LA-UR-16-22788

Matter-Radiation Interactions in Extremes
MaRIE 1.0
CD-0 Pre-Conceptual Design Introduction

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Outline

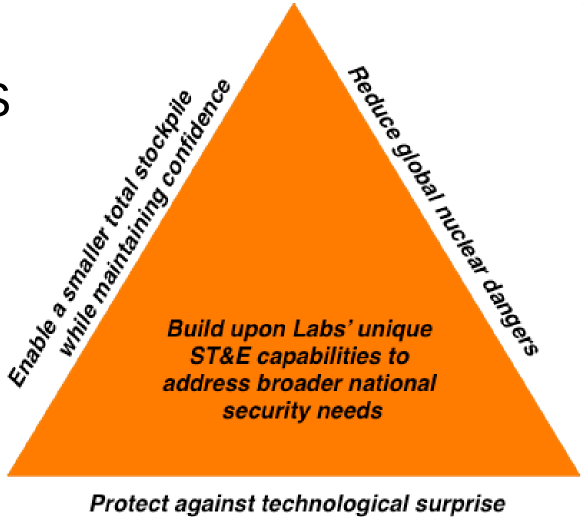
- MaRIE Mission Drivers
- MaRIE XFEL Preconceptual Design Overview
- Technical Risk Reduction
- MaRIE Project Status
- Summary

At the inception of the Stockpile Stewardship Program, stockpile performance was the primary mission driver; post-2020 mission drivers are more diverse

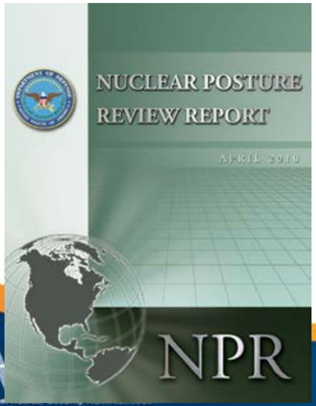
- **Stewardship Past: *Underwriting the STS****
  - Emphasis on performance and reliability: The STS
  - Dominant concern: *hubris*

Button → Boom

We cannot afford the same.



- **Stewardship Future: *Underwriting the life cycle***
  - Broadened emphasis: From "Ore to Disposition" and others' stockpiles
  - Dominant concern: *paralysis.* Preventing loss of confidence where we should have it



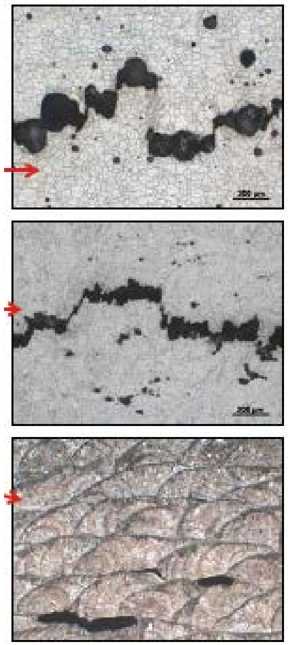
Production → Button → Boom → Disposition

To afford the mission, the way we do it must change!

*Stockpile-to-Target Sequence

MaRIE will address the control of performance and production of materials at the <u>mesoscale</u>

Performance of additively-manufactured (AM) structural components



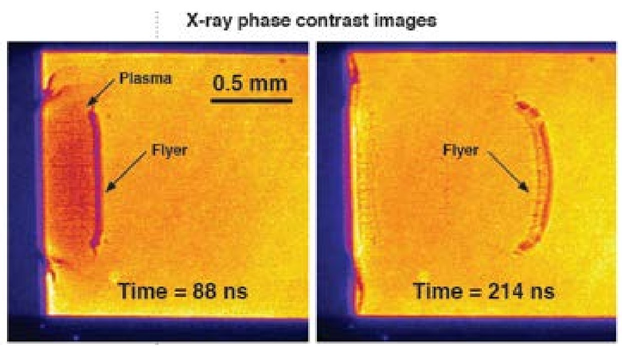
Wrought

AM Annealed

AM

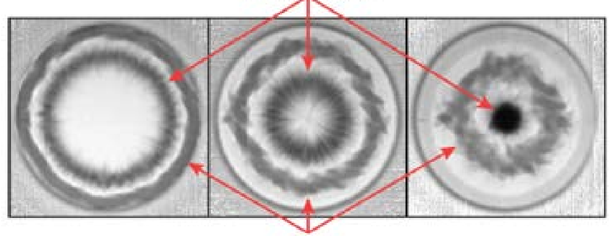
Damage in wrought vs additively-manufactured steel

Detonator performance and safety in LEPs



Movies of functioning slapper detonators

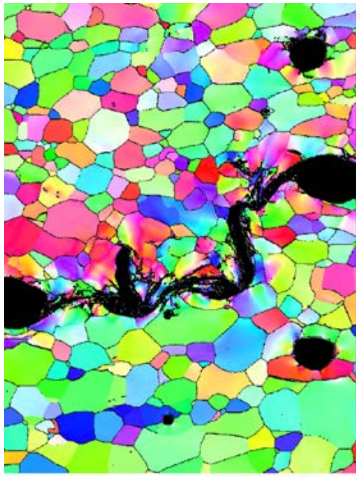
Ejecta and Mix in aged components under re-use

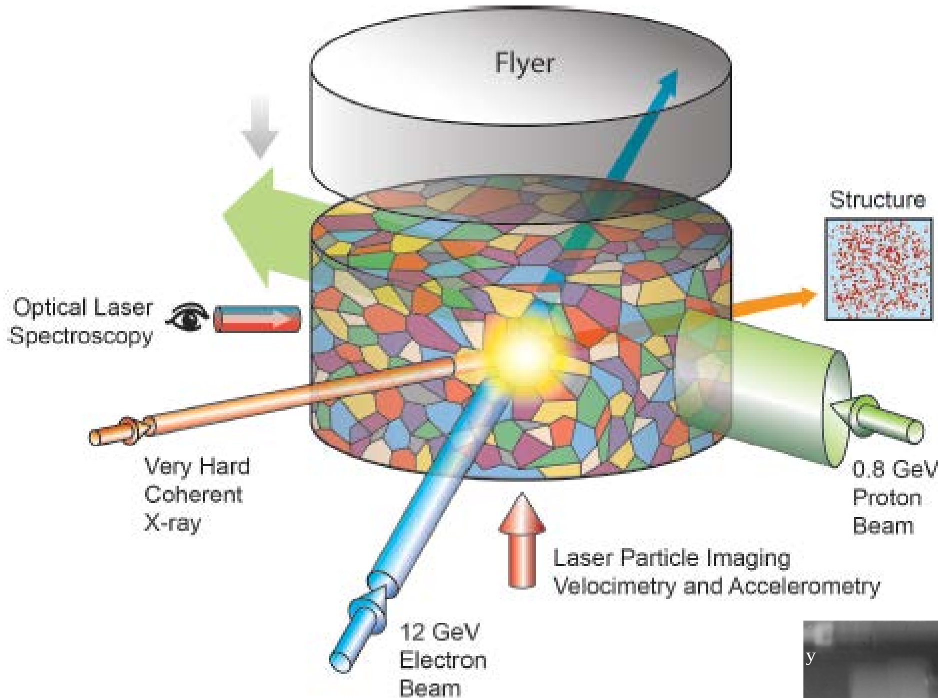


Movies of ejecta in convergent geometry

MaRIE fills a critical gap in length scales between the integral scale addressed by DARHT and the molecular scale addressed by facilities such as NIF.

Challenging experiments using multiple probes are planned to observe and characterize the dynamic microstructure and phase evolution of materials.





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

The model:

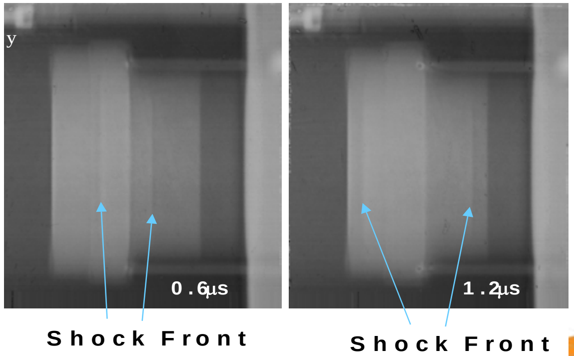
Accurate sub-grain models of microstructure evolution coupled to molecular dynamics.

The goal

Predict dynamic microstructure and damage evolution.

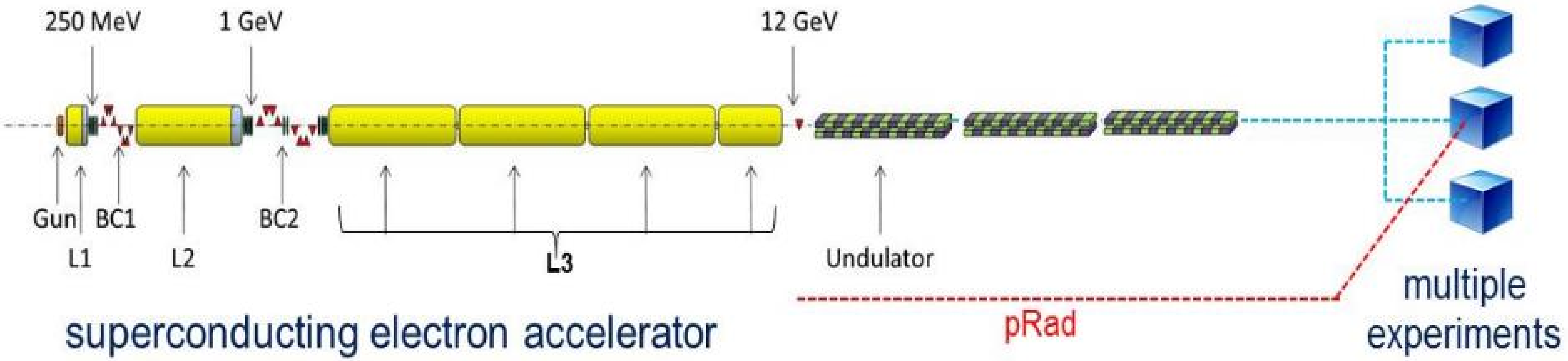
The first experiment

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

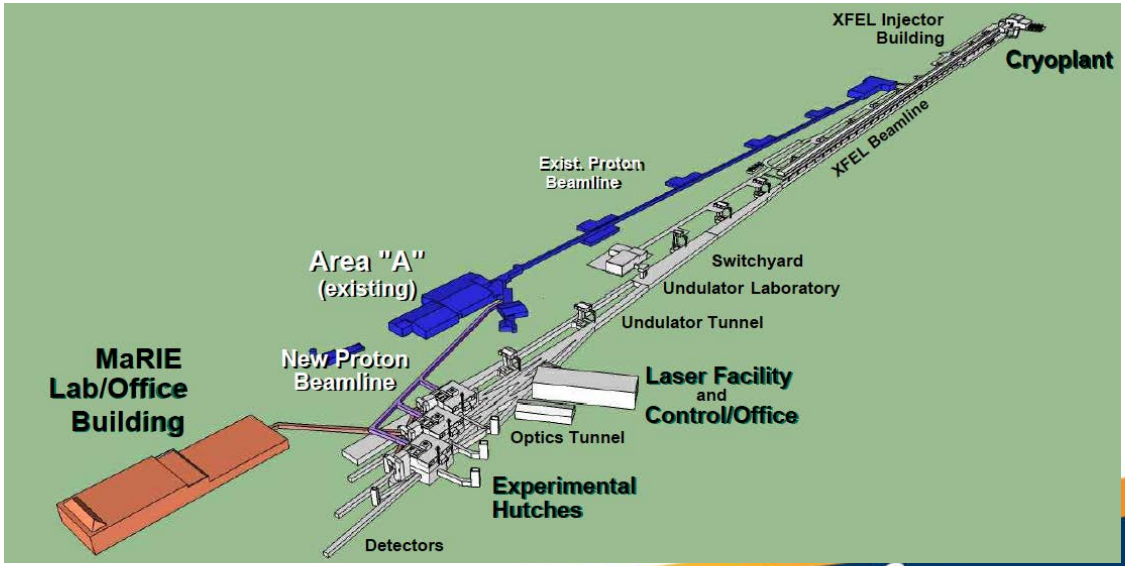


MaRIE will allow us to break apart the problem.

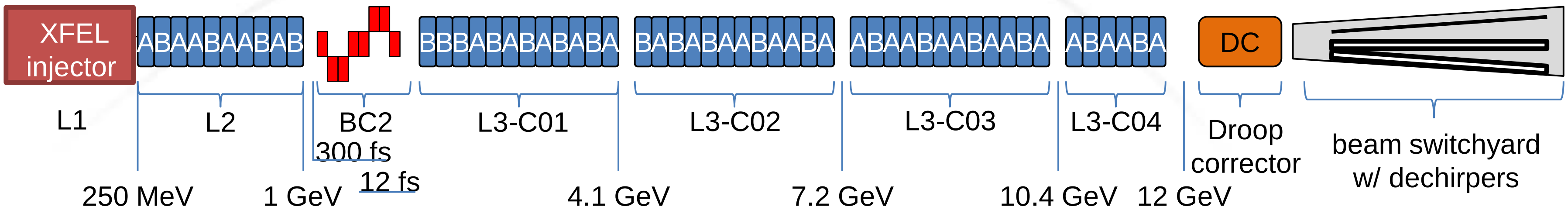
MaRIE will provide this capability by building a 12-GeV electron linac feeding a 42-keV XFEL to new experimental facilities



Our pre-conceptual reference design would be located on the north side of the LANSCE mesa, leveraging the capabilities of that proton/neutron facility.



We have used existing programmatic equipment to help translate pre-conceptual physics designs to realistic cost ranges



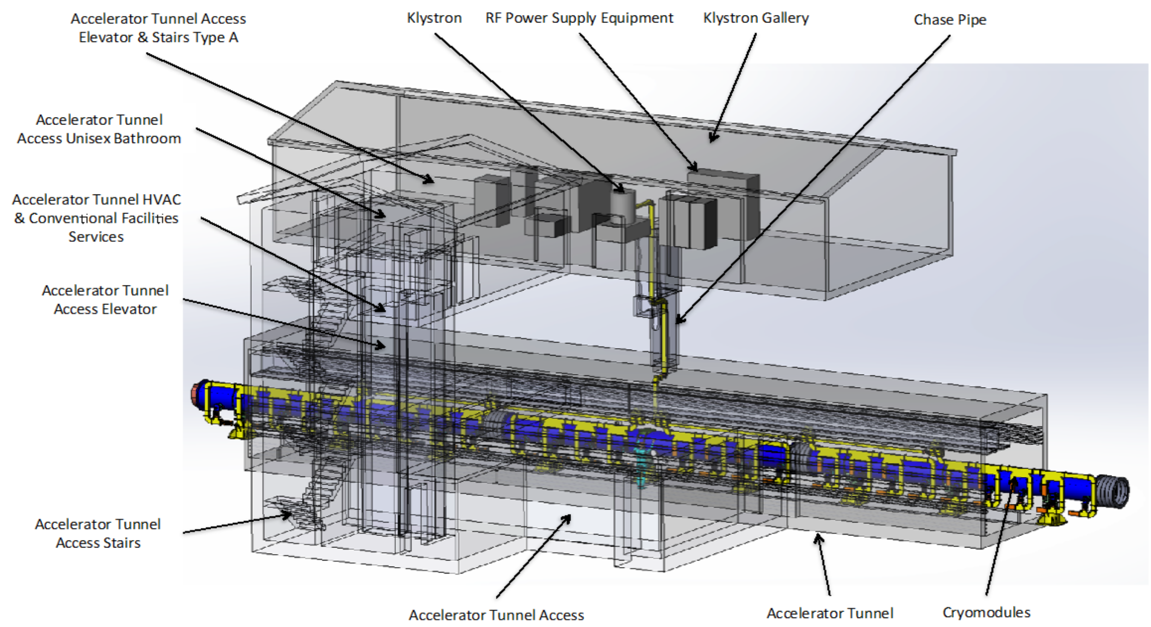
A 9-cavity ILC cryomodule, "A"-type

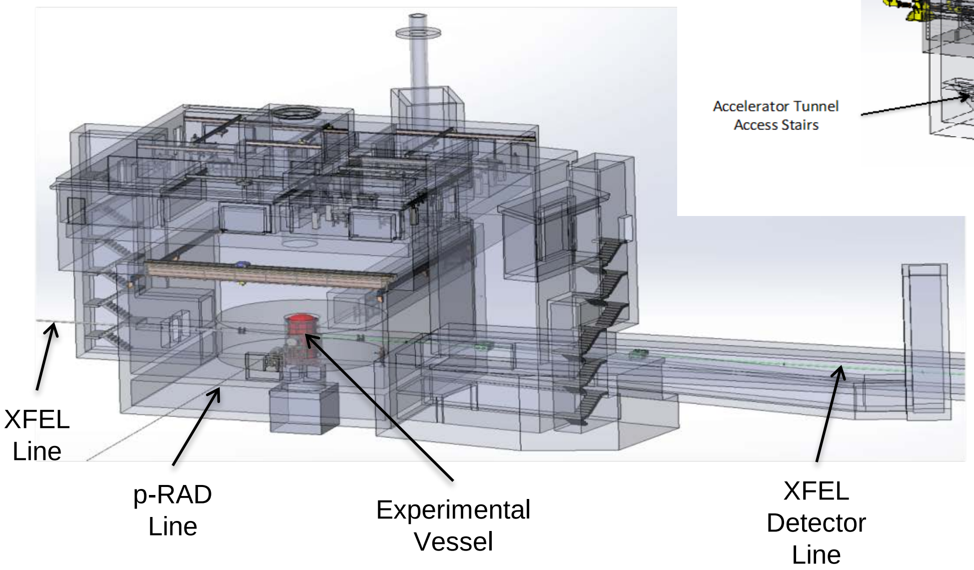
B 8-cavity ILC cryomodule, with quad / corrector / BPM, "B"-type

European XFEL RF Systems and Cryomodules

AOT also led the effort to define conventional facilities, experimental systems, pre-operations and operational costs

Isometric views of the accelerator tunnel and klystron gallery and the Multi-Probe Diagnostic Hall





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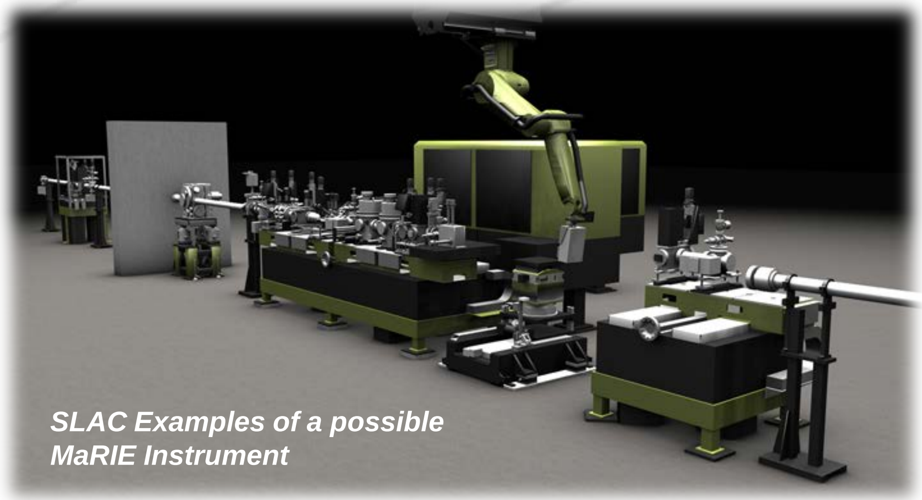
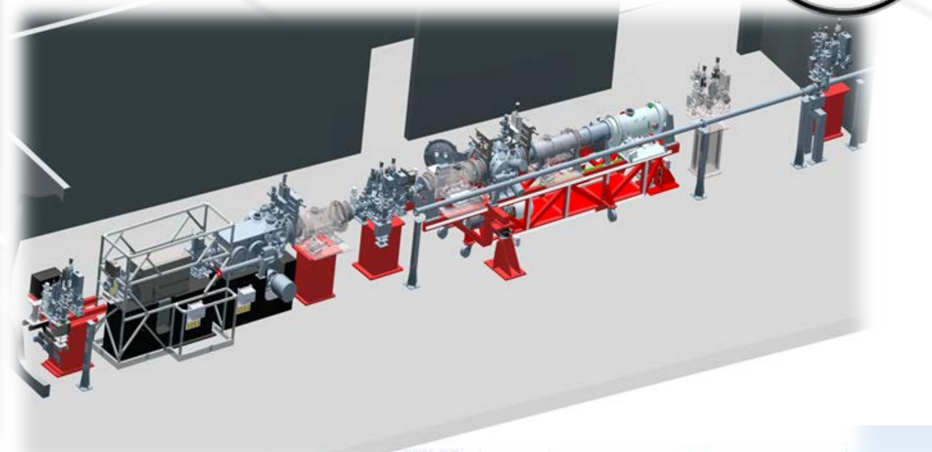
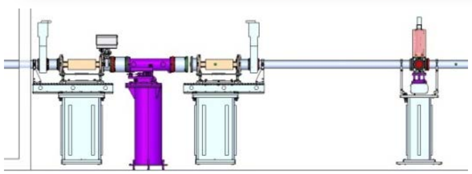
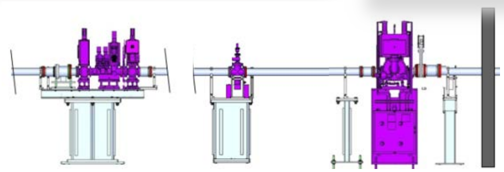
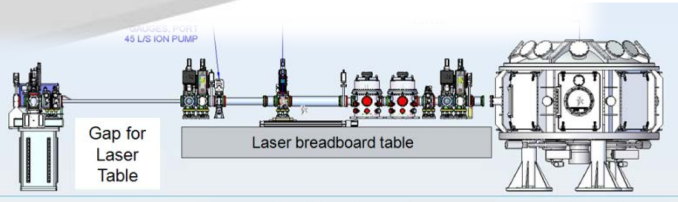
Experimental facilities equipment is based on existing hardware at LANL, SLAC, and ANL with planned improvements through R&D.



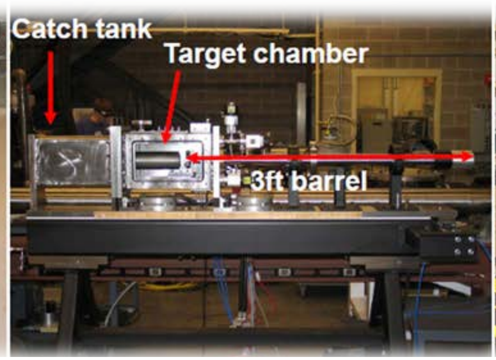






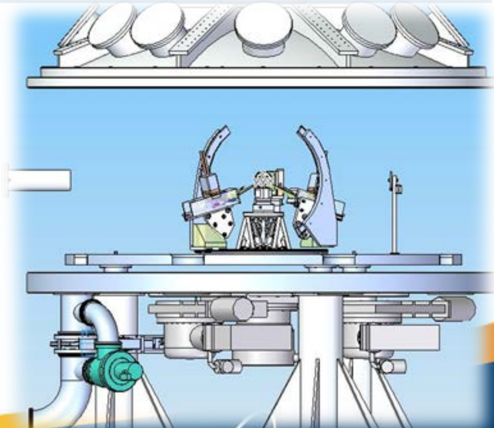


XRD Powder Gun



Gun used at APS

Pulser



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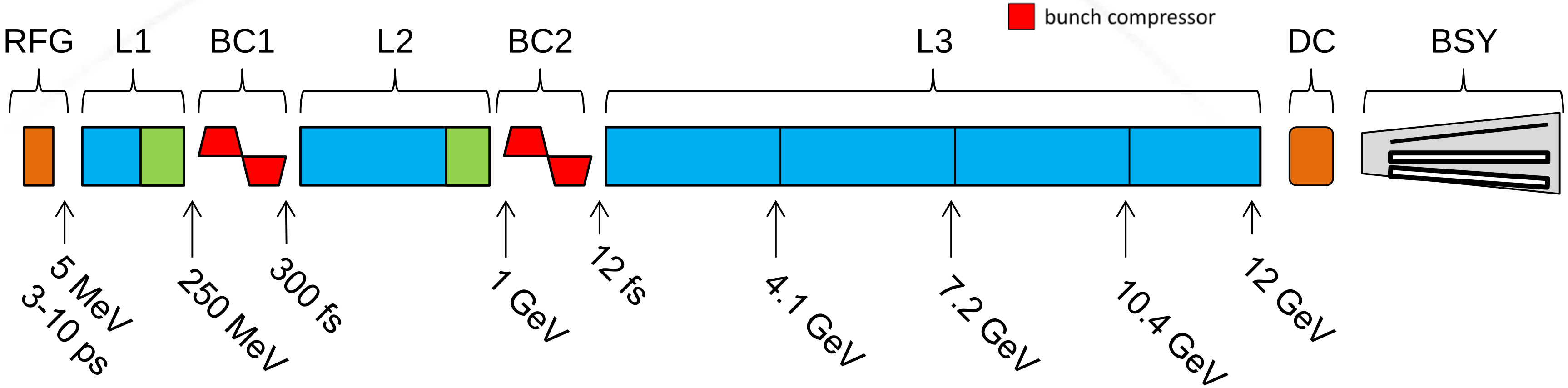
MaRIE is based on established high-performance linac designs.

1.3 GHz copper
1.3 GHz SCRF
3.9 GHz SCRF
bunch compressor

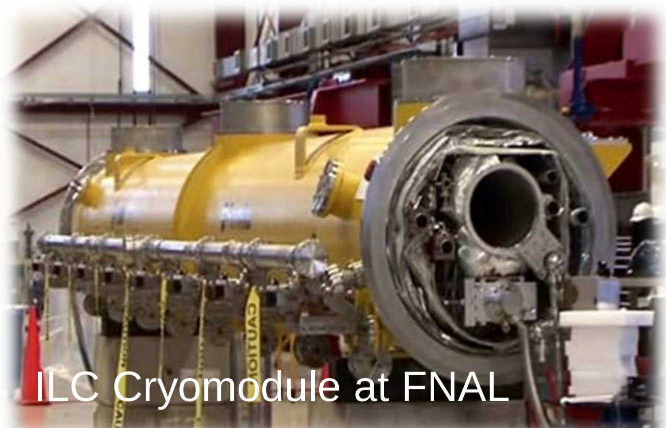
RFG photocathode electron gun
DC droop corrector
BSY beam switchyard



A 9-cavity ILC cryomodule, “A”-type

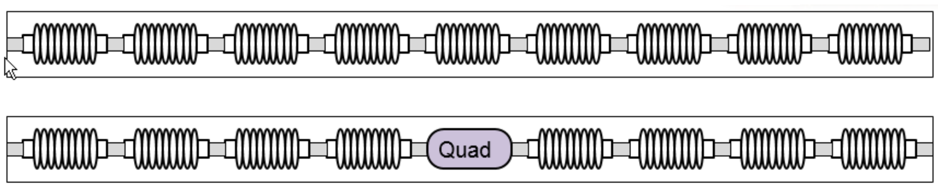
B 8-cavity ILC cryomodule, with quad / corrector / BPM, “B”-type

	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

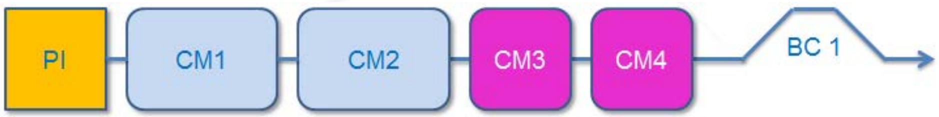


“A”

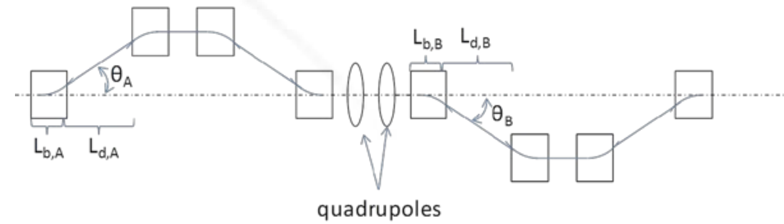
“B”



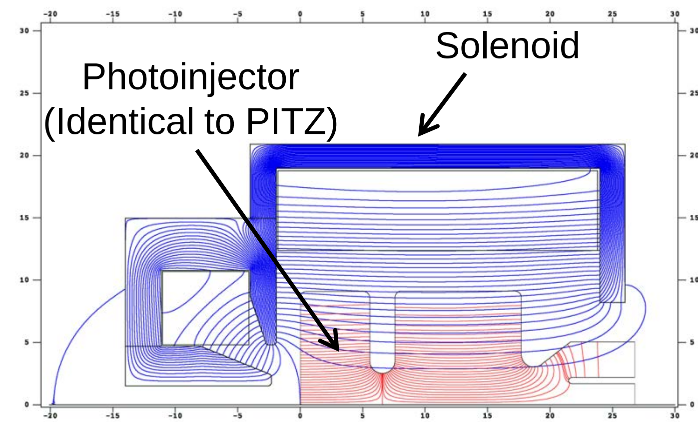
The MaRIE XFEL injector uses several innovations to meet performance requirements.



- **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.

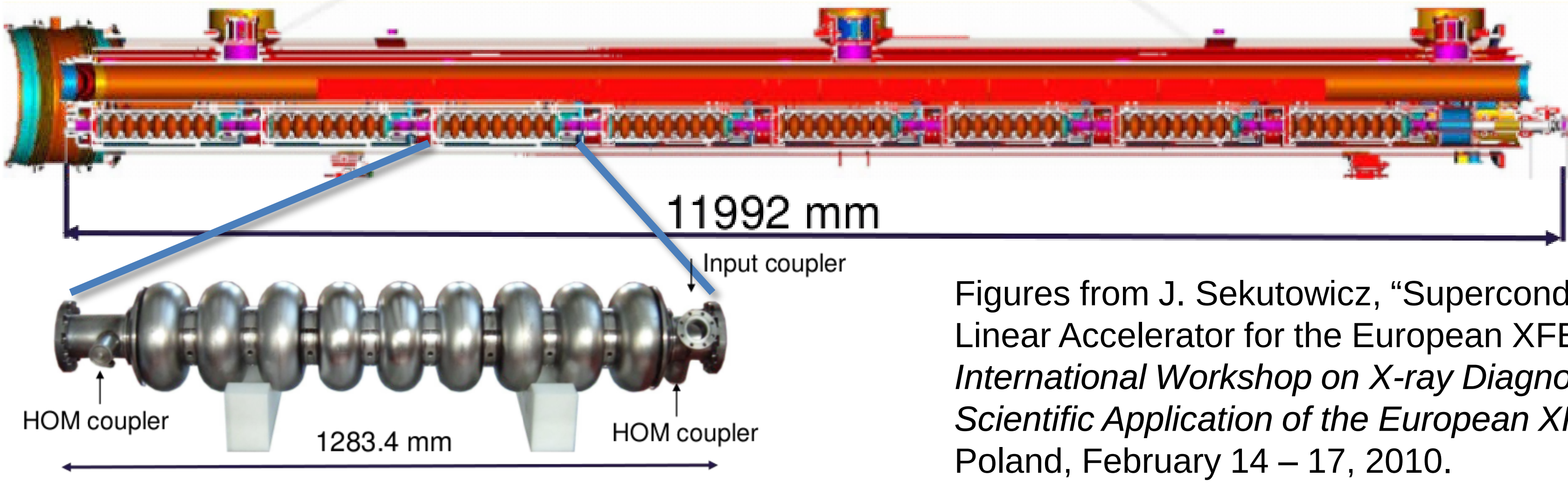


Double reversed-chicane helps reduce time-dependent dispersion from CSR wake.



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

1.3-GHz Cryomodule based on ILC and DESY XFEL



Figures from J. Sekutowicz, “Superconducting Linear Accelerator for the European XFEL”, *International Workshop on X-ray Diagnostics and Scientific Application of the European XFEL*, Ryn Poland, February 14 – 17, 2010.

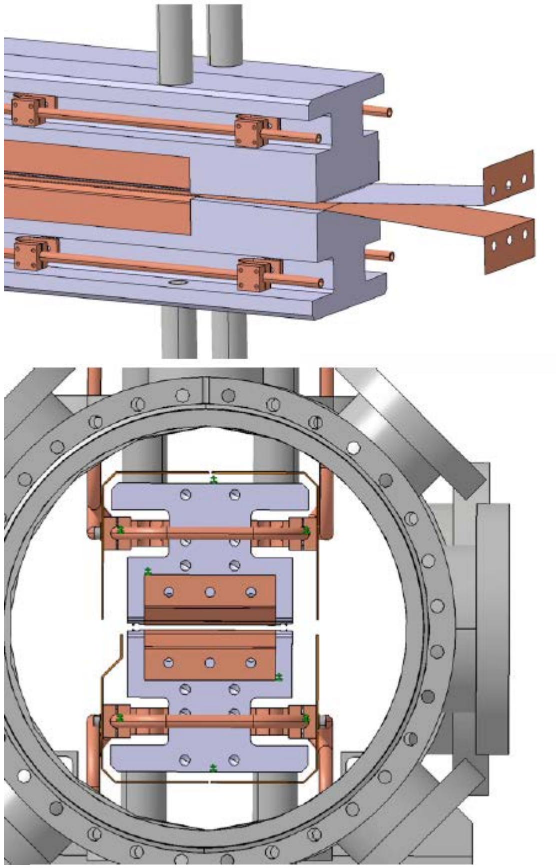
- 1.3-GHz Cryomodule has slots for 9, 9 cell accelerating cavities.
  - **Type A**
    - All 9 slots filled with accelerating cavities.
    - Injector uses Type-A cryomodules in present concept.
    - CM1 has independent phase and amplitude control for each cavity. (This allows for more efficient use of CM1, but may not be strictly necessary.)
  - **Type B**
    - 8 slots filled with accelerating cavities.
    - One slot reserved for a quad/BPM/steering magnet.

3.9-GHz Cryomodule

- Will be used to linearize the beam phase space.
- Cryomodules contain 4 accelerating cavities.
- Accelerating cavity scaled from 1.3-GHz cavity.
- Routine operation at FLASH with 18.9 to 19.7 MV/m average gradient.
- Capable of 22 MV/m average gradient.
- Fabricated by FNAL.

E. Harms, "3.9 GHz Cryomodule for FLASH", *FNAL-LBNL joint meeting on SRF Cavities and Cryomodules*, March 25, 2012.

The MaRIE undulators are based on SwissFEL U15.

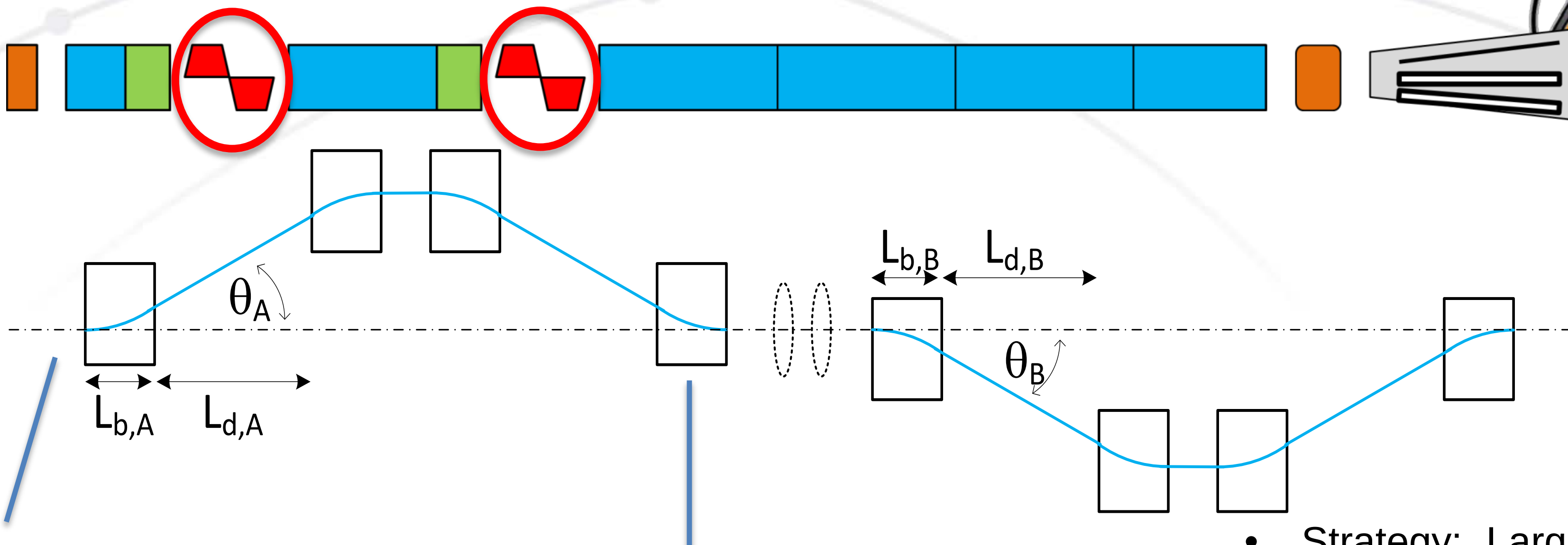


Courtesy of T. Schmidt

	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

- PM material = VACODYM 863 TP with Dy infusion
- B_r = 1.25 tesla; intrinsic H_c > 2,300 kA/m
- Pole material = vanadium permendur
- Wakefield shield and RF fingers = 0.1-mm CuNi foils with 50-μm copper as the RF surface.

MaRIE bunch compressors extend conventional designs.



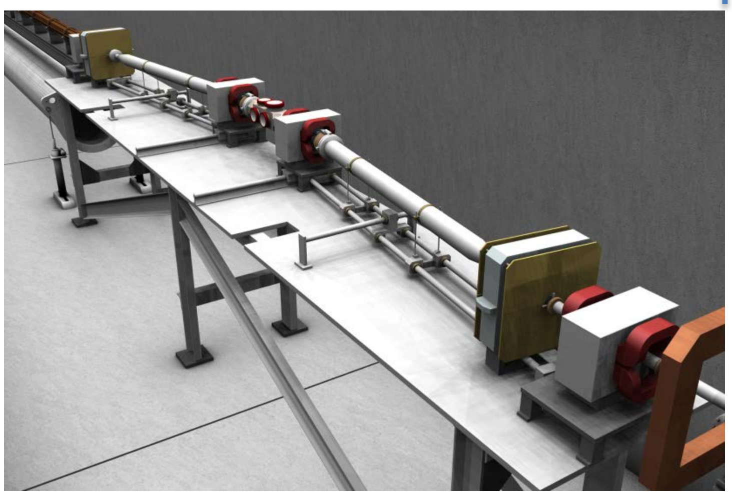
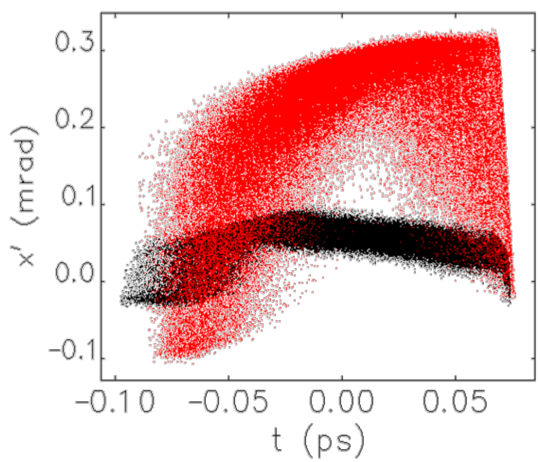
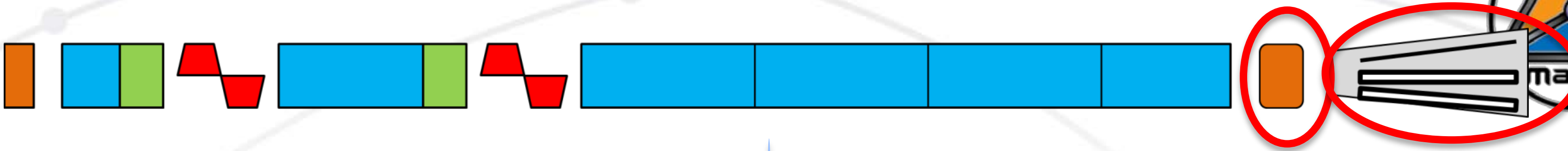


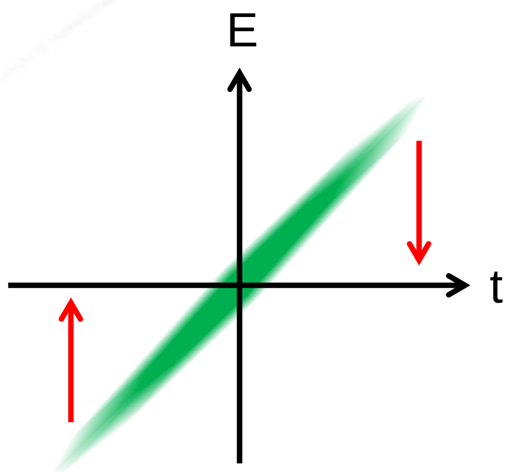
image courtesy SLAC



- Strategy: Large chirp / small R_{56}; Dual chicane for wake cancellation
- Known issues: Microbunching; residual chirp
- Open questions: Will wake cancellation work in practice?

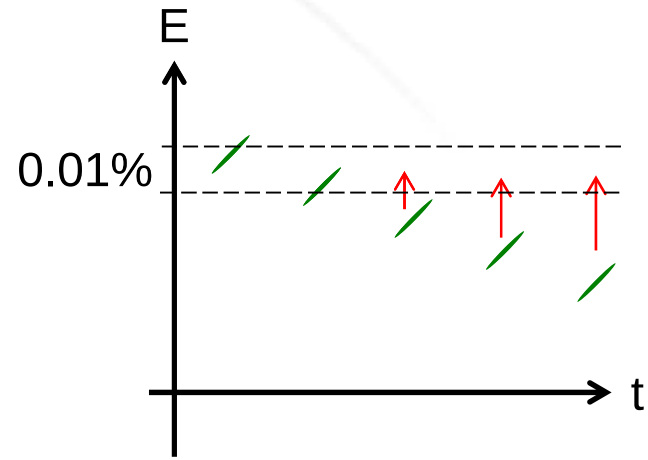
Energy spread and drift mitigation pose unique-to-MaRIE challenges.





Strategy: Use corrugated pipe dechirper to remove post-compressor energy spread

Open questions: tuning, practical implementation, wakefields



Strategy: Use short TW copper linac section to boost "drooped" bunches

Open questions: needed pre-BC2? how flexible can it be?

R. L. Sheffield, "Enabling cost-effective high-current burst-mode operation in superconducting accelerators," *NIM A 785 (2015)*

Spatial and Temporal resolutions for MaRIE multi-probe mesoscale experiments are defined by analysis of the measurement techniques.

	Metals Manufacture and Age aware performance	HE certification and qualification	Turbulent Materials Mixing	Welding and Additive Manufacturing
resolution	100 nm - 20 μm	100 nm - 20 μm	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	7 μsec	15 μsec	100 μsec
sample thickness	> 250 μm	> 10 μm – 6 cm	1 – 10 cm	0.1 to 10 mm
species	Be - Pu	Typically C, H, O, N	Noble gases, Ga, Be	Be - Pu

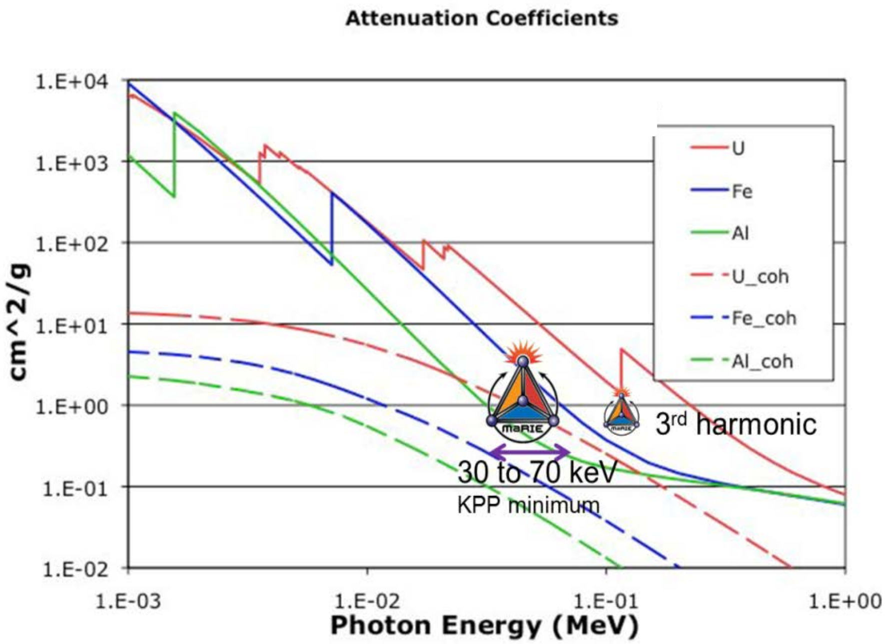
	spatial resolution	Framing time	sample thickness# Z=13	sample thickness# Z=26	sample thickness# Z=92
prad*	> 20 μm	50 nsec	15 cm / 0.8 GeV	3 cm / 0.8 GeV	1 cm / 0.8 GeV
erad*	> 1 μm	> 25 nsec	6 cm / 12 GeV	5 mm / 12 GeV	1 mm / 12 GeV
X ray	> 0.1 μm	< 100 psec	>10 μm/ 8 keV 2 cm/ 42 keV	500 μm/42 KeV 4 mm/122 KeV	200 μm/42 KeV 2 mm/122 KeV

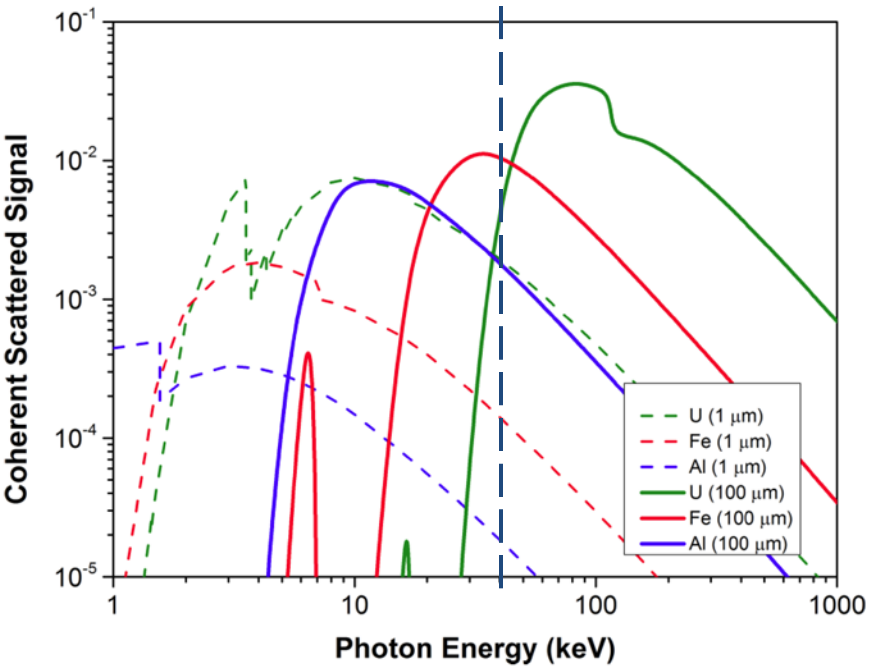
X-ray-only End Station measurement requirements require ms-long macropulses

Requirement	Multi-probe End Stations	X-ray only End Stations
Time scale for single image	< 0.1 ps	< 0.1 ps
# of closely spaced bunches	30 within 1µs	30 within 1 µs
Nominal micropulse repetition rate within macropulse	41 MHz	41 MHz
Minimum # of closely spaced pulses and pulse separation	2 within 300 ps	Not specified
Maximum macropulse length	100 µs	1 ms
Macropulse repetition rate	10 Hz	10 Hz
Expected typical spot diameter(s) at target (microns)	10 to 1000	10 to 1000
XFEL density resolution	5%	5%
Minimum imaging resolution	<0.1 mm	<0.1 µm
Materials of interest	Be to Pu	Be to Pu
eRad pulse separation/micropulse charge	4.6 ns/0.4 nC	N/A
eRad density resolution	2%	N/A
eRad imaging resolution	<1 mm	N/A

A superconducting linac can cost effectively meet the long macropulse requirements.

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





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 ~$2x10^{10}$.

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 *μ*m (dashed lines) and 100 *μ*m (solid lines)

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

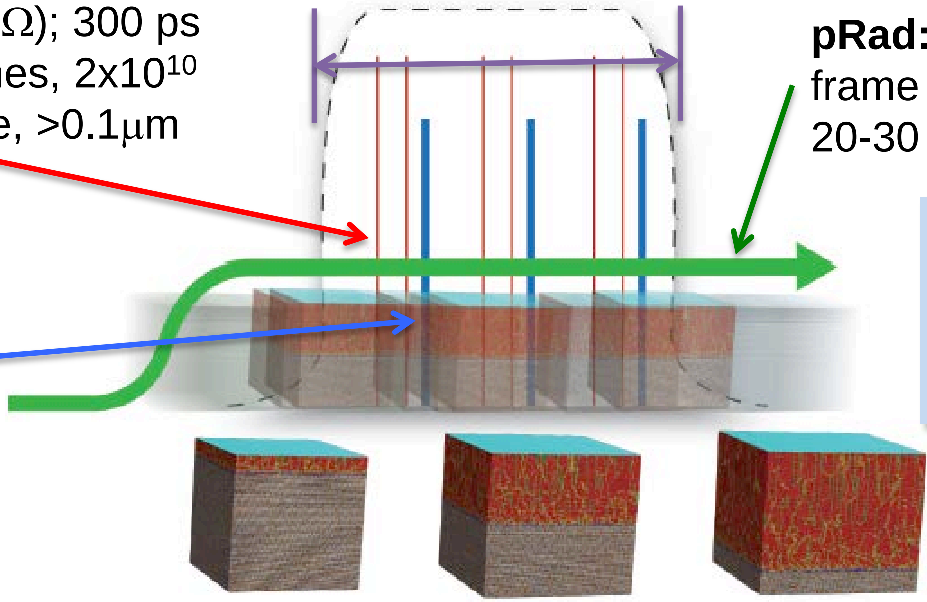
42-keV x-ray photons (red), 12-GeV electrons (blue), and 0.8-GeV protons (green) will be multiplexed to interrogate a single dynamic event.

Macropulse, variable, <1ms

XFEL: 42-126 keV (3Ω); 300 ps frame speed, 30 frames, 2×10^{10} photons @50 fs/pulse, >0.1μm resolution

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

eRad: 12 Gev, 25 ns frame speed, 30 frames, >1 μm resolution, 0.4 nC/pulse



Each probe beam covers a different parameter range for sample interrogation.

Adds significant machine costs:

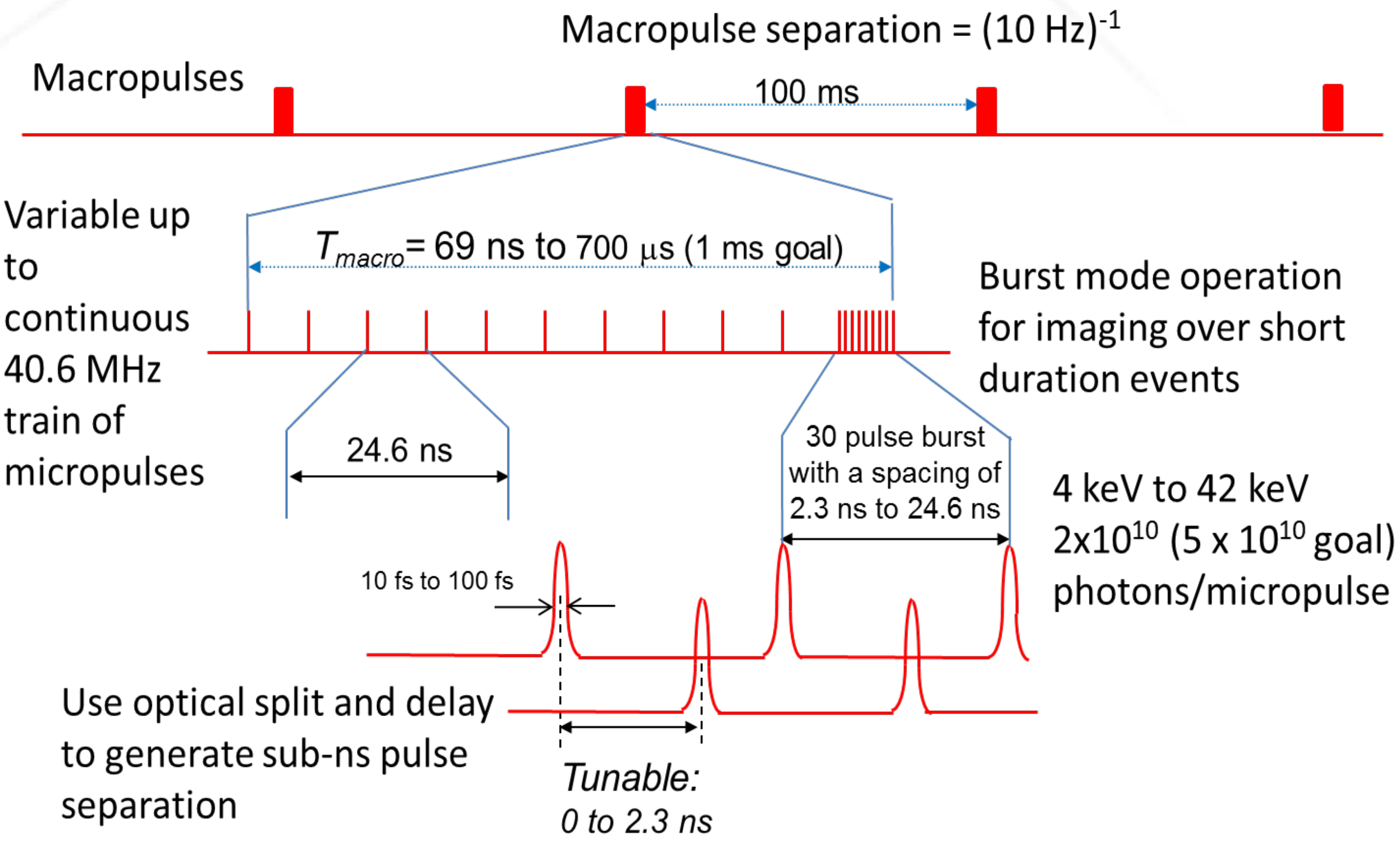
- Requires another injector

- 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

Flexible x-ray and multi-probe pulse structures, including high repetition rates, will be required to study time-dependent phenomena at multiple scales.



Key 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 20000	Energy	4 to 42 keV (3rd harmonic: 126 keV)
Linac fundamental frequency	1.3 GHz	RMS slice energy spread	≤ 0.01%	# per bunch	$5x10^{10}$ (3rd harmonic: $1x10^{8}$
Linac type	Superconducting	Macropulse to macropulse energy variation	≤ 0.02%	% Transverse coherence	70%
SC L-band cavity gradient	31.5 MV/m	Pulse energy variation within a macropulse	≤ 0.01%	Pulse length	≤ 100 fs
Maximum beamline angle	2.0 degrees @ 12 GeV	Min. bunch separation	2.3 ns	Bandwidth	$2x10^{-4}$
Maximum macropulse duration	0.1 ms	Dropped bunch rate	$1x10^{-3}$	Divergence	≤ 1 μrad
Electron source	Photoinjector	Normalized rms slice emittance	≤ 0.2 micron	Polarization	linear
XFEL bunch charge	0.2 nC	Macropulse repetition rate	10 Hz	Tunability	1%/ms
eRad pulse charge	0.4 nC	eRad energy spread	$5x10^{-4}$		
eRad normalized emittance	< 1000 microns	eRad minimum bunch separation	4.6 ns		

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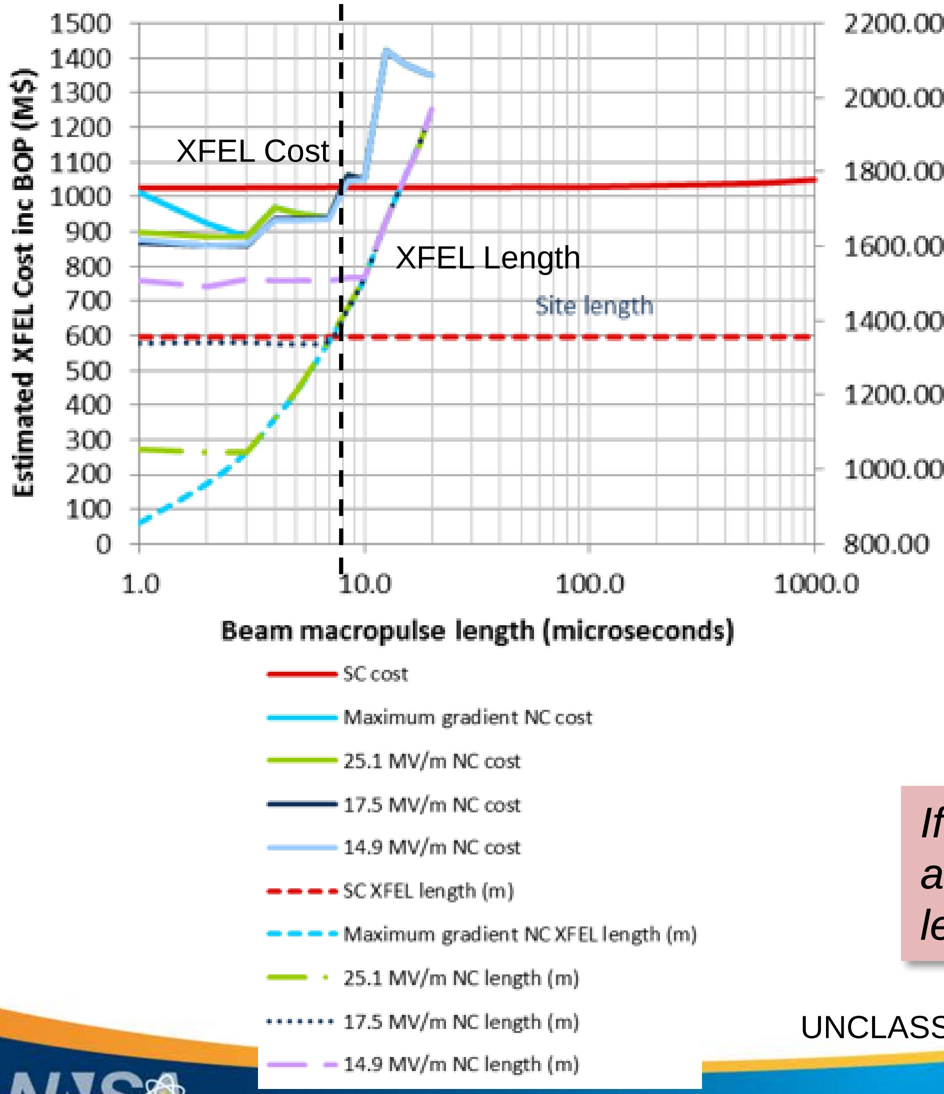
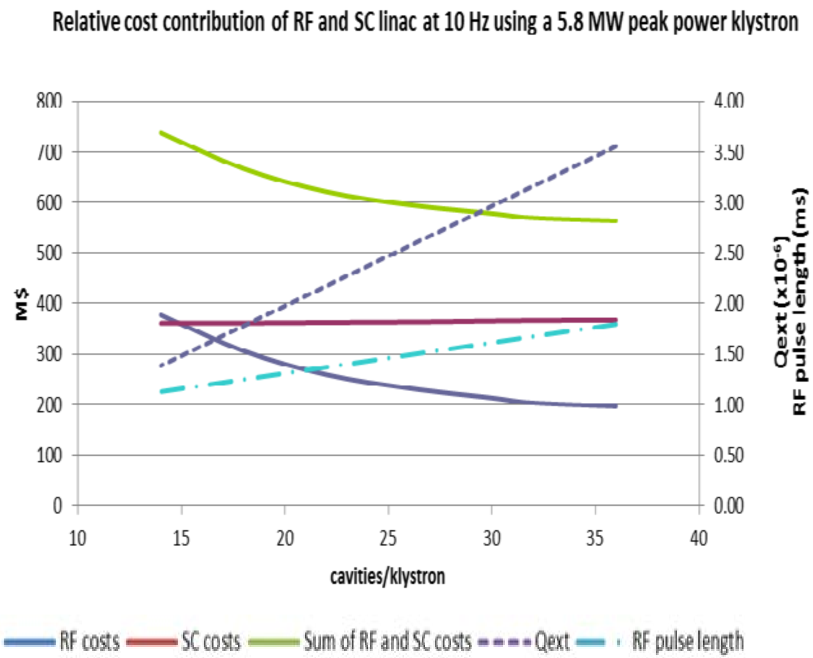
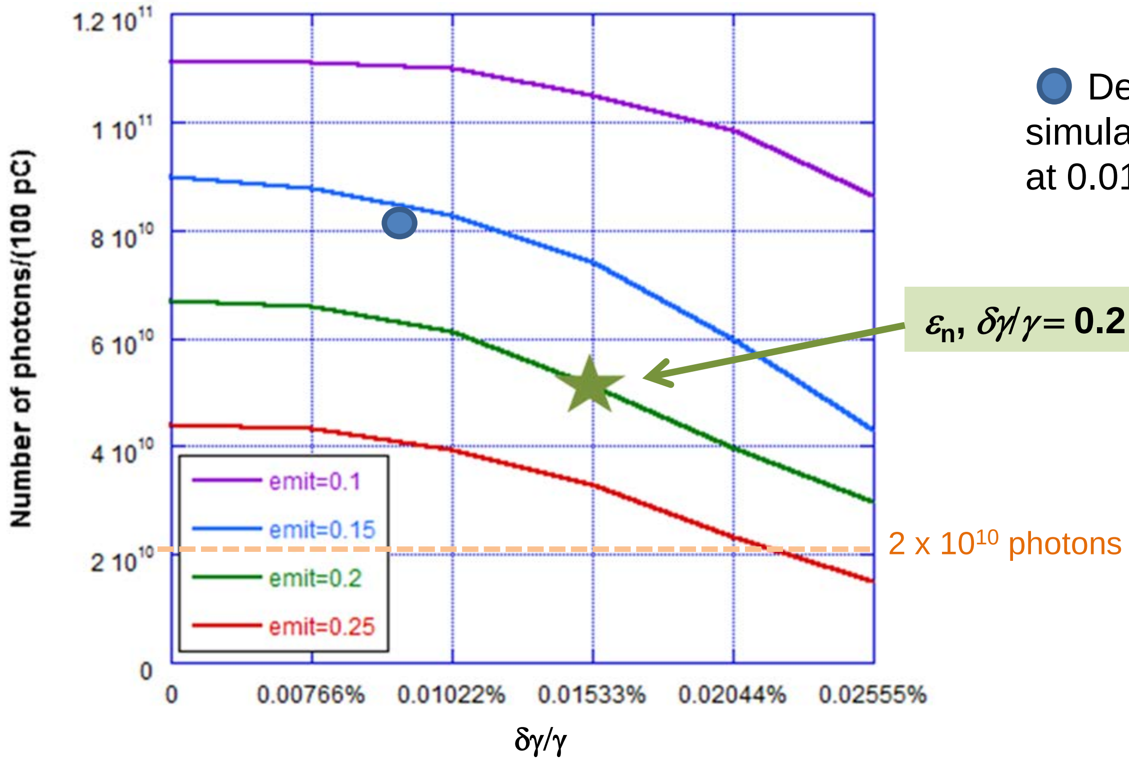
A parametric model was used to evaluate linac design space and for technology down-select, such as cost versus pulse length, SC vs. NC, etc.





If overall accelerator length and costs are the major constraints, for macropulse lengths > 7 μs a SC linac is optimal.

Time-independent GENESIS simulations show that >2x10[10] 42-keV photons within 0.015% bandwidth can be obtained using expected electron beam parameters.

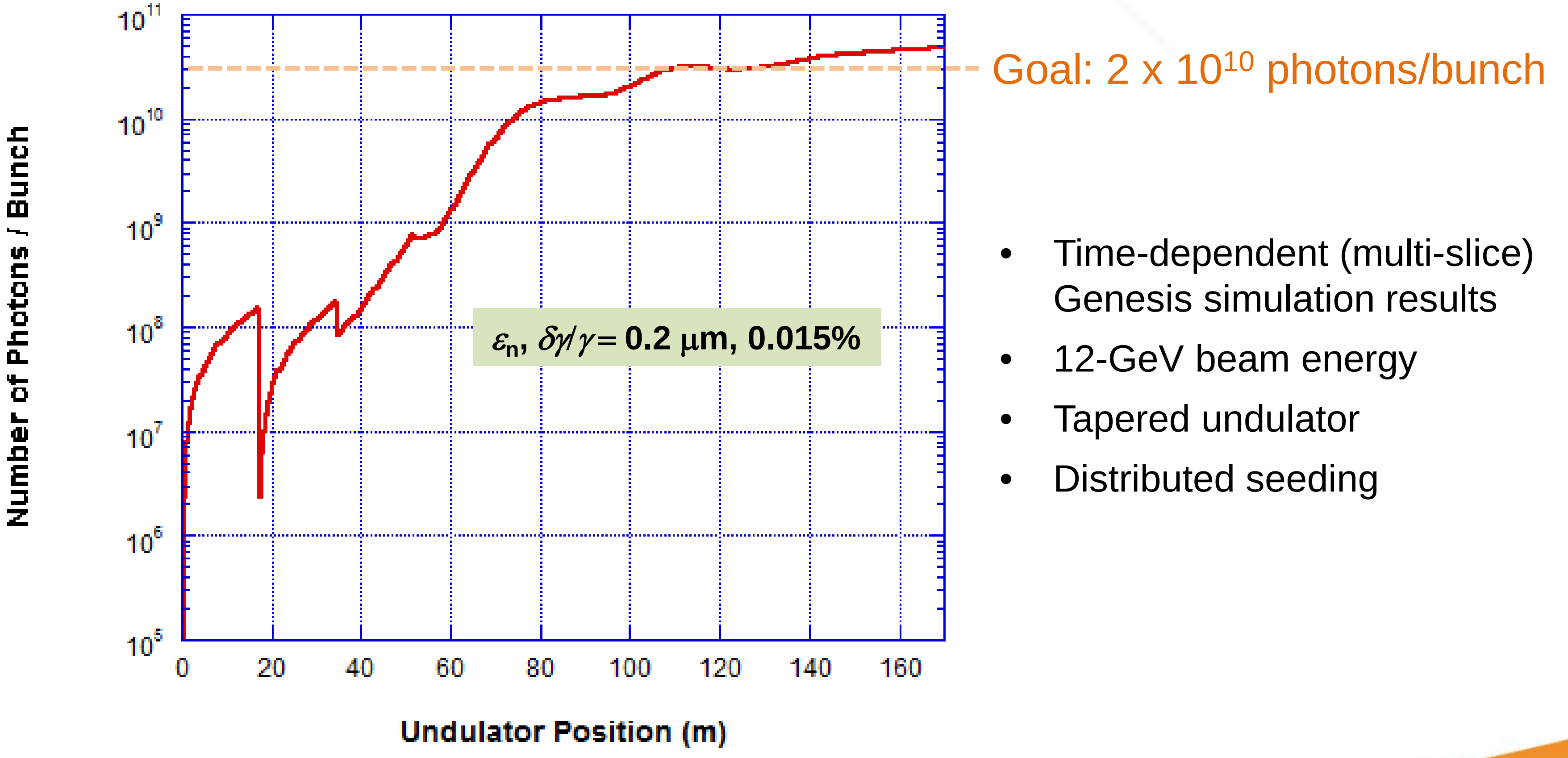


Design Goal: Electron beam simulations give 0.1 μm emittance at 0.01% energy spread.

Planned: X-ray flux using nominal emittance of 0.2 μm for 100 pC scaled from PITZ photoinjector.

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

XFEL performance risks associated with beam emittance can be mitigated through undulator tapering after saturation



- Time-dependent (multi-slice) Genesis simulation results
- 12-GeV beam energy
- Tapered undulator
- Distributed seeding

MaRIE Critical Technology Element Priorities

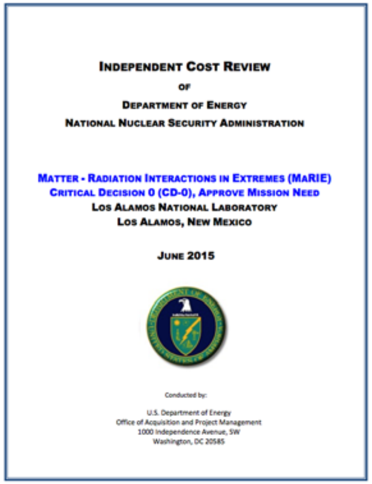
To do the following prioritization we used the following metrics:

- **Does it drive schedule, does it need to start soon to avoid delaying the project? Red most important**
- **How significantly does it affect a key risk of the project? Red most important, then yellow**
- **Will our sponsor, NNSA, see value in the work independent of the MaRIE project?**
- **Will strategic partners (SC Lab interest) be drawn to work with us by this project?**

	KPP	Schedule?	Risk?	NNSA	SC
Undulator and Distributed Seeding	FEL Photon Quantity		Red		✓
Start-to-End (S2E) Simulations of XFEL	Photon Beam Energy	Red	Red		✓
High-Energy and Ultrafast Imaging Camera	# of bunches and pulses		Red	✓	✓
Photo-Injector Design Test	Linac Electron and Photon Beam Energy	Red	Red		✓
X-ray optics	# of closely spaced pulses	Yellow	Yellow		✓
Long-Range Wakefields	# of closely spaced pulse		Yellow		✓
Bunch Compression/De-Chirping	Photon Beam Energy, FEL Photon Quantity		Yellow		✓
Microbunching Mitigation with Laser Heater	FEL Photon Quantity		Yellow		✓
Bulk Thermometry of Dynamic Materials with Laser-Driven NRS				✓	
Development of Charged Particle Radiography for the Study of Small and Fast Physical Processes	Multiple probes	Yellow		✓	
Long-Pulse Laser Technology Development	Sample subject to time-dependent change		Red	✓	
Multidimensional Dynamic Imaging	Multiple probes	Yellow		✓	✓
High Voltage Converter Modulator Development	[operational cost]				✓

DOE-Office of Project Management, Oversight, and Assessments (PMOA) staff completed an Independent Cost Review (ICR) in June

- The ICR team concluded the MaRIE project team prepared a credible and comprehensive cost estimate for the projected scope definition that exceeds what is expected at CD-0.
  - “The MaRIE CD-0 package exceeded DOE's expectations”
  - “The preliminary cost estimate range addressed current known costs and was well documented.”
  - “Considering the comprehensive and advanced state of the point estimate at CD-0, the ICR team recommends expanding the upper end of the range +30% above the point estimate.”
  - “DOE-PMOA recommends an estimated ROM = $1.9 - $3.7B.”



INDEPENDENT COST REVIEW
OF
DEPARTMENT OF ENERGY
NATIONAL NUCLEAR SECURITY ADMINISTRATION

MATTER - RADIATION INTERACTIONS IN EXTREMES (MARIE)
CRITICAL DECISION 0 (CD-0), APPROVE MISSION NEED
LOS ALAMOS NATIONAL LABORATORY
LOS ALAMOS, NEW MEXICO

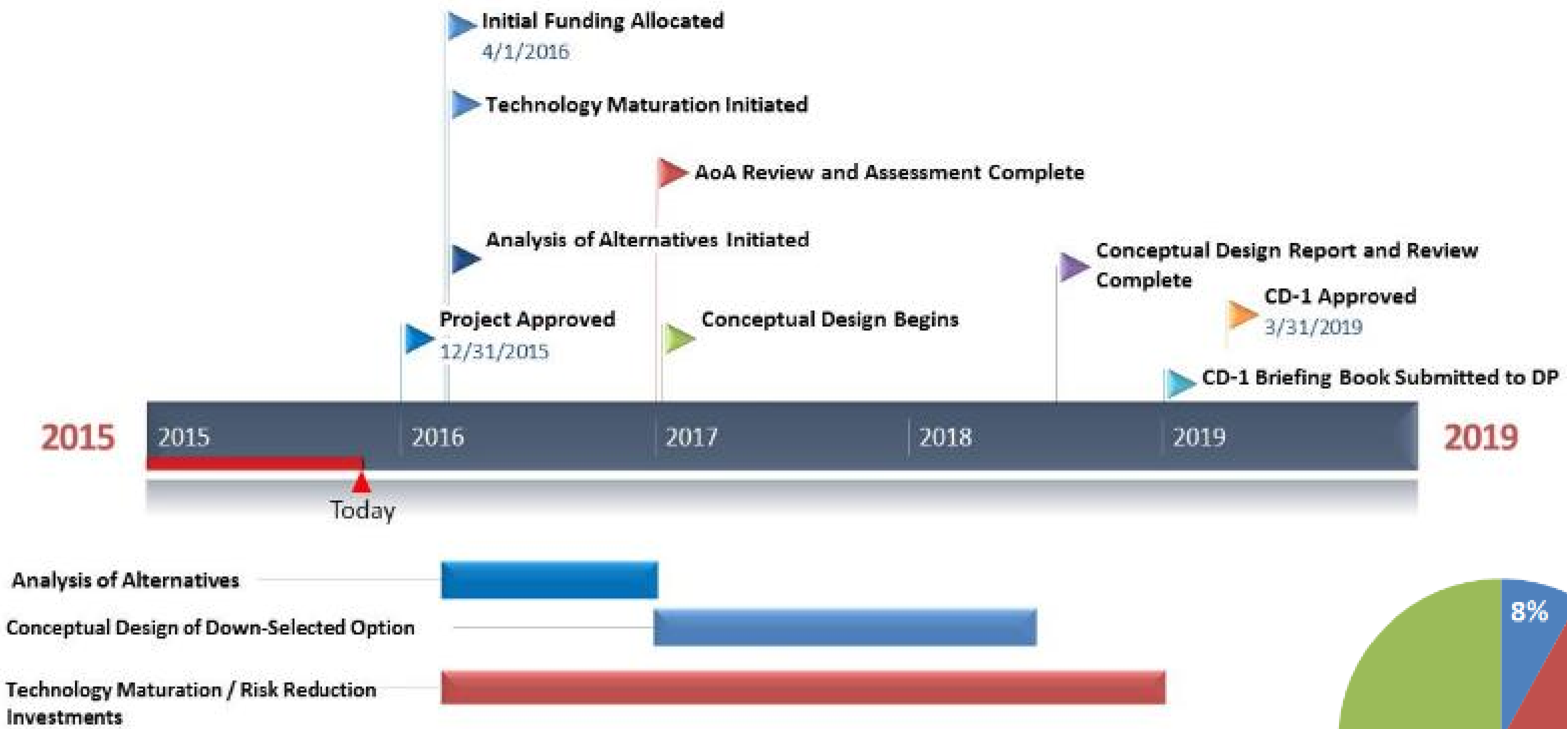
JUNE 2015

Conducted by:

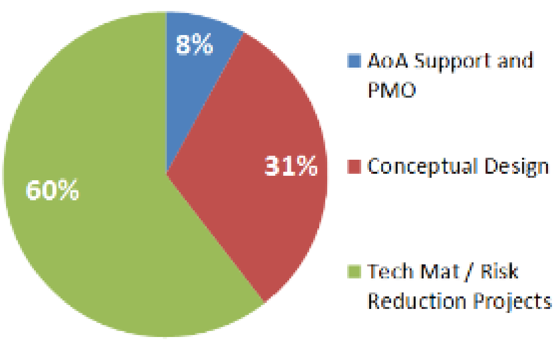
U.S. Department of Energy
Office of Acquisition and Project Management
1000 Independence Avenue, SW
Washington, DC 20585

We have a proposed near-term schedule to complete conceptual design

Cost Estimate between CD-0 and CD-1 is $110 - $150M. This includes investments in Technology Maturation / R&D projects, completion of an Analysis of Alternatives, and a subsequent Conceptual Design report.



	FY16	FY17	FY18	FY19
Low Range	$5 mil	$15 mil	$45 mil	$45 mil
High Range	$10 mil	$20 mil	$60 mil	$60 mil



Many SC projects are similar to MaRIE 1.0 in scale and complexity and provide benchmarks as well as potential partners

- Basic approach proposed will be to meet essential requirements, then *maximize* science capability within TPC and schedule, i.e. "***design to budget***".
- Project will benefit from rigorous SC Project Management Methods including robust Peer Reviews.
- Implementing the SC Process is our proposed risk mitigation approach to lower the risk for MaRIE and meet TPC as the next NNSA Project.

Successful Project Management Practices
in
Office of Science

Daniel R. Lehman, Contractor
L. Edward Temple Jr.
Project Advisor to the Director, ANL

http://science.energy.gov/opa

February 2015

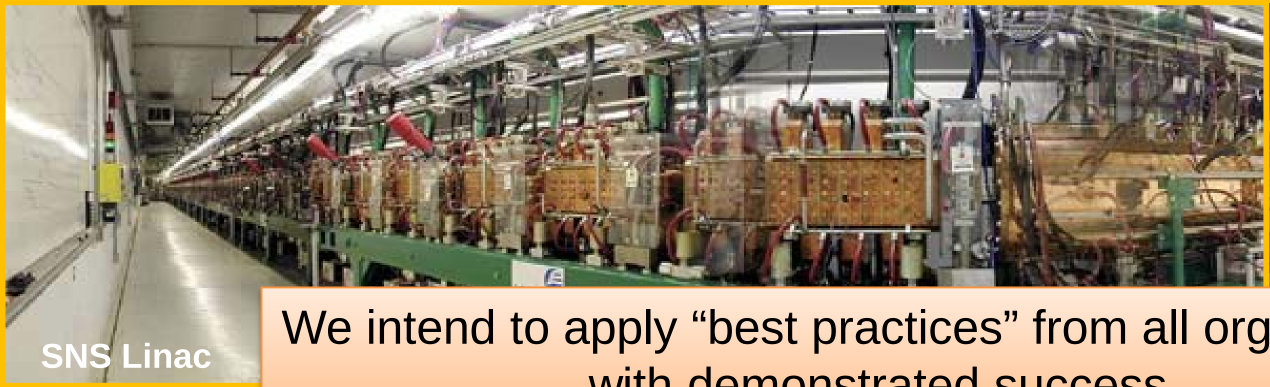
Topic

Primary Factors for Successful Project Completion

- Clear Ownership, Accountability, and Responsibilities
- Effective Front-End Planning
- Appropriate Project Contingencies
- Sufficient and Stable Funding
- Regular Independent Oversight

Office of Science Peer Reviews

Office of Science 2



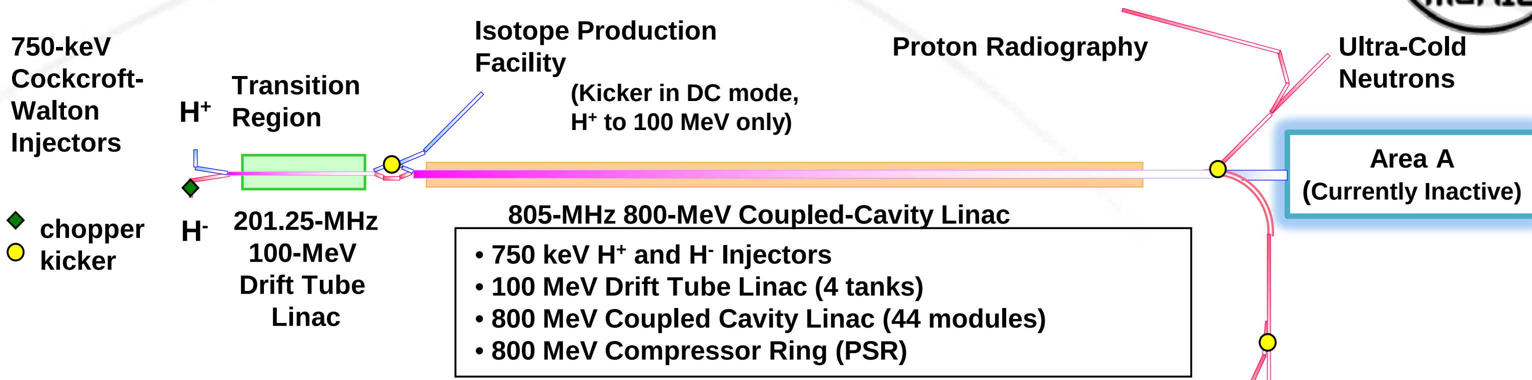
We intend to apply "best practices" from all organizations with demonstrated success.

Summary

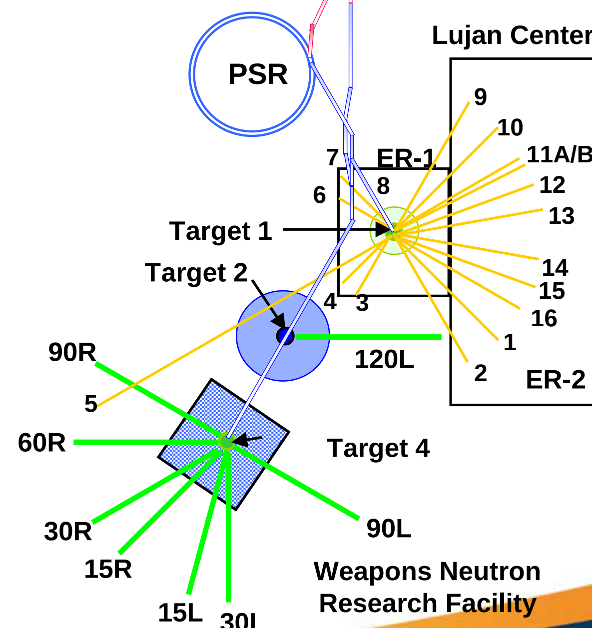
- There is a clear, compelling mission need and outstanding scientific opportunity.
- At least one viable technical approach, an accelerator with XFEL, is well understood and R&D has been identified to address the important technical issues.
- Critical Decision 0 approved by Deputy Secretary on February 18.
  - ROM: $1.9 to 3.7 B; CD-4: mid 2020's
- LANL's robust engineering capability was vital in preparing the MaRIE 1.0 CD-0 project scope definition
- Now that CD-0 is approved, <u>planning</u> for the project definition phase is underway
- It's time for wider engagement in MaRIE. Formal recognition of mission need will allow the entire DOE "network of Labs" to engage on requirements, alternatives, and technology risk reduction.

Backup Slides

LANSCE Facility Overview



Area	Typical Repetition Rate (Hz)	Typical Pulse Length (μs)	Linac Beam Species	Typical Chopping Pattern	Average Beam Current (μA)	Nominal Energy (MeV)	Avg Beam Power (kW)
Lujan	20	625	H-	290 ns / 358 ns	100 - 125	800	80-100
WNR Tgt 4	≤ 40, present 100, future	625	H-	1 μpulse every ~1.8 μs	≤ 2	800	< 1.6
UCN	20	625	H-	Lujan-like beam to unchopped	< 5	800	< 4
pRad	~1	625	H-	60-ns bursts every ~1 μs	< 1	800	< 1
IPF	≤ 100 pulsed or DC mode	625	H+	NA	≤ 250	100	≤ 25
Area A Inactive	≤ 100	625	H+	NA	1000	800	~800



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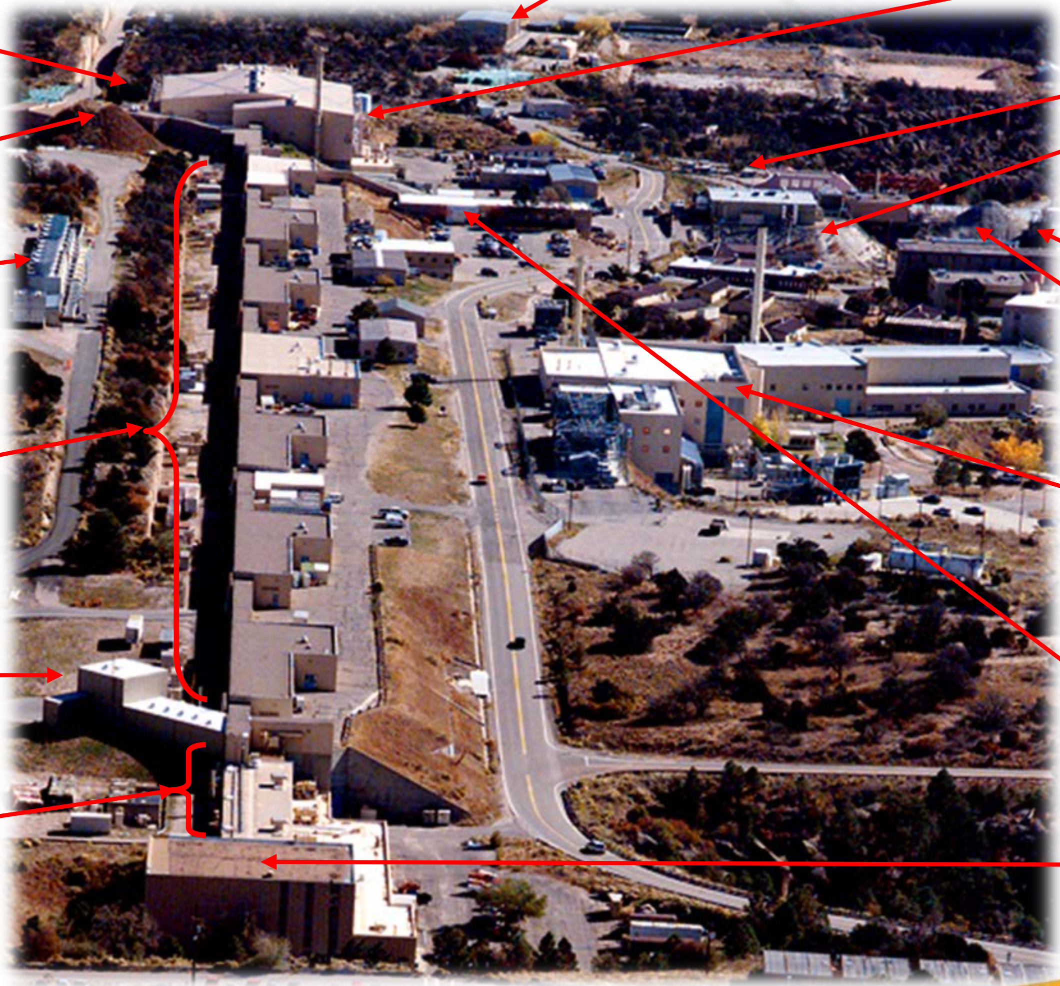
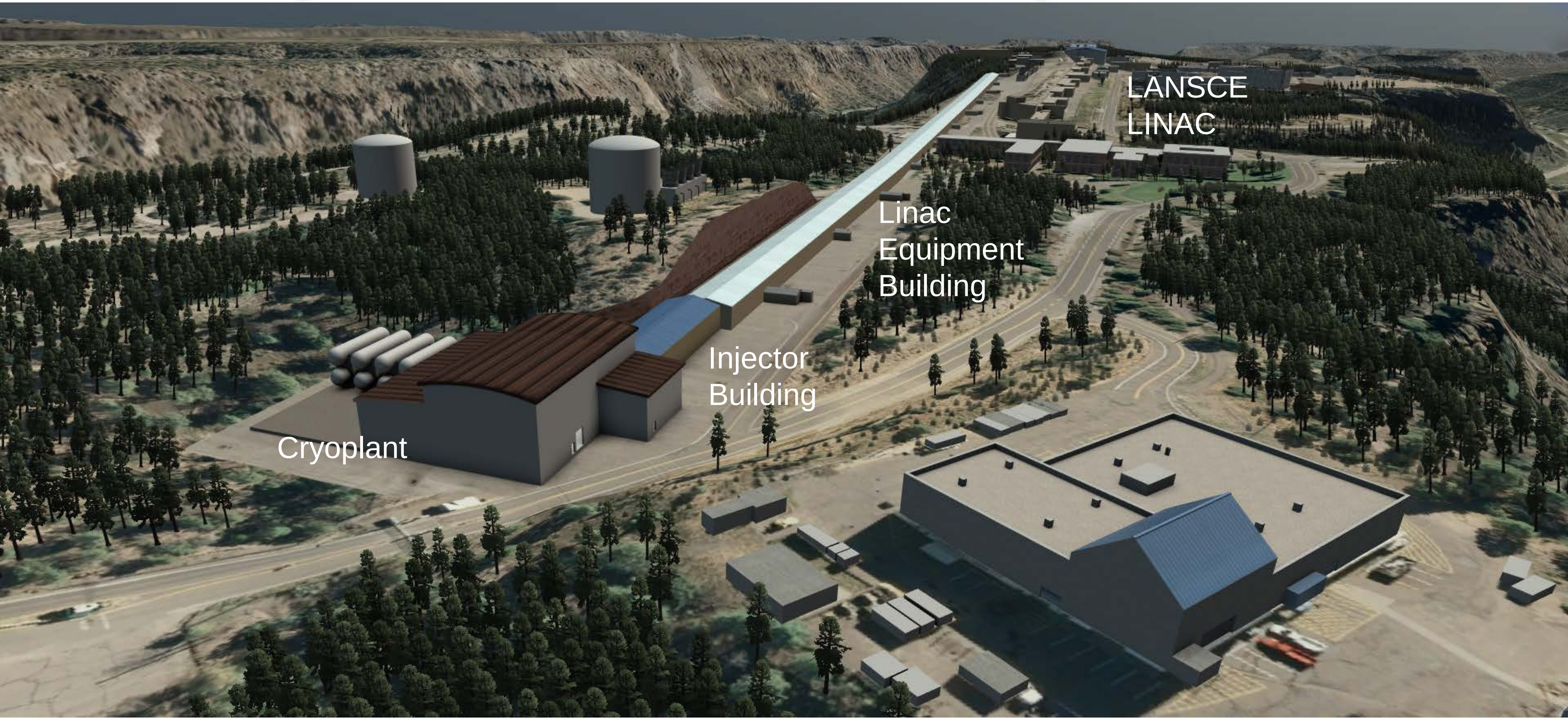
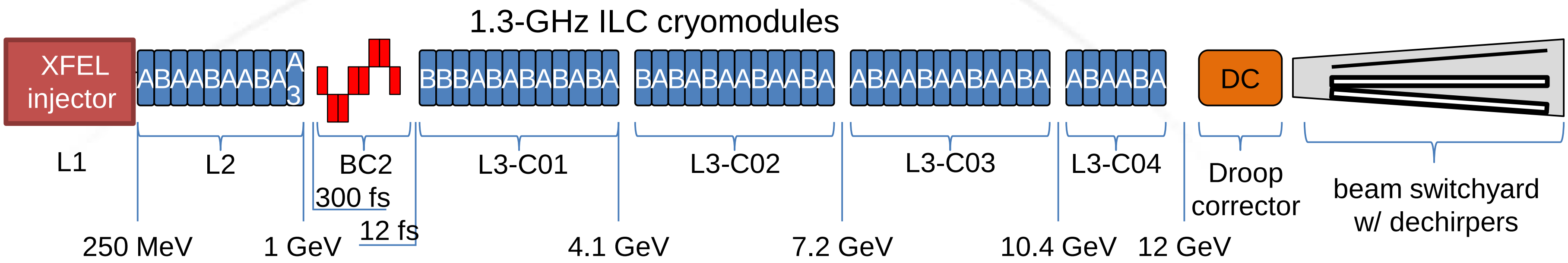
The LANSCE accelerator provides flexible time-structured beams from 100-800 MeV to >20 active experimental stations.



Artist Rendition of MaRIE Conventional Facilities



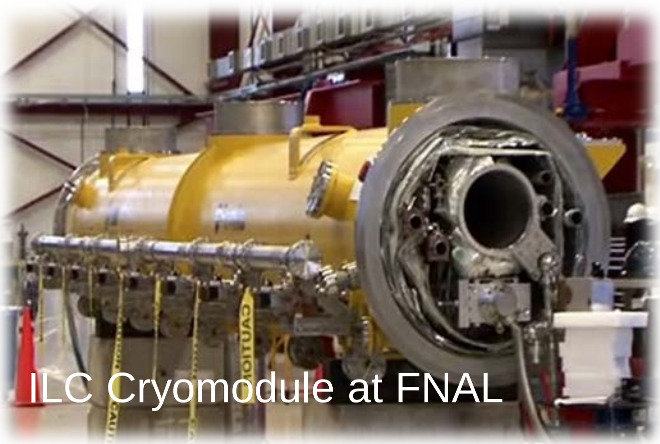
An XFEL pre-conceptual reference design that meets the MaRIE performance requirements has been developed.



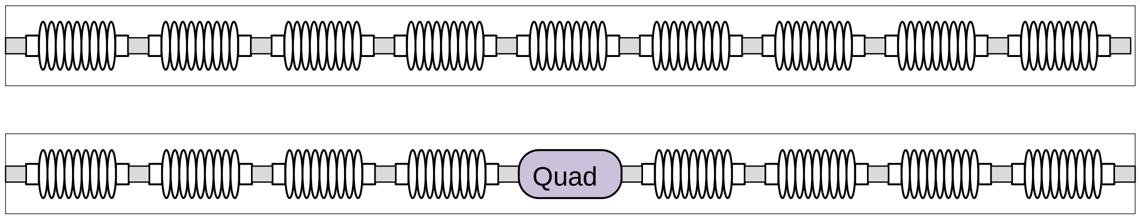
A — 9-cavity ILC cryomodule, “A”-type

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



“A”
“B”



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