LA-UR-16-27235

The Los Alamos Multi-Probe Facility for Matter-Radiation Interactions in Extremes (MaRIE)

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LINAC'16
Lansing, Michigan
September 25-30, 2016

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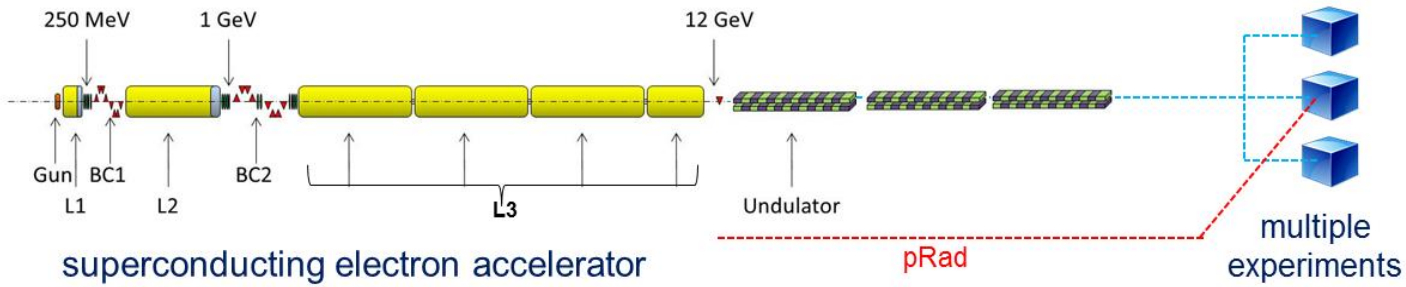
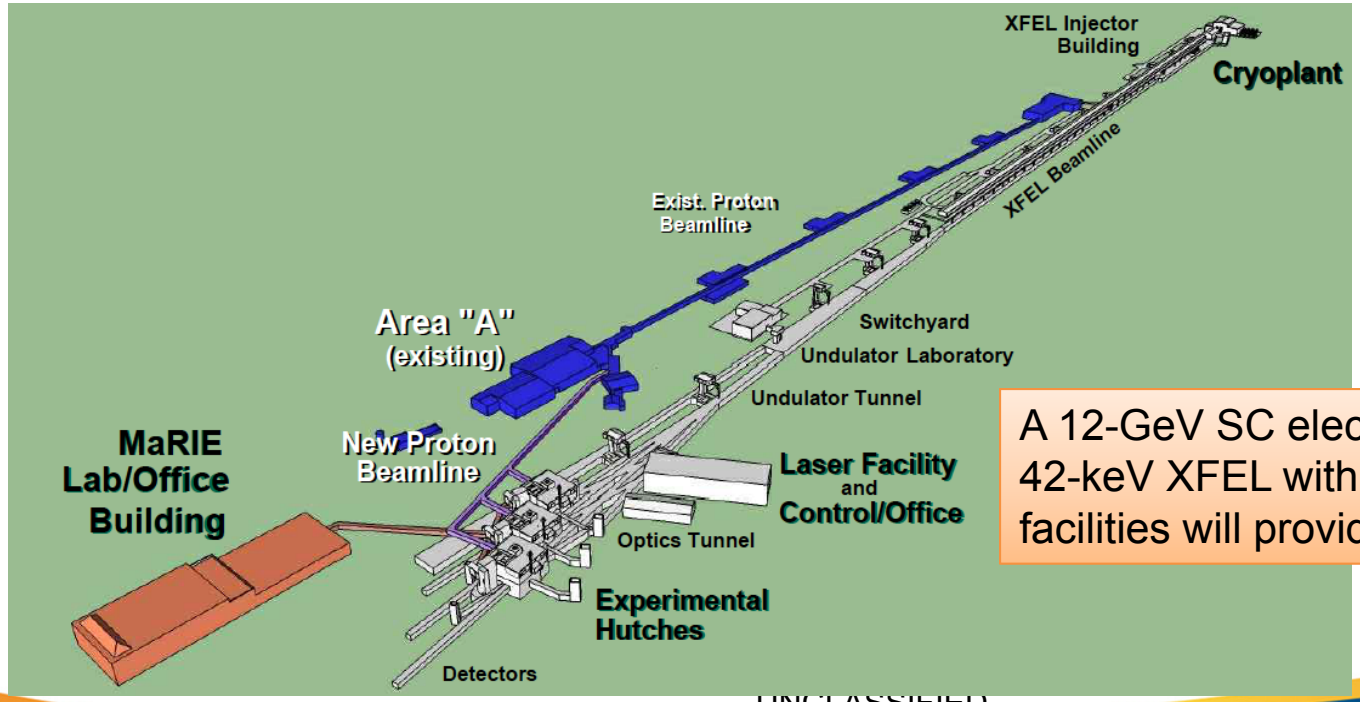
Outline

- MaRIE Overview & Requirements
- MaRIE XFEL Preconceptual Reference Design
- MaRIE Status

MaRIE at LANSCE would leverage existing proton and neutron capabilities to provide a next-generation, multi-probe facility.

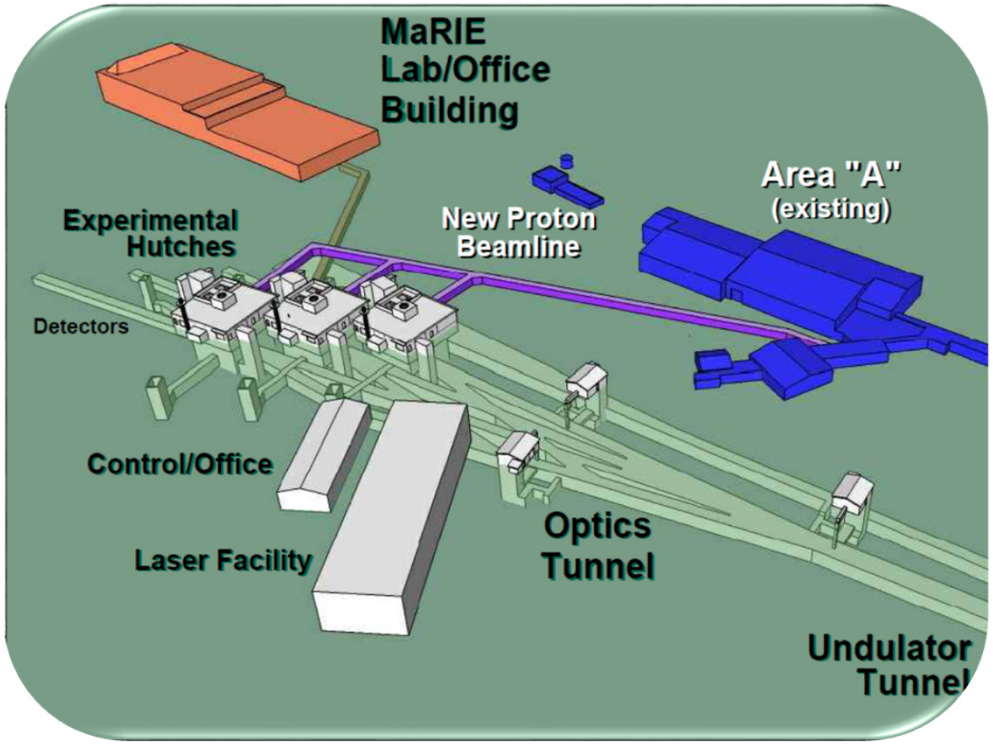




A 12-GeV SC electron linac feeding a 42-keV XFEL with new experimental facilities will provide this new capability.

MaRIE would provide a transformational facility for materials research at the mesoscale.

- World's highest energy x-ray scattering capability (**42-keV XFEL**)
- High repetition frequency with simultaneous charged particle dynamic imaging
- Experimental hutches for simultaneous, multi-probe measurements of in-situ transient phenomena in relevant dynamic extremes
- Comprehensive, integrated resources for materials synthesis and control, with national security infrastructure
- Materials discovery, design, and process capability

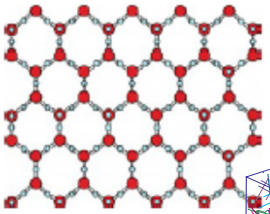


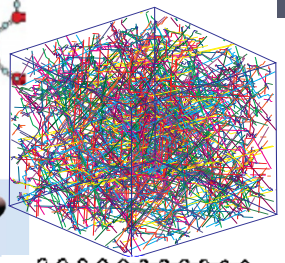
What is the mesoscale?

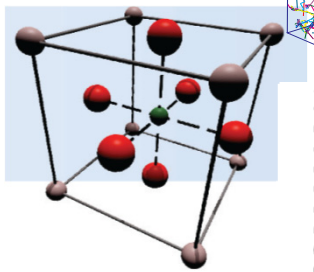
Atomic

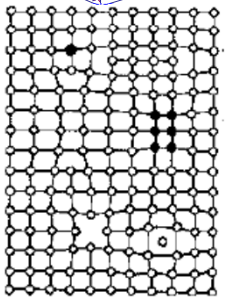
Mesoscale

Macroscale

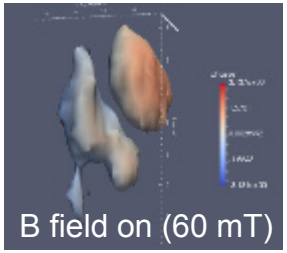




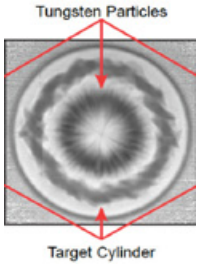




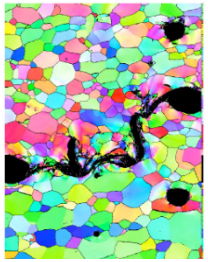
Simple Perfect Homogeneous



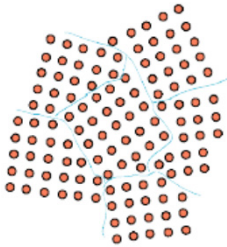
Emergent Phenomena

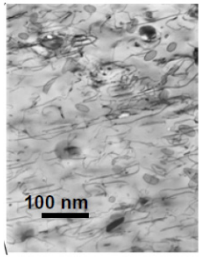


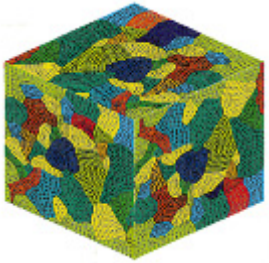
Extreme Environments

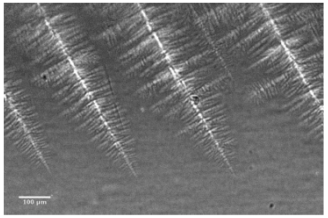


Defects and Interfaces

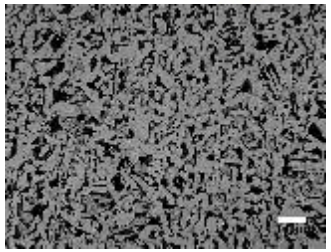




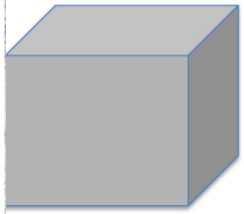




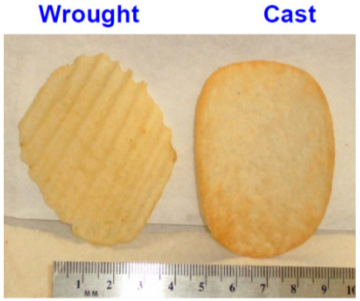
Internal features Interacting



phase separation



bulk



Continuum Bulk Behavior

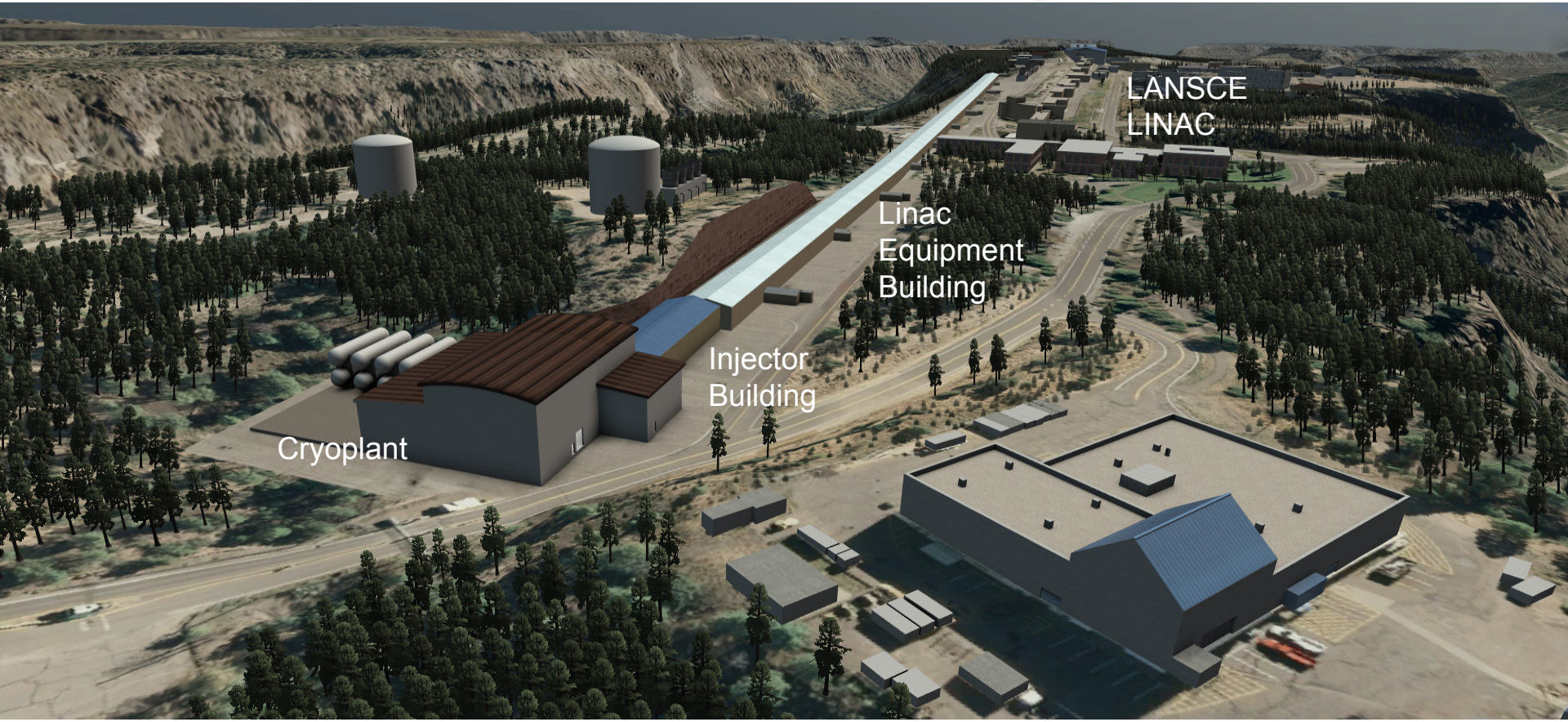
10^{-10} 10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1}

Nanometer — Micron — Millimeter+

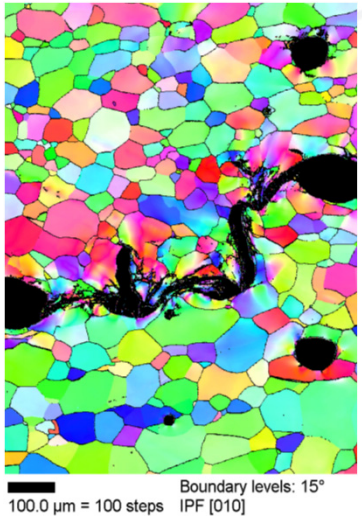
Hard X-ray FEL Parameters

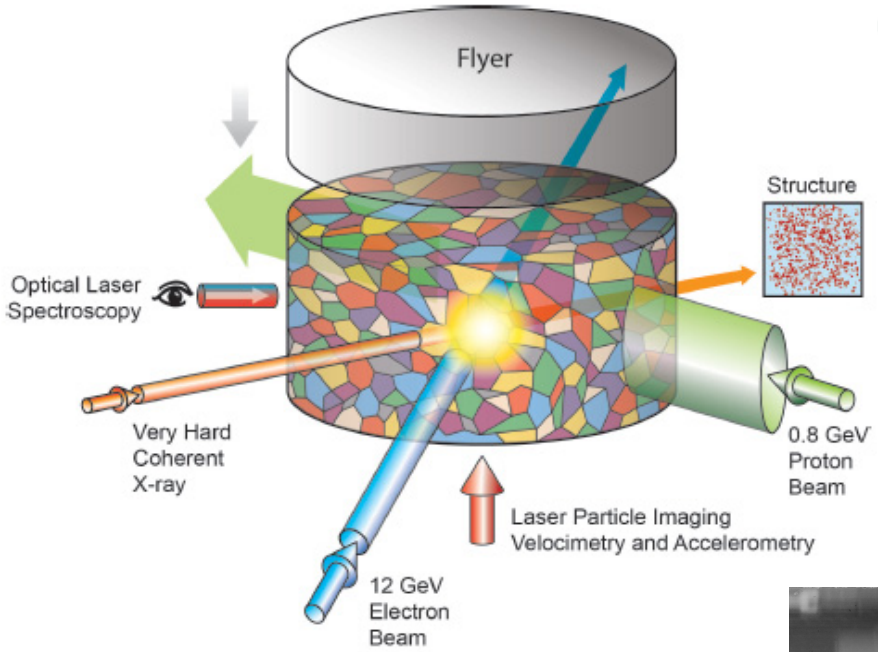
	LCLS-I	SACLA	EXFEL 2016	PAL XFEL 2016	SwissFEL 2017	LCLS-II 2019 SRF / NCRF	MaRIE 202x
X-ray energy Pulse energy photons/pulse	12.8 keV 0.93 mJ 5E11	19.5 keV 0.03 mJ 1E10	24.7 keV 1 mJ 2.5E11	20.6 keV 0.08 mJ 2.5E10	12.4 keV 1.4 mJ 7E11	5 / 25 keV 0.025 / 0.3 mJ 3E10 / 7E10	**42 keV** **0.35 mJ** **5E10**
Undulator period K_{rms}	3.0 cm 2.5	1.8 cm 0.94	4.0 cm 1.4	2.44 cm 0.94	1.5 cm 1.1	2.6 cm 0.43 / 1.5	**1.86 cm** **0.86**
Electron beam energy	16.9 GeV	8.5 GeV	17.5 GeV	10 GeV	5.8 GeV	4 / 15 GeV	**12 GeV**
Linac type Linac length	NCRF S-band 1 km	NCRF C-band 0.4 km	SRF L-band 1.7 km	NCRF S-band 0.78 km	NCRF C-band 0.46 km	SRF / NCRF 0.4 / 1 km	**TBD** **<1.4 km**
Gun type Cathode	NCRF S-band Cu photo	Pulsed DC CeB_6	NCRF L-band Cs_2Te photo	NCRF S-band Cu photo	NCRF S-band Cu photo	VHF / S-band Cs_2Te / Cu	**TBD**
RF pulse Rep. rate	<1 μs 120 Hz	<1 μs 30 Hz	600 μs 10 Hz	< 1 μs 60 Hz	< 1 μs 100 Hz	CW / <1 μs 930 kHz / 120 Hz	**TBD**
# pulses/RF	1-2	1-2	2,700	1-2	1-2	N/A / 1-2	**TBD**
Bunch charge	150 pC	30 pC	250 pC	100 pC	200 pC	20 / 130 pC	**100 pC**
Bunch length	43 fs	<10 fs	50 fs	43 fs	42 fs	20 / 33 fs	**33 fs**
Norm. slice emittance	0.4 μm	0.6 μm	0.6 μm	<0.5 μm	0.2 μm	0.14 / 0.48 μm	**0.2 μm**

Artist Rendition of MaRIE Conventional Facilities



Challenging experiments are planned to observe the *dynamic microstructure* and *phase evolution* in materials down to the sub-granular level while connecting to the macroscale.



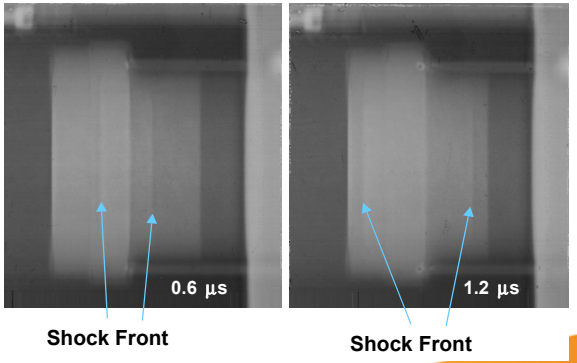


Requirements:
Sub-µm spatial resolution
100's – 1000's-µm samples
Sub-ns time resolution,
~30 frames in
1−10-µs duration

The model:
Accurate sub-grain models of microstructure evolution coupled to molecular dynamics.

The goal
Predict dynamic microstructure and damage evolution.

The first experiment
Multiple, simultaneous dynamic *in situ* diagnostics with resolution at the scale of nucleation sites (< 1 µm; ps – ns)



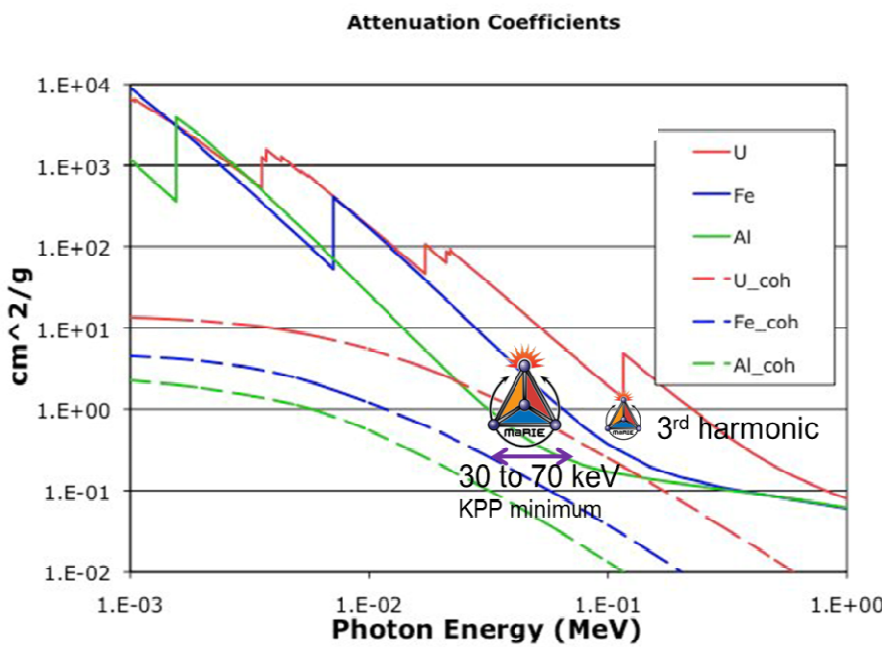
MaRIE will allow us to break apart the problem.

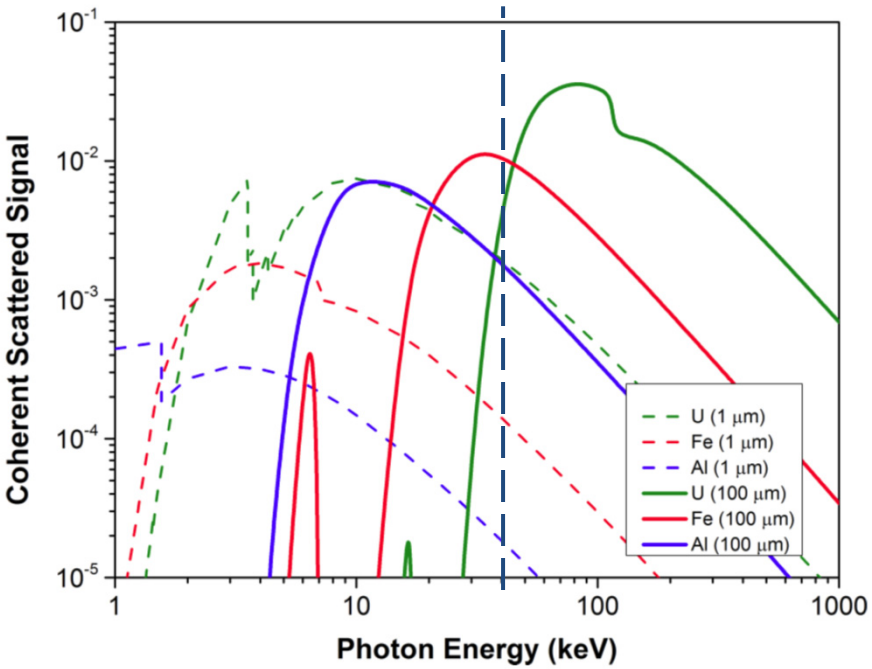
Spatial and temporal resolutions for MaRIE mesoscale experiments are defined by analysis of the possible measurement techniques.

	Metals Manufacture and Age aware performance	HE certification and qualification	Turbulent Materials Mixing	Welding and Additive Manufacturing
Spatial resolution	<100 nm - 20 µm	100 nm - 20 mm	500 nm	<1 µm – 100 µm
Field of View	100 µm - 1 mm	100 µm - 2 mm	1 mm	0.3 mm – 1 cm
# of frames	up to 30	up to 30	up to 30	1000 per second
min pulse sep	< 300 psec	< 500 psec	30 nsec	10 nsec
macropulse length	10 µsec	100 µsec	15 µsec	1 msec
sample thickness	> 250 µm	> 10 µm – 6 cm	1 – 10 cm	0.1 to 10 mm
Repetition rate	<1 Hz	< 1 Hz	10 Hz	10 Hz
species	Be - Pu	Typically C, H, O, N	Noble gases, Ga, Be	Be - Pu

	spatial resolution	Framing time	Density resolution	sample thickness Z=13	sample thickness Z=26	sample thickness Z=92
pRad	< 50 µm	50 nsec	2%	15 cm / 0.8 GeV	3 cm / 0.8 GeV	1 cm / 0.8 GeV
eRad	< 1 µm	> 25 nsec	5%	6 cm / 12 GeV	5 mm / 12 GeV	1 mm / 12 GeV
X ray	< 1 µm	< 100 psec	5%	>10 µm/ 8 keV 2 cm/ 42 keV	500 mm/42 KeV 4 mm/122 KeV	200 mm/42 KeV 2 mm/122 KeV

The 42-keV photon energy and flux are a trade-off between maximizing elastic scattering for diffraction, minimizing absorptive heating, and sample thickness.





High resolution requires a minimum number of coherently scattered photons per sub-ps pulse. This sets the incident number of photons on a sample of ~2×10^{10}.

Coherent scattering signal (fraction of incident photons coherently scattered just once) as a function of incident photon energy for various materials at thicknesses of 1 μm (dashed lines) and 100 μm (solid lines)

J. L. Barber *et al.*, Phys. Rev. B **89** (2014) 184105

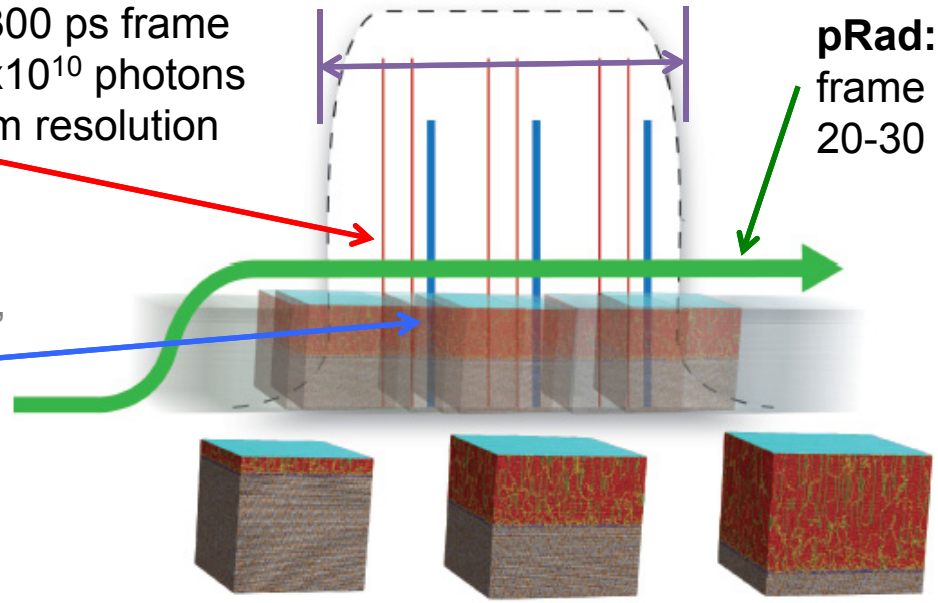
Multiple probes allows sampling of different temporal and spatial regimes: 42-keV x-ray photons (red), 12-GeV electrons (blue), and 0.8-GeV protons (green)

Macropulse <100μs

XFEL: 42-126 keV; 300 ps frame speed, 30 frames, $2x10^{10}$ photons @50 fs/pulse, >0.1μm resolution

pRad: 800 MeV, 5-50 ns frame speed, 30 frames, 20-30 μm resolution

eRad: 12 GeV, 25 ns frame speed, 30 frames, >1 μm resolution, 2 nC/pulse

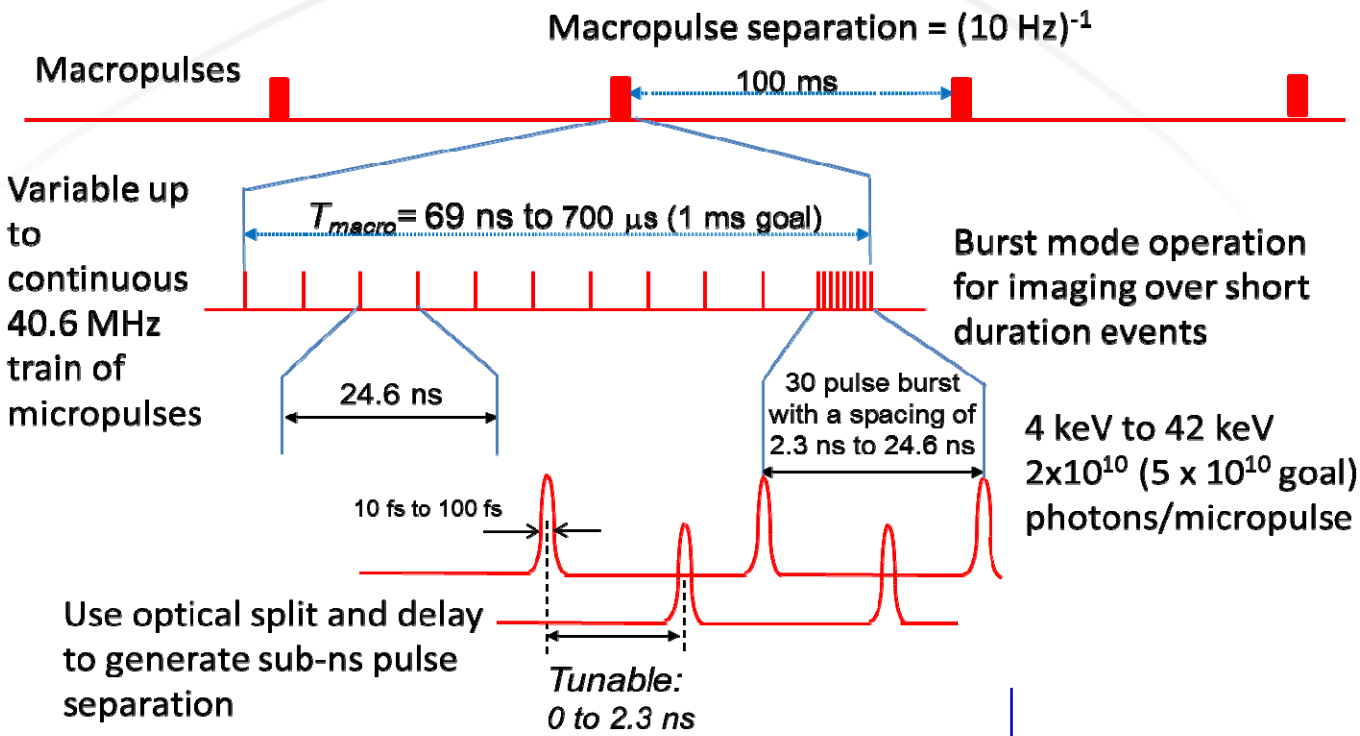


Adds significant machine costs:

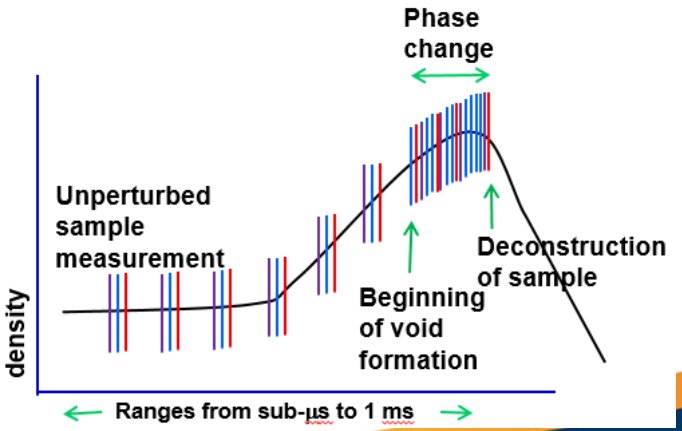
- Requires another injector
- Impacts XFEL beamline design
- Increases experimental hall complexity & cost

- **XFEL** has **sub-ps** pulse lengths, **sub-ns** pulse spacing, **sub-micron** resolution, but is limited in sample thickness at 42 keV to < 0.1 mm for high-Z materials
- **eRad** has **~10-ps** pulse lengths, **~20-ns** pulse spacing, ≤**1-μm** resolution, penetrate ≤ 2 mm high-Z materials
- pRad has **50-ns** pulse lengths, **100-ns** pulse spacing, **>10-μm** resolution, penetrate >1 cm high-Z materials

The MaRIE pulse format needs to be very flexible.



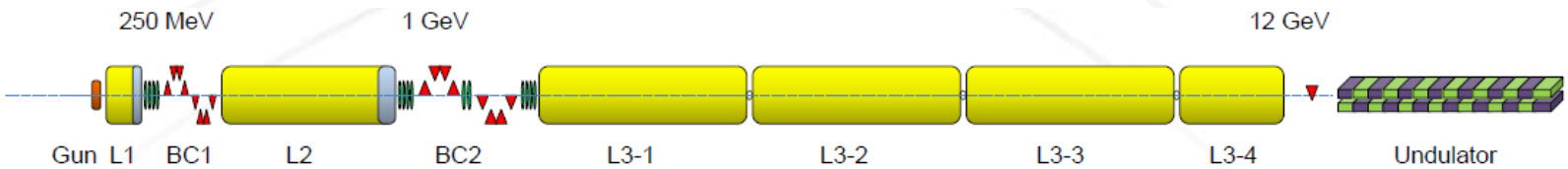
- **700-μsec macropulse requires a superconducting accelerator**
- **Variable pulse format will require a room-temperature "droop corrector"**
- **Assuming 0.2 nC/pulse as the main eRad option**



Performance Parameters derived from the measurements quantify the accelerator/XFEL requirements.

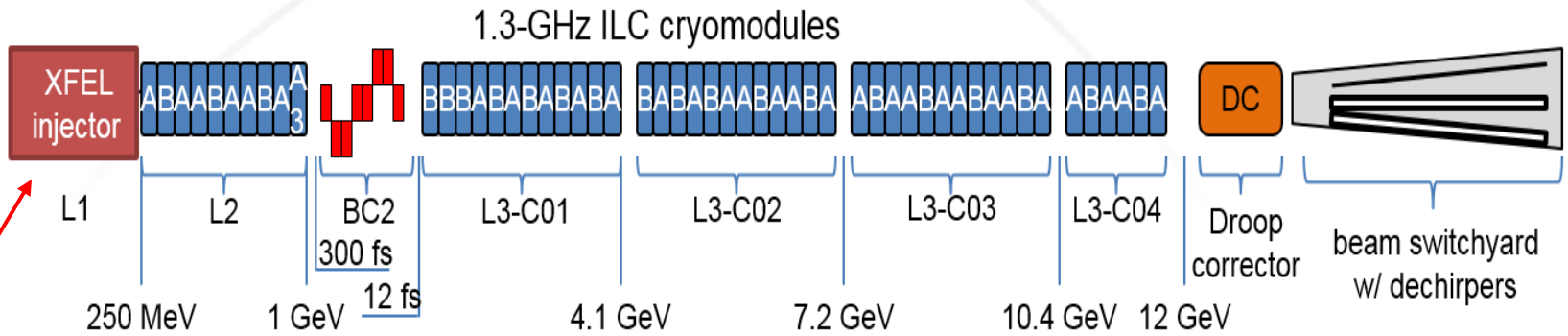
Electron Beam Requirements				Photon Requirements	
Energy	12 GeV	# of bunches per macropulse	10 to 100	Energy	4 to 42 KeV
Linac fundamental frequency	1.3 GHz	RMS slice energy spread	$\leq$ 0.015%	# per bunch	5×10^{10}
Linac type	Superconducting	Macropulse to macropulse energy variation	$\leq$ 0.02%	% Transverse coherence	70%
SC L-band cavity gradient	31.5 MV/m	Pulse energy variation within a macropulse	$\leq$ 0.01%	Pulse length	$\leq$ 100 fs
Maximum beamline angle	2.0 degrees, max. @ 12 GeV	Min. bunch separation	2.3 ns	Bandwidth	5×10^{-4}
Maximum macropulse duration	1 ms	Dropped bunch rate	1×10^{-3}	Divergence	$\leq$ 1 µrad
Electron source	Photoinjector	Normalized rms slice emittance	$\leq$ 0.2 micron	Polarization	linear
Maximum bunch charge	0.2 nC	Maximum repetition rate	10 Hz	Tuneability	1%/ms

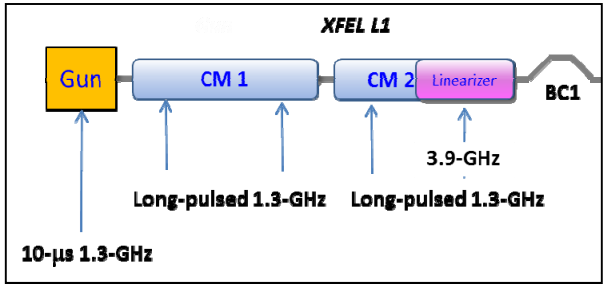
Performance Parameters derived from the measurements quantify the accelerator/XFEL requirements.



Parameter	Symbol	Value	Unit
Electron beam energy	E_b	12	GeV
Peak current	I_{pk}	3	kA
Bunch charge	Q	100	pC
Slice normalized emittance	ε_n	0.2	µm
Slice energy spread	σ_γ/γ	0.015%	
Undulator period	λ_u	18.6	mm
Peak undulator parameter	K	1.22	
Wavelength	λ	0.2936	Å
1-D FEL gain parameter	ρ	0.05%	
3-D gain length	L_{G3D}	2.5	m

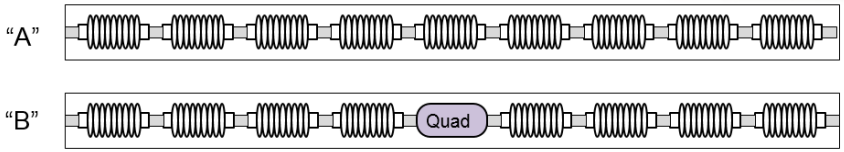
An XFEL pre-conceptual reference design that meets the MaRIE performance requirements has been developed.





A 9-cavity ILC cryomodule, "A"-type

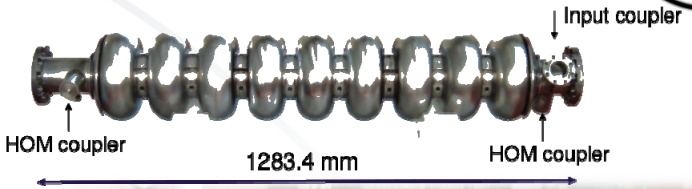
B 8-cavity ILC cryomodule, with quad / corrector / BPM, "B"-type

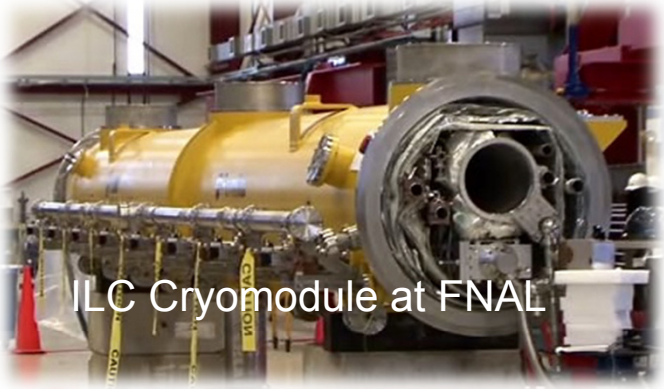


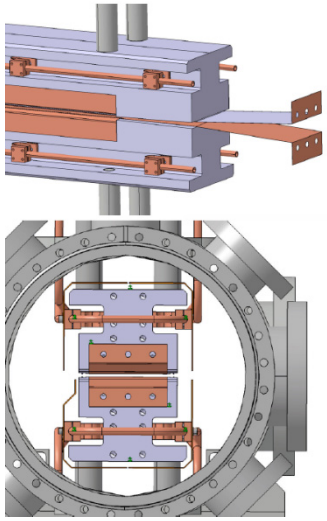
	1.3-GHz cavities	3.9-GHz cavities
L1 (X-FEL)	11	9
L1 (eRad)	11	9
L2	78	9
L3	360	0
Total	460	27

MaRIE pre-conceptual reference design is based on current technology.

- Accelerating cavities and cryomodules based on 1.3-GHz ILC and DESY XFEL designs
- FLASH 3.9-GHz cryomodules to linearize the beam phase space
- Undulator design based on SwissFEL U15







	Symbol	Value
Undulator period	λ_u	18.6 mm
Undulator magnetic field	B_0	0.7 T
rms (peak) undulator parameter	K_{rms} (K_{peak})	0.86 (1.22)
FEL resonance wavelength	λ_0	0.2934 Å
FEL (Pierce) parameter	ρ	0.0005
Calculated 3D gain length	L_G	2.6 m
Calculated 3D saturated power	P_S	9 GW
FEL pulse energy at saturation	W_p	0.3 mJ

Courtesy of T. Schmidt

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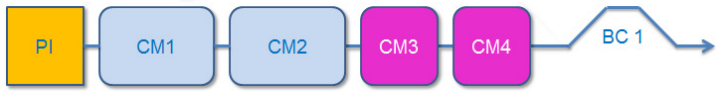
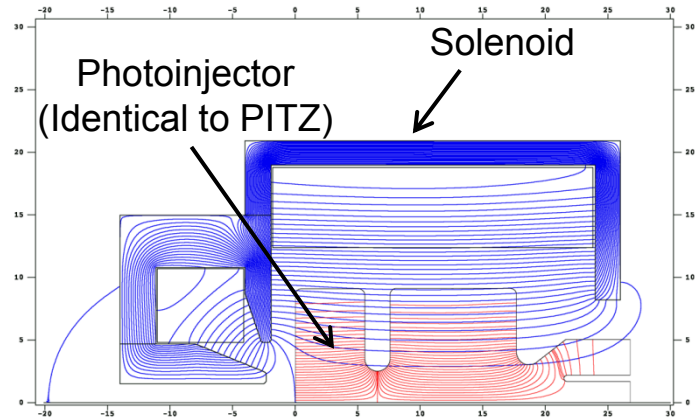
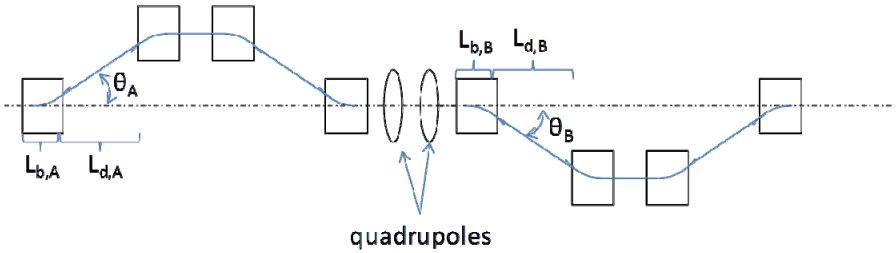
The MaRIE XFEL injector pre-conceptual design incorporates several innovations to meet performance requirements.



- **Photoinjector (PI)**
  - 1.3-GHz, normal conducting.
  - Long pulse (100 μs) operation, 60 MV/m gradient at cathode.
- **Cryomodules 1 & 2 (CM1 & CM2)**
  - 1.3-GHz superconducting.
  - Capture beam from PI, accelerate and introduce energy slew for BC1.
- **Cryomodules 3 & 4 (CM3 & CM4)**
  - 3.9-GHz superconducting.
  - Linearize beam energy slew for BC1.
- **Bunch compressor 1 (BC1)**
  - ~ 20x compression at ~ 250 MeV.



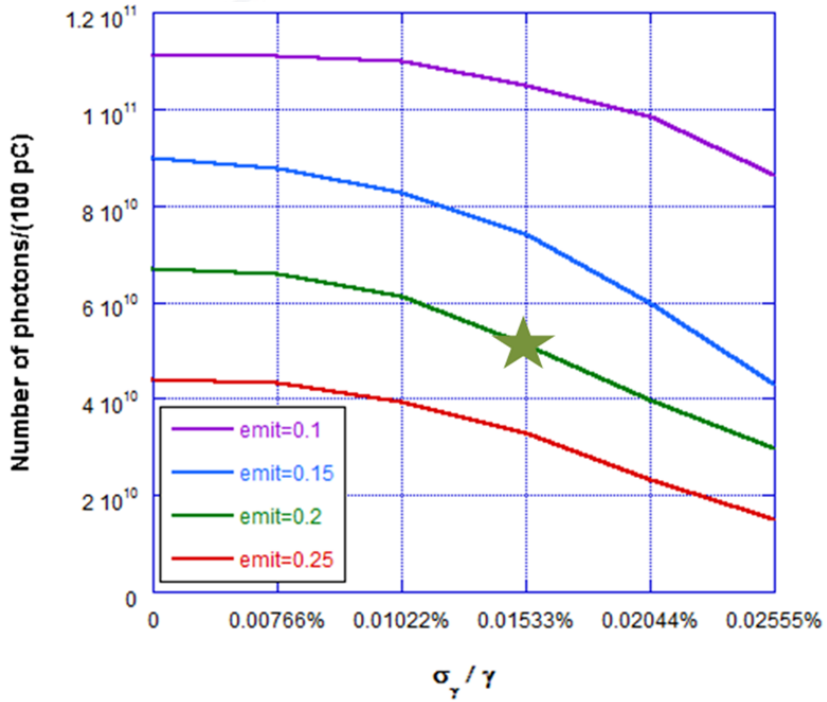
The MaRIE photoinjector design is based on the PITZ photoinjector with a modified solenoid configuration.

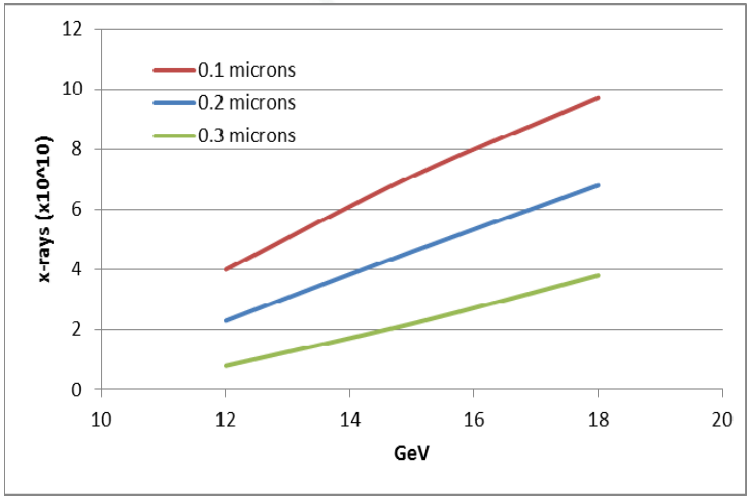


Double reversed-chicane helps reduce time-dependent dispersion from CSR wake.

Pre-conceptual design assumes 100 pC because we need a small emittance and small energy spread.

Time-Independent GENESIS Simulation Results





We can gain photons by going to higher electron beam energy

Photon requirements: 5×10^{10} 42-keV photons
0.02% bandwidth

Beam parameters: **100 pC, 30 fsec, 3.4 kA**
0.015% energy spread
0.20 μm emittance

150-m tunnel contingency to go to 15 GeV in the future; worth ~2x photons.

We have contingency in emittance, energy spread, and tunnel length.

Significant technical challenges remain to meet the MaRIE performance goals.

- **Microbunch Instability** – dominant challenge; made harder because of our tight energy-spread limit; suppression ideas include laser heater to pre-compress bunch, use residual dispersion (LBNL), “microbunch” the beam and eliminate BC2 (e-SASE)
- **CSR** – novel bunch compressor design; propose demo at BNL
- **Wakefields** – important for MaRIE XFEL, not important for other XFELs; long-range wakefields may limit the bunch spacing due to poor compressor or induced energy spread; propose measurement at FNAL
- **Emittance** – we need the brightest electron injector ever; plans for injector test facility at LANL
- **Distributed Seeding** – new concept; propose demo at SLAC
- **Droop Corrector** – short Cu linac (3 m) to compensate during shortest macropulse lengths; needed due to variable pulse format
- **Dechirper** – old concept; relatively low risk; propose demo at BNL

MaRIE Status

- Project presently in the pre-conceptual planning phase.
- We have a pre-conceptual accelerator/XFEL reference design appropriate for this phase of the project that meets the requirements.
- Cost & Schedule estimates are based largely on current technology (supported by several cost and project reviews in 2015).
- Following US Dept. of Energy, National Nuclear Security Agency (NNSA) guidance regarding submission of a large construction project, including DOE Order 413.3B requirements and process.
- Several workshops held this past year on MaRIE experiments and accelerator/XFEL design and requirements.
- External requirements review this week with other NNSA Labs.
- Beginning to initiate discussions with potential partner labs (and others).

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