accelerator producing electron-beam energy of approximately 2 GeV, requires a bright electron beam with low emittance, low energy spread, and high peak current. This, together with the requirement of a high repetition rate, drives the need for an R&D program. Critical work is required in the physics of low-emittance beams, free-electron lasers, photocathodes, high-repetition-rate electron-gun systems, laser systems, CW superconducting rf cryomodules, diagnostics, and short-period undulators. Already, research in some of these areas has resulted in advances and novel approaches with potential applications to future facilities—the high-repetition-rate rf gun described below, for example—and a broad R&D program will likely produce much more.

LBNL staff are currently pursuing R&D for future X-ray FELs, and our strategy is to address the most fundamental challenges that are the cost drivers and performance limitations of FEL facilities. An internally funded R&D program is aimed at investigating accelerator physics and technologies in key areas in which R&D is critically needed and for which the impact could be the greatest. These activities are summarized below.

Photocathode design

The aim of this program is to improve beam quality through the development of a cathode that produces a beam with very low thermal emittance. We also aim to increase the quantum efficiency up to the point at which conventional laser technology can be used to produce tailored electron pulses at a MHz repetition rate. As a first step, we have investigated metallic photocathodes and determined that photocurrent at the very low photon energies typically used is dominated by surface states. This has led directly to a prediction of the minimum transverse momentum and to a direction for producing lower emittance through the use of other crystalline surfaces. These studies will be extended to metallic systems in which the surface electric field is manipulated using plasmonic interactions and to semiconductor systems. The latter have the advantage that some degree of thermalization can take place, resulting in colder emission. This work is based on understanding the near-Fermi-surface electronic structure, through use of very-low-energy photoelectron spectroscopy and through electronic structure modeling. In addition, we have developed modeling techniques to better understand the impact of the scattering of electrons after they leave the cathode surface [11].

VHF photo gun

We are developing a design for a high-brightness, high-repetition-rate electron gun that uses a normal-conducting rf structure in the very-high-frequency (VHF) range, at approximately 100 MHz [12]. The gun cavity has quarter-wave coaxial geometry, which is a mature rf technology. The lower frequency results in a larger cavity compared to the more common designs operating at ~1 to ~3 GHz. A significant benefit of using a larger cavity is a dramatic reduction in the power density on the cavity walls, which allows CW operation of the gun, and thus a bunch repetition rate of up to the rf frequency (dependent on photocathode-laser time structure). Calculations show that a VHF gun can achieve an accelerating gradient at the cathode of approximately $20 \text{ MV}\cdot\text{m}^{-1}$, and that an injector based on such a gun can provide beam of excellent quality.

Electron-beam delivery systems

The production of electron beams for X-ray FELs is a difficult and elaborate process consisting of electron generation, acceleration, compression, and transport. A significant understanding of the underlying physics, such as space-charge effects, wake fields, and coherent synchrotron radiation (CSR) has been gained over the past decade [13–17]. Significant improvements in electron-beam quality may be needed to build a cost-effective VUV/soft-X-ray FEL facility. We are improving our understanding of beam phase-space evolution and ways to control and manipulate emittances, using both theoretical approaches and high-resolution numerical modeling. We have developed a parallel code suite, IMPACT [18–19], for advanced supercomputer modeling of high-intensity, high-brightness beams in rf linacs and photoinjectors. An example is provided by 100-million-macroparticle simulations of the microbunching instability, simulations that cannot be sensibly performed on today’s single-processor computers. Figure 2 shows a multiprocessor simulation using IMPACT. The figure shows the sensitivity of the evolution of the microbunching instability to macroparticle number. We are augmenting our present particle-loading approach with “quiet-start” techniques, and in parallel we are also developing a direct Vlasov-Maxwell solution.

After leaving the accelerator, electron beams will be switched into each FEL in the array, in a time-sliced manner dependent on user needs. Techniques for switching the electron beam between FELs are being studied using pulsed ferrite magnets in a linear array.

FEL design

Our goal is to develop design concepts for flexible photon-beam performance, based on a number of FEL configurations, fed by a low-energy electron accelerator, that would provide experimentalists a variety of configurations, including high-flux time-domain pulses of femtosecond to 0.1 femtosecond duration and high-resolution frequency-domain outputs with close to transform-limited meV bandwidth. SASE, seeded, regenerative-amplifier, and oscillator techniques are being simulated and developed using GINGER and GENESIS simulation codes. Start-to-end modeling of the electron beam is critical in determining realistic FEL performance capabilities. These studies are performed in conjunction with the development of beam delivery systems.

Timing and synchronization systems

To produce an ultrastable timing and synchronization system with jitter reduced to the few femtosecond level, we have developed a laser-based scheme with optical signals distributed over a stabilized optical fiber [20–21]. Transmission of precise frequency and timing signals over distances of hundreds of meters, stabilized to a few femtoseconds (a few parts in 10^8), is accomplished by measuring the phase delay in an optical fiber and actively compensating for differences with a piezoelectric modulator.

In our scheme, illustrated in Figure 3, phase differences at optical frequency are down-converted to 110 MHz. At present, a 4-km fiber link has been stabilized to the femtosecond

level. Two kilometers of fiber in this link passes under several roads and through several buildings at LBNL, demonstrating that the fiber stabilization system is robust under real-world conditions. Techniques for synchronization of laser systems using CW optical signals, propagated over stabilized optical fiber links, are described in Ref. 22. Further developments will include integration with controls and low-level rf systems as well as high-resolution diagnostics of photon and electron beams, to provide enhanced feedback control of the integrated laser/accelerator systems. We are planning to develop and implement similar systems at the Linac Coherent Light Source [23] and FERMI@Elettra [24].

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Table 1: Performance requirements and research needs driving specifications for future light sources

Performance category	Quantification	Required for:
Ultrafast time resolution and laser synchronization	<100 fs and ~100 as	All dynamics studies <ul style="list-style-type: none"> • Attosecond to picosecond time scales • Duration/bandwidth control
High repetition rate	10–100 kHz	Time-resolved spectroscopy <ul style="list-style-type: none"> • high repetition rate for signal averaging • repetition rate limited by sample recovery/replacement • flux per pulse limited by damage and nonlinear effects Inelastic X-ray scattering Lensless imaging
High average flux	$\sim 10^{15}$ ph/s/0.1% BW (~third-gen. SR)	Time-resolved spectroscopy X-ray emission spectroscopy— RIXS/XES (at 0.5-eV resolution) <ul style="list-style-type: none"> • flux per pulse limited by damage and nonlinear effects
Very high average flux	$\gg 10^{15}$ ph/s/0.1% BW (\gg third-gen. SR)	Inelastic X-ray scattering—IXS X-ray emission spectroscopy— RIXS/XES (<10-meV resolution) Lensless imaging <ul style="list-style-type: none"> • flux per pulse limited by damage and nonlinear effects
Tunability	100 eV–10 keV	X-ray spectroscopy (electronic and atomic structure) <ul style="list-style-type: none"> • Soft X-ray: XANES, EXAFS (TM L-edges) • Hard X-ray: EXAFS (TM K-edges)
Polarization control	Adjustable circular/linear	All X-ray dichroism spectroscopy
Coherence	Full transverse and longitudinal	Energy resolution (temporal transform limit) Chirped/shaped-pulse experiments Lensless imaging (spatial and temporal coherence)
Stability	<10% pulse amplitude <0.1 $\sigma_{x,y}$ alignment	Extraction of small signals from background

Table 2: Performance goals for a future seeded FEL facility

	Short-pulse beamlines	High-resolution beamlines	Sub-femtosecond beamlines
Wavelength range (nm)	200–1	200–1	40–1
Repetition rate ¹ (kHz)	100	100	1-100
Peak power (GW)	1	1	0.1–0.3
Intensity stability ²	5%	5%	TBD
Timing stability ^{3,4} (fs)	10	10	TBD
Pulse length ⁵ (fs)	10–100	100–1000	~0.1
Bandwidth	2–3 x transform limit	2–3 x transform limit	transform limit
Harmonics ⁶	≤ few%	≤ few%	≤ few%
Source position stability	<10% source size	<10% source size	<10% source size
Spot size (μm)	~50	~50	~50
Divergence (μrad)	~5	~5	~5
Polarization	Variable, linear/circular	Variable, linear/circular	Variable, linear/circular
Wavelength stability ⁷	TBD	TBD	TBD
Background signal ⁸	small	small	TBD

¹Initial experiments may be at lower rate; the linac and other infrastructure will accommodate higher bunch-repetition rates

²Most experiments will incorporate a pulse energy measurement

³Stabilized timing and synchronization systems will provide timing signals with 10-fs stability with respect to the seeded FEL output

⁴Timing stability for the attosecond mode will be developed in an R&D plan

⁵Capabilities for pulse durations in the range of a few femtoseconds and a hundred attoseconds to be explored in an R&D plan

⁶Third harmonic may be used to achieve wavelengths shorter than 1 nm at reduced flux

⁷Currently under detailed study

⁸Dependent on FEL configuration and mode of operation

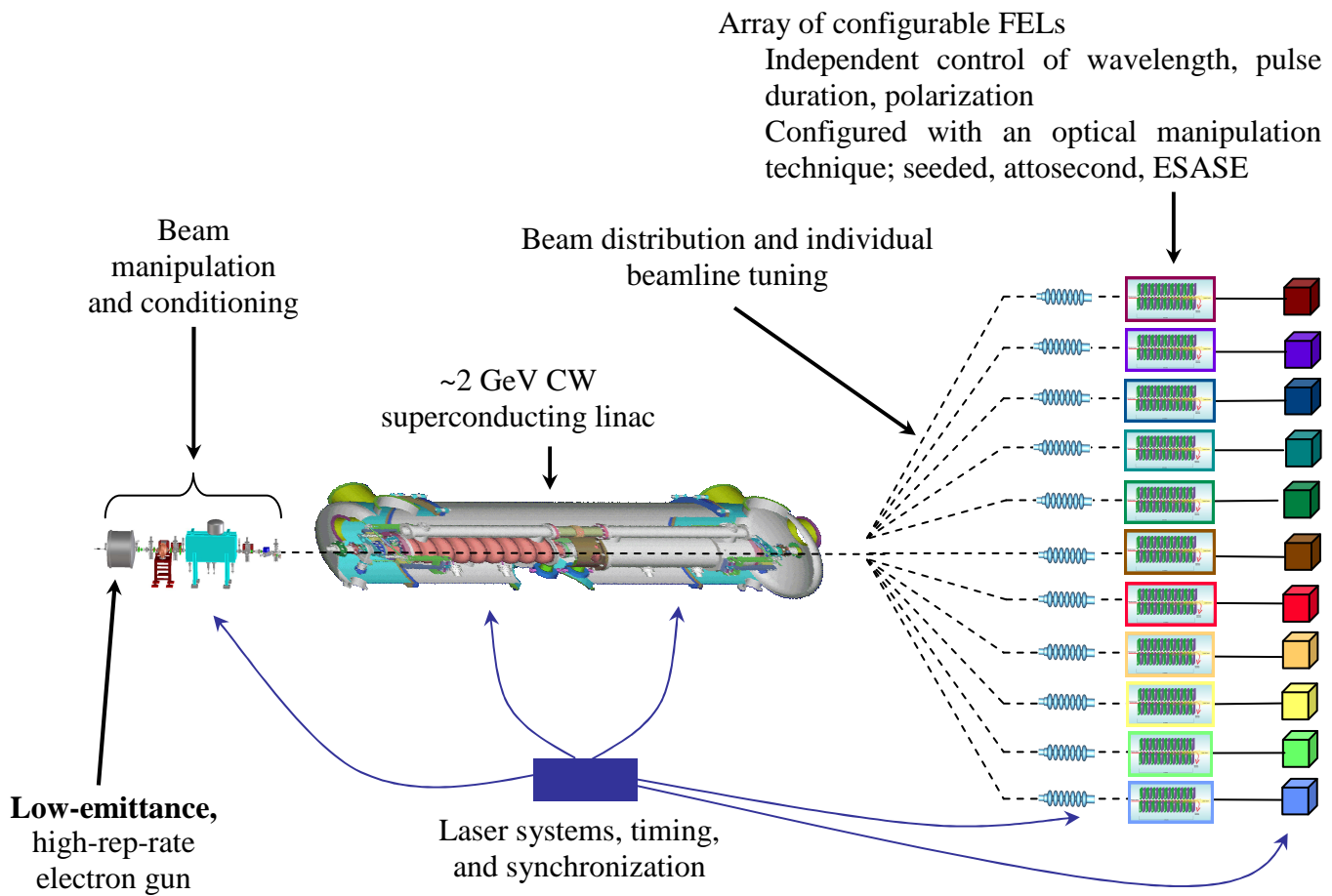


Figure 1: Schematic of a light source facility based on a high-pulse-repetition-rate, seeded FEL.

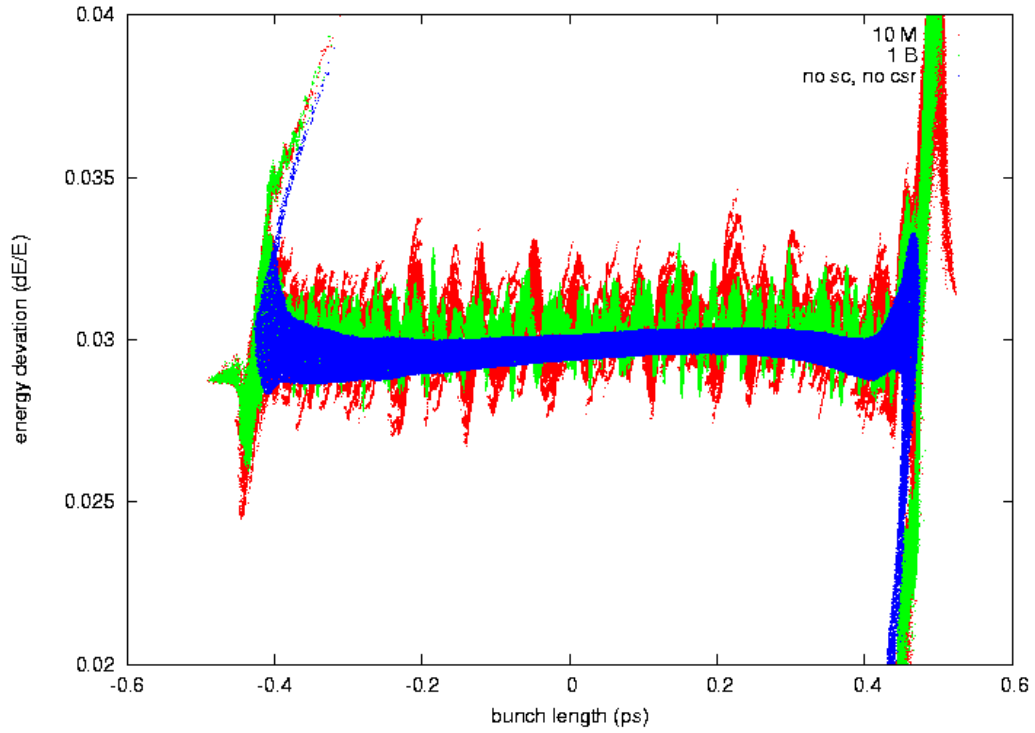


Figure 2: Longitudinal phase-space distribution calculated using 10 million (red) and 1 billion (green) macroparticle IMPACT simulations. Blue shows the model with no space-charge or CSR effects.

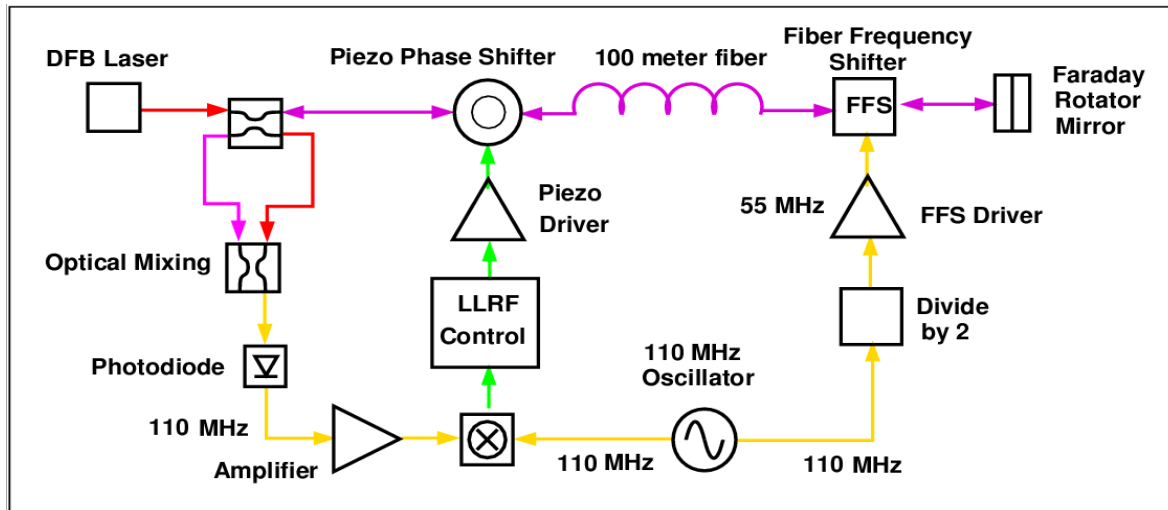


Figure 3: Schematic of the frequency-offset method for distribution of timing and synchronization signals with femtosecond-scale timing stability over long distances (100-m fiber in this example, extendable to km scale).