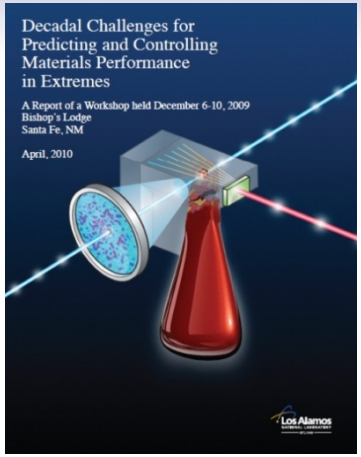


Current Status of the MaRIE

(Matter-Radiation Interactions in Extremes)

Science Facility at Los Alamos National Laboratory

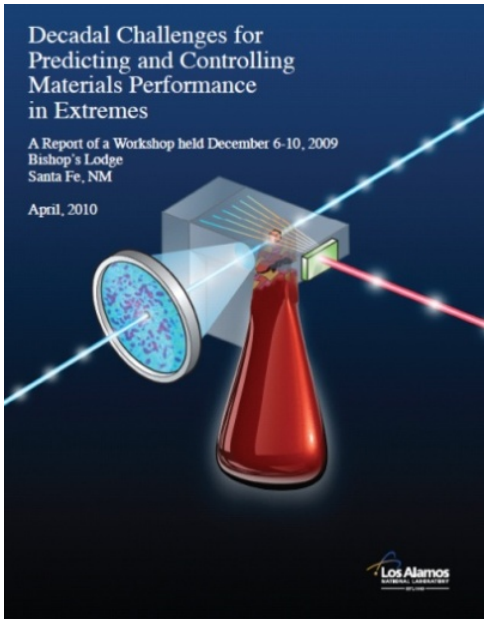
Petr M. Anisimov, Cris W. Barnes, Bruce E. Carlsten, Patrick L. Colestock, Leanne D. Duffy, Henry P. Freund, Frank Krawczyk, John W. Lewellen, Quinn R. Marksteiner, Matthew T. Reiten, Donald J. Rej, John L. Sarrao, Richard L. Sheffield, Evgenya I. Simakov, Steven J. Russell, and Nikolai A. Yampolsky

Outline (credit: largely from Russell's MaRIE talk at 2013 HBEB)

- MaRIE (**Ma**tter-**R**adiation **I**nteraction in **E**xtremes)
  - *Why build it?*
  - *What is it?*
- MaRIE 1.0: First Steps.
- MaRIE 1.0 X-Ray Free Electron Laser
  - *Current baseline concept.*
  - *Status of the design.*

The intent of MaRIE is to move materials research from an era of observation of performance to control of properties

- **The confluence of improved experimental capabilities (e.g. 4th generation light sources, controlled synthesis and characterization, …) and simulation advances are providing remarkable insights at length and time scales previously inaccessible**



New capabilities will be needed to realize this vision:

In situ, dynamic measurements

simultaneous scattering & imaging

of well-controlled and characterized materials

advanced synthesis and characterization

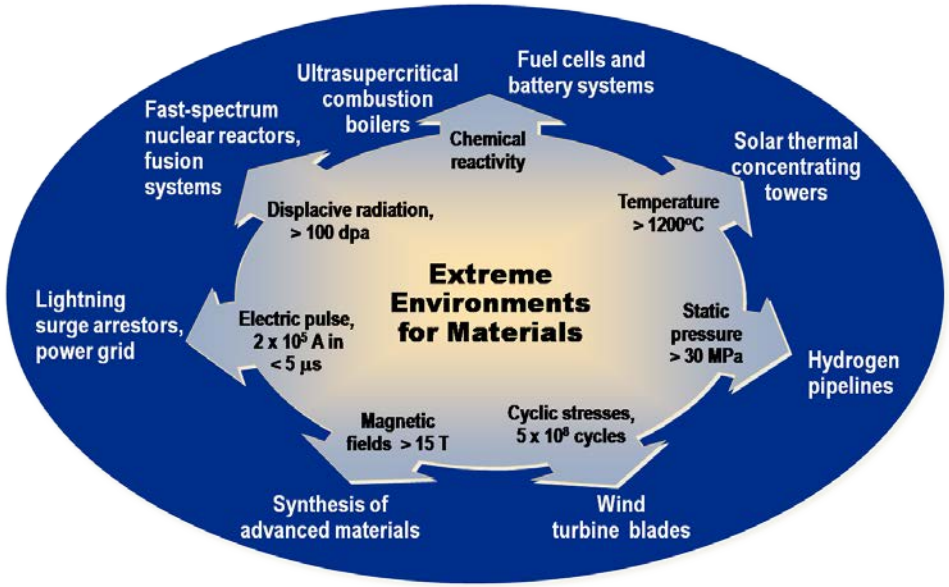
in extreme environments

dynamic loading, irradiation

coupled with predictive modeling and simulation

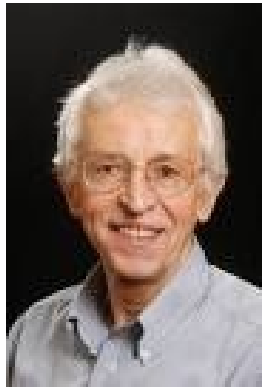
materials design & discovery

The needs for materials in extremes are many; the challenge is common: revolutionary advances in controlled functionality



"Physicists perform elegant experiments on crummy samples while materials scientists perform crummy experiments on elegant samples"

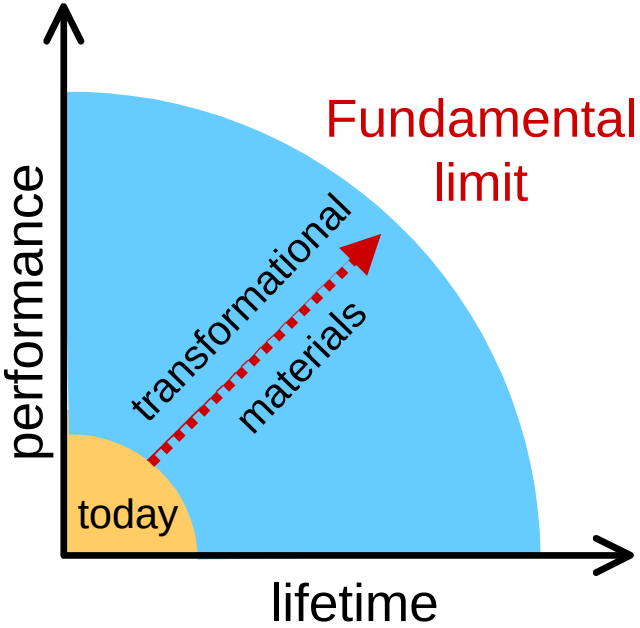
-Sig Hecker
Former LANL Director
(materials scientist)



We need to enable a transition:

from observation and validation

to prediction and control



MaRIE builds on existing facilities to provide unique experimental materials science tools

First x-ray scattering capability at high energy and high repetition frequency with simultaneous charged particle dynamic imaging

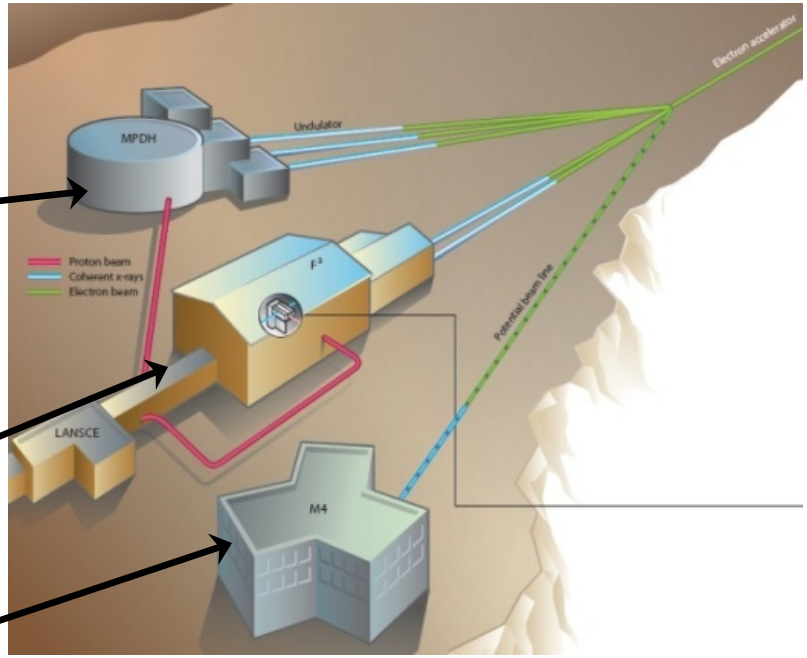
(**MPDH**: Multi-Probe Diagnostic Hall)

Unique in-situ diagnostics and irradiation environments beyond best planned facilities

(**F^3**: Fission and Fusion Materials Facility)

Comprehensive, integrated resource for materials synthesis and control, with national security infrastructure

(**M4**: Making, Measuring & Modeling Materials Facility)



Very hard x-ray free electron laser
Simultaneous photon-proton imaging measurements
Spallation neutron-based irradiation capability
In-situ, transient radiation damage measurements
Materials design and discovery capability

MaRIE will provide unprecedented international user resources

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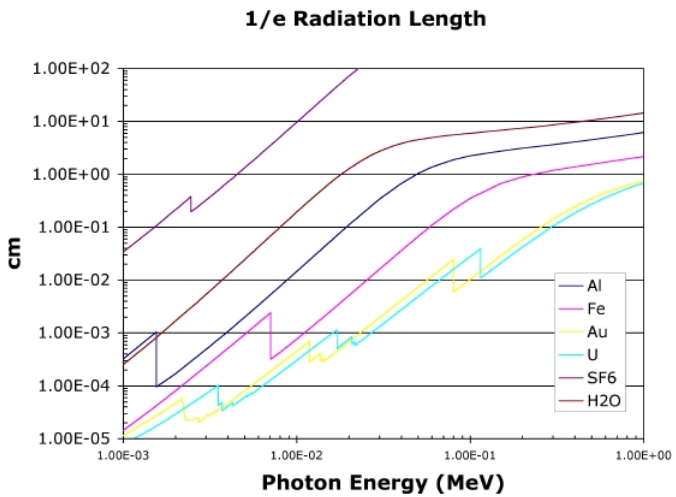
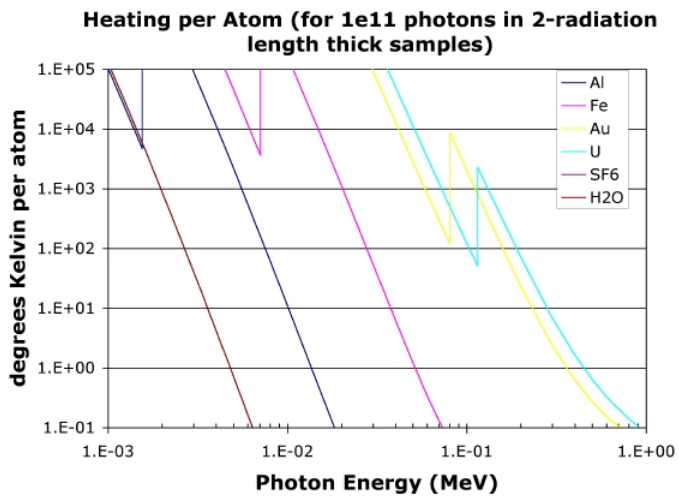
Why a 42 keV X-FEL?

MaRIE seeks to probe *inside* multigranular samples of condensed matter that represent bulk performance properties with sub-granular resolution. With grain sizes of tens of microns, "multigranular" means 10 or more grains, and hence samples of few hundred microns to a millimeter in thickness. For medium-Z elements, this requires photon energy of ~50 keV or above.

This high energy also serves to reduce the absorbed energy per atom per photon in the probing, and allows multiple measurements on the same sample. Interest in studying transient phenomena implies very bright sources, such as an XFEL.





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Where does MaRIE 1.0 stand?

Year old memo from NNSA provides guidance on moving MaRIE 1.0 to CD-0 in FY13.

Department of Energy
National Nuclear Security Administration
Washington, DC 20585

DEC 0 3 2012

MEMORANDUM FOR PARNEY ALBRIGHT
DIRECTOR, LAWRENCE LIVERMORE NATIONAL LABORATORY

PAUL HOMMERT
PRESIDENT AND DIRECTOR, SANDIA NATIONAL LABORATORIES

CHARLES McMILLAN
DIRECTOR, LOS ALAMOS NATIONAL LABORATORY

FROM: DONALD COOK
DEPUTY ADMINISTRATOR
FOR DEFENSE PROGRAMS

SUBJECT: Future Experimental Facilities: Decisions following the 2012 Review

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•
•

Based on these considerations, MaRIE will move to CD-0 this fiscal year *provided* that we first have the commitments and plans needed for fully realizing MaRIE's potential value. Acceptance of MaRIE for CD-0 will require a letter from the directors of Los Alamos National Laboratory (LANL) and Lawrence Livermore National Laboratory (LLNL) that describes your commitment and plan for advancing the process and science of certification to make use of MaRIE.

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MaRIE 1.0

- To achieve full facility capability, MaRIE would cost ~$2B.
- The focus of MaRIE 1.0 is to bring the Multi-Probe Diagnostic Hall (MPDH) online. The part of the MPDH that is new is a 12-GeV electron linac driving a 42-keV (0.3Å) x-ray free electron laser (X-FEL). The X-FEL is the cornerstone of MaRIE 1.0 (about $1B total).
- MaRIE is an NNSA facility. Various government issues are conspiring against us; CD-0 is likely pushed off to FY16, the Laboratory is continuing to develop the compelling CD-0 message.
- Most of the design work is on hold. We are considering changes to MaRIE requirements which may lead to a L-band SC system (the following slides describe our S-band RT baseline design).

MaRIE photon needs can be met by an X-FEL (10^{10} photons and 10^{-3} bandwidth for MaRIE 1.0 XFEL)

	MPDH	FFF		M4	
Energy/Range (keV)	50	<10 - >50	10-400	0.1-1.5	10-50
Photons per image	10^{11}	10^{11}	10^{9}	10^{9}	10^{11}
Time scale for single image	50 fs	>1 s	0.001 s	10-500 fs	50 fs
Energy Bandwidth ($\Delta E/E$)	10^{-4}	10^{-4}	10^{-3}	10^{-4}	10^{-4}
Beam divergence	1 μrad	1 μrad	< 10 μrad	< 10 μrad	1 μrad
Trans. coherence (TC) or spatial res.	TC	TC	1-100 μm	TC	TC
Single pulse # of images/duration	30/1.5 μs	-	-	-	-
Multiple pulse rep. rate/duration	120 Hz/day	0.01 Hz/mo.	60 Hz/secs	1 KHz/day	10 Hz/days
Longitudinal coherence	yes	yes	no	yes	yes
Polarization	linear	linear	no	Linear/circular	linear
Tunability in energy ($\Delta E/E$/time)	2%/pulse	fixed	fixed	10%/s	10x/day

- Photon energy - set by gr/cm^2 of sample and atomic number
- Photon number for an image - typically set by signal to noise in detector and size of detector
- Time scale for an image - fundamentally breaks down to transient phenomena, less than ps, and semi-steady state phenomena, seconds to months
- Bandwidth - set by resolution requirements in diffraction and/or imaging
- Beam divergence - set by photon number loss due to stand-off of source/detector or resolution loss in diffraction
- Source transverse size/transverse coherence - the source spot size will set the transverse spatial resolution, if transversely coherent then this limitation is not applicable so transverse coherence can be traded off with source spot size and photon number
- Number of images/rep rate/duration – images needed for single shot experiments/image rep rate/ duration of experiment on sample
- Repetition rate - how often full images are required
- Longitudinal coherence – 3D imaging
- Polarization - required for some measurements
- Tunability – time required to change the photon energy a fixed percentage

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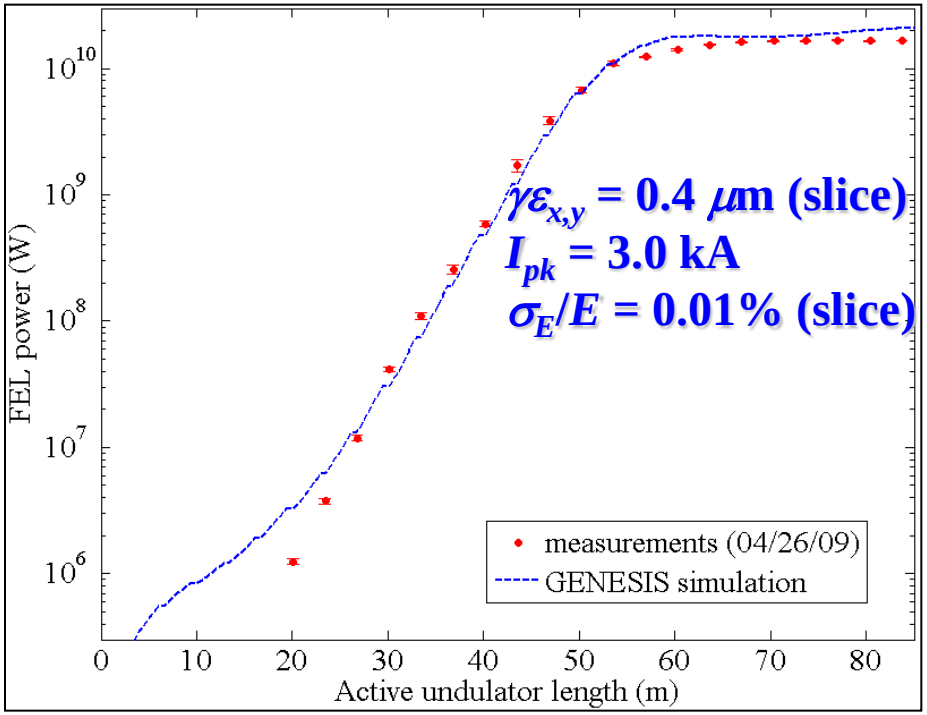
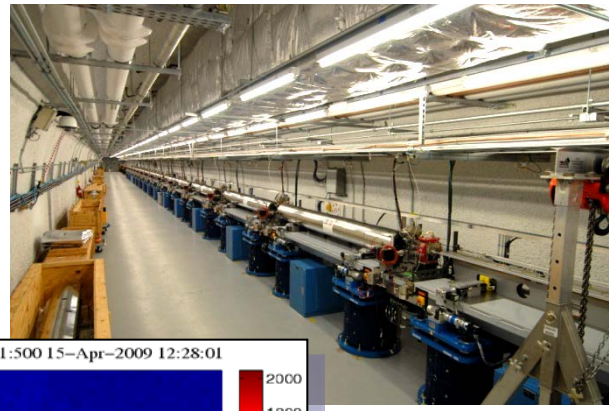
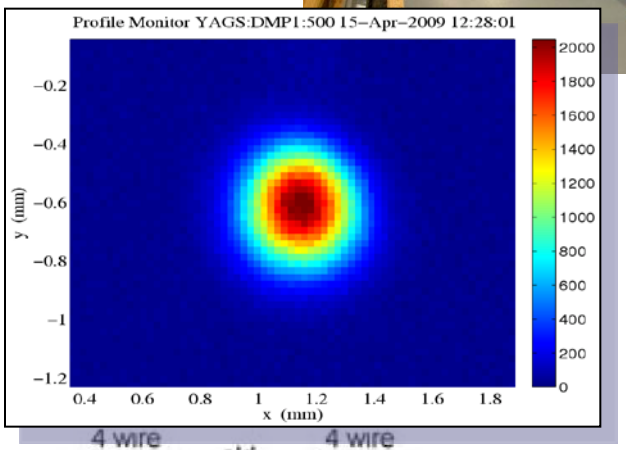
MaRIE 1.0 requirements

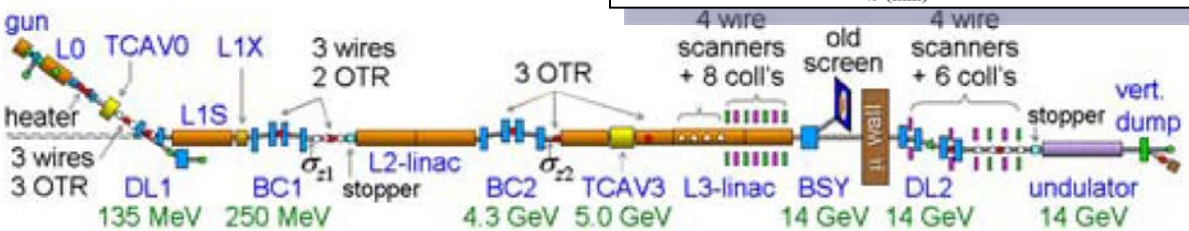
- 10^{-4} bandwidth
- 2 10^{10} 42 keV X-rays (no requirement at 126 keV) (impact: emittance 0.1 μm, energy spread 0.015% for 100 pC electron bunches)
- 100-pC bunches interleaved with 2-nC bunches for electron radiography
- 10-μsec RF pulse window
- Up to 30 100-pC bunches in the RF pulse
- Minimum X-ray spacing is ~ 400 psec; can split the X-rays so minimum electron bunch spacing is ~ 800 psec (L-band)
- **Want strong short-range wakes and weak long-range wakes**

The MaRIE X-FEL is motivated by the success of the LCLS 0.8 to 8 keV X-FEL









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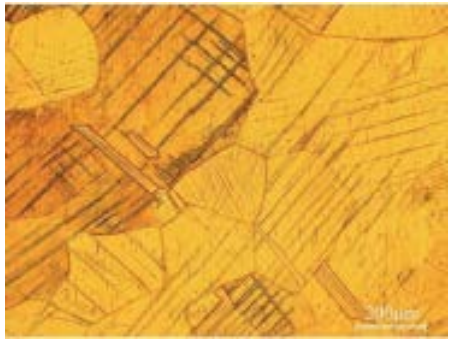
The MaRIE X-FEL requires tiny emittances

Beam energy is typically chosen because of two constraints:

$$\frac{\varepsilon_{beam}}{\gamma} = \varepsilon_{lab} \leq \frac{\lambda_{x-ray}}{4} = \frac{\lambda_{wiggler}}{8\gamma^2}\left(K^2+1\right)$$



The choice for beam energy (γ) is dominated by the beam emittance, not wiggler period (which can go down to 1 cm)

Energy diffusion limits how high the beam energy can be (~ 20 GeV); to reduce cost we're pushing the beam energy lower to 12 GeV. The overlap constraint puts a very extreme condition on the beam emittance (ideally ~ 0.1 μm at 12 GeV).

$$\left\langle \frac{d}{dz}\left(\delta\mathcal{E}\right)_{QF}^2 \right\rangle = \frac{55 e\hbar\gamma^4 r_e^2 B_w^3}{24\sqrt{3} m_e c}$$

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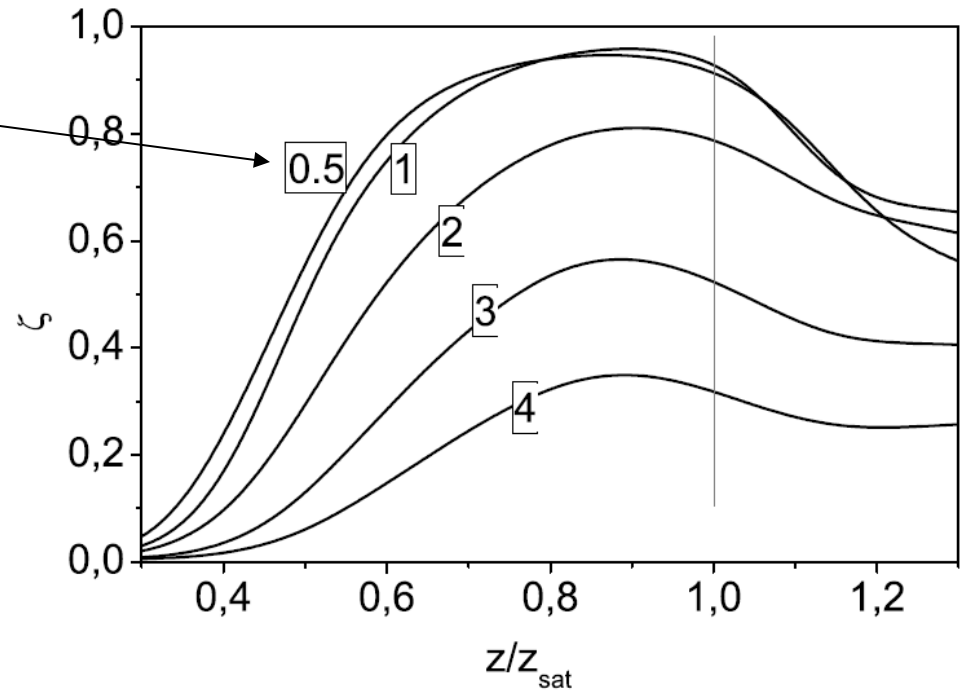
Transverse coherency also requires tiny emittances

$$\hat{\varepsilon} = 2\pi\varepsilon_n / \gamma\lambda_{X-ray}$$

$$\zeta = \frac{\iint |\Gamma(r_\perp r'_\perp)|^2 \langle I(r_\perp) I(r'_\perp)\rangle dr_\perp dr'_\perp}{\left[\int \langle I(r_\perp)\rangle dr_\perp\right]^2}$$



An emittance of 0.1 μm is an emittance ratio of about 1 for the figure above (at 12 GeV). MaRIE 1.0 XFEL baseline emittance (0.2 μm) leads to a transverse coherency of about 0.8.

The MaRIE X-FEL is an aggressive extrapolation of LCLS parameters

	UNIT	LCLS	MARIE 1.0 baseline
Wavelength	Å	1.5	0.293
Beam energy	GeV	14.35	12.0
Bunch charge	pC	250*	100
Pulse length (FWHM)	fs	80*	30
Peak current	kA	3.0*	3.4
Normalized rms emittance	mm-mrad	0.3-0.4	0.2
Energy spread	%	0.01	0.01
Undulator period	cm	3	1.86
Peak magnetic field	T	1.25	0.70
Undulator parameter, a_w		2.48	0.86
Gain length, 1D (3D)	m	(3.3)*	(6.0)
Saturation length	m	65	80
Peak power at fundamental	GW	30*	8
Pulse energy	mJ	2.5*	0.24
# of photons at fundamental		2×10^{12}*	2×10^{10}

Y. Ding, HBEB, 11/09

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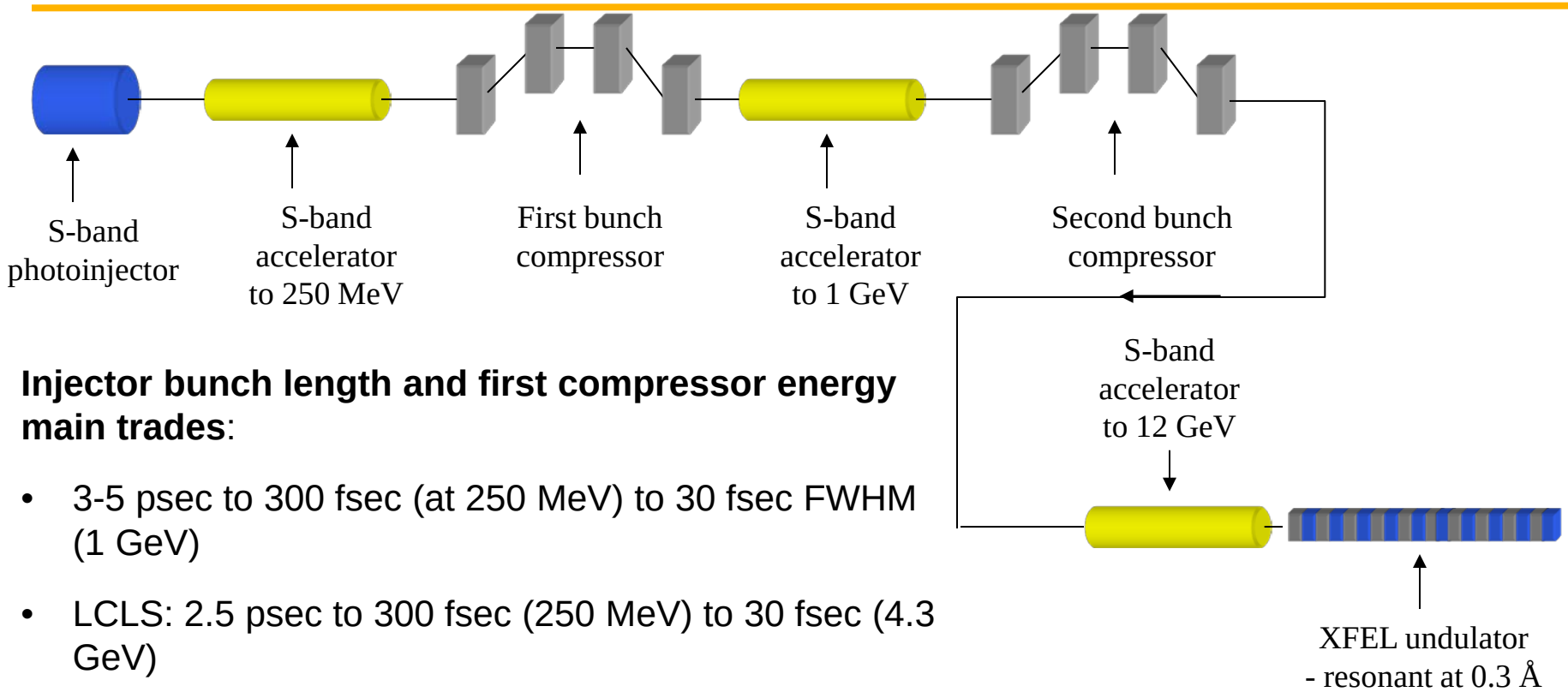
The baseline MaRIE X-FEL is LCLS inspired



Injector bunch length and first compressor energy main trades:

- 3-5 psec to 300 fsec (at 250 MeV) to 30 fsec FWHM (1 GeV)
- LCLS: 2.5 psec to 300 fsec (250 MeV) to 30 fsec (4.3 GeV)

1 GeV comes from our CSR and ISR studies

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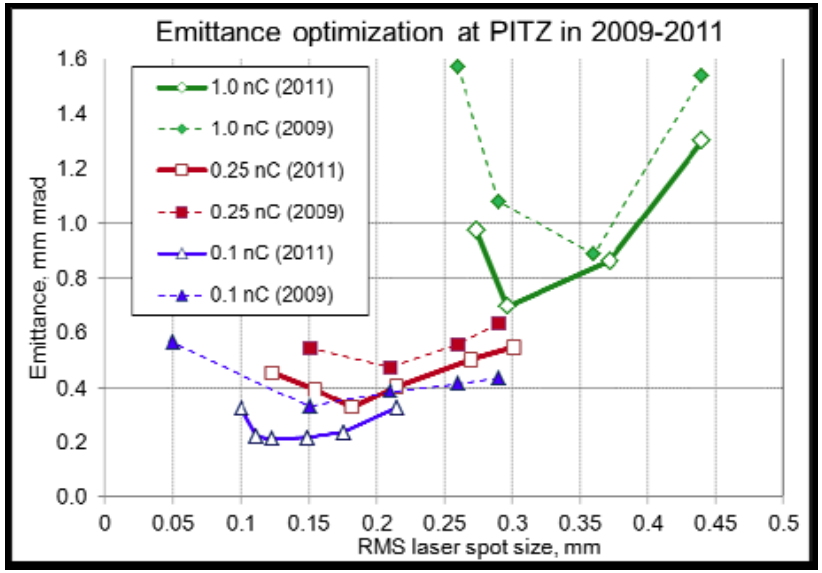
Where does the design stand now?

- We have a preliminary injector design to 250 MeV.
- We have a preliminary design for bunch compressors 1 and 2.
- We have a preliminary start-to-end simulation of the accelerator to 12 GeV.
- We have a preliminary design of the undulator and simulations of the X-FEL performance.

The photoinjector is a scaled version of the PITZ injector (Russell)

Emittance requirements demonstrated at PITZ, DESY.

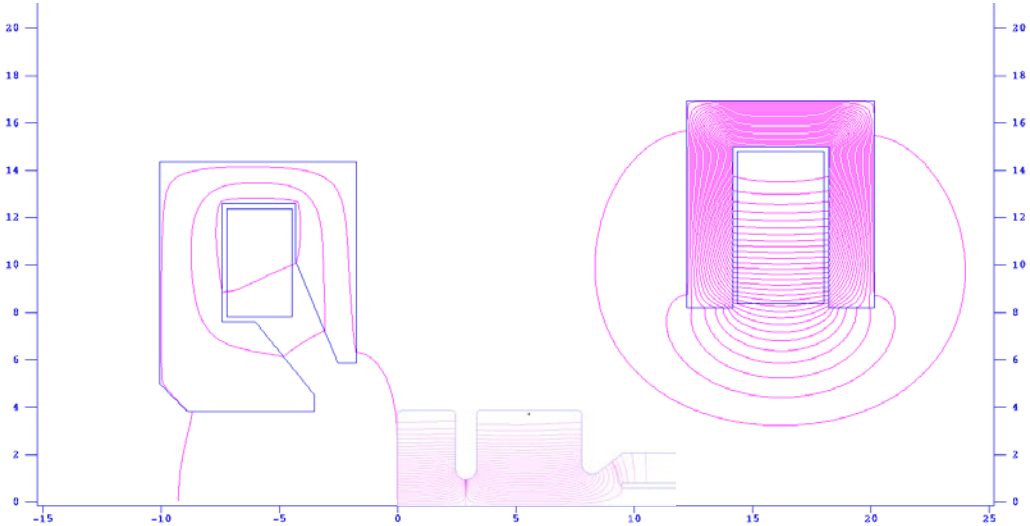


M. Krasilnikov, et. al., ***Experimentally minimized beam emittance from an L-band photoinjector***, *Phys. Rev. STAB*, **15,**, p. 100701 (2012).

We scaled the PITZ design, optimized for 1 nC, to 2856 MHz and 0.1 nC:

J. Rosenzweig and E. Colby, ***Charge and Wavelength Scaling of RF Photoinjectors: A Design Tool***, *Proceedings of the 1995 Particle Accelerator Conference,* p. 957.

We achieved a 0.12 μm simulated normalized RMS



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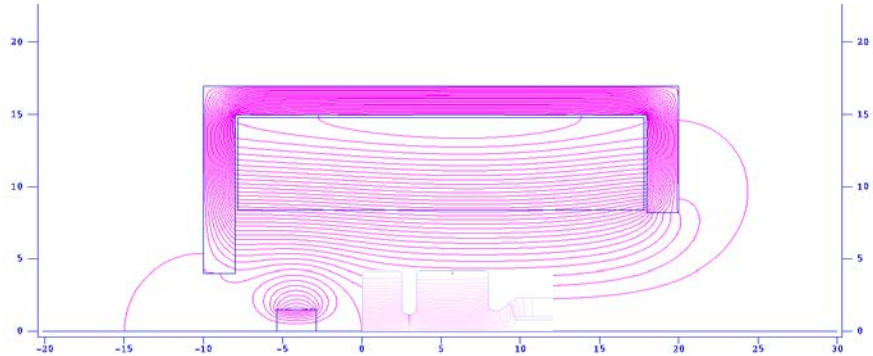
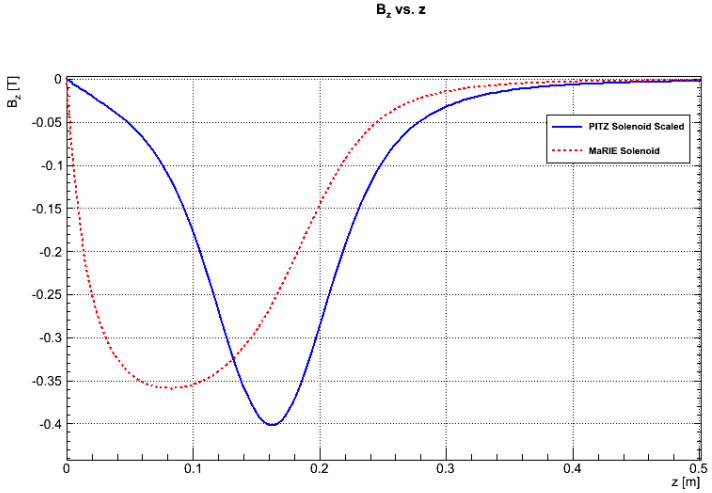
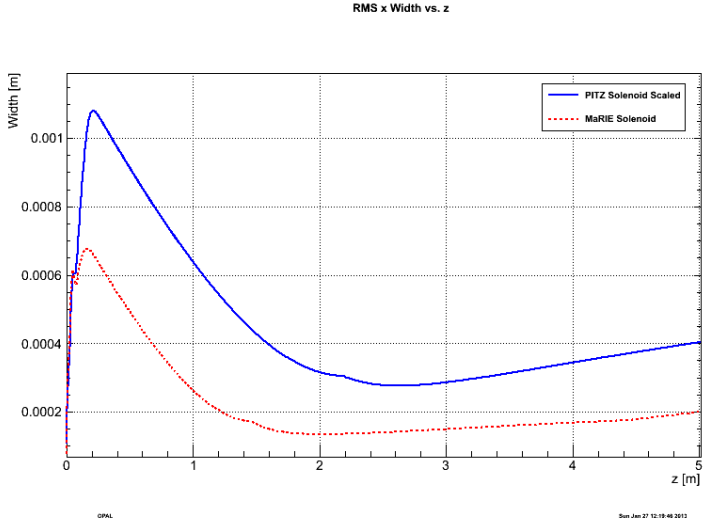
With a redesign of the photoinjector solenoid, we achieved even lower emittances





By using a permanent magnet as our bucking solenoid, we can ramp up the magnetic field more rapidly. In turn, the beam envelope stays smaller through the injector.



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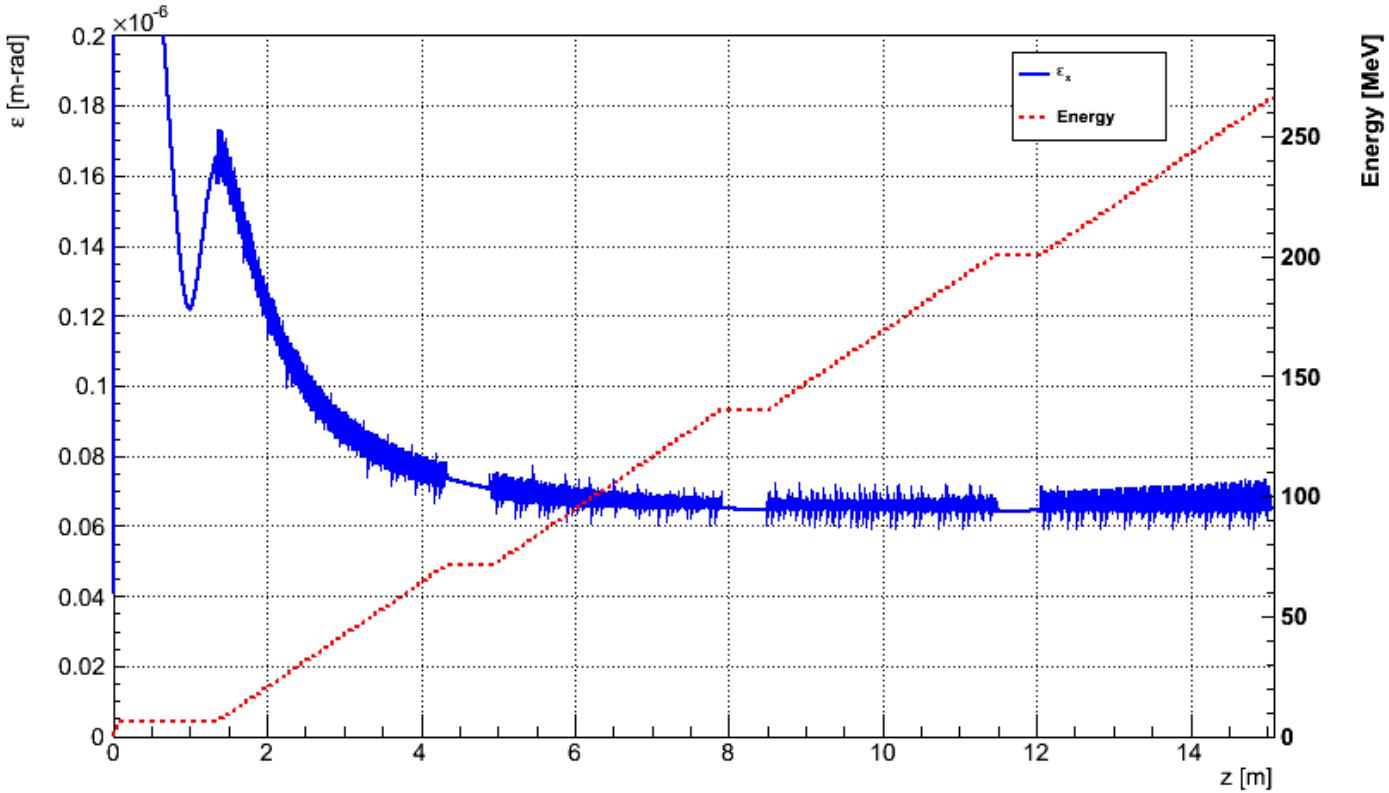
With a redesign of the photoinjector solenoid, we achieved even lower emittances

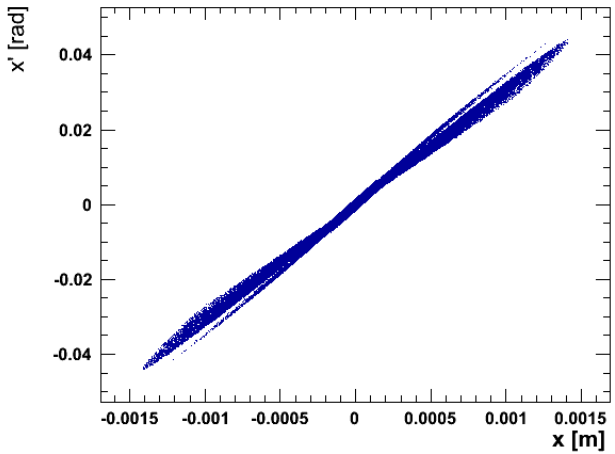
Normalized Emittance and Energy vs. z (OPAL*)



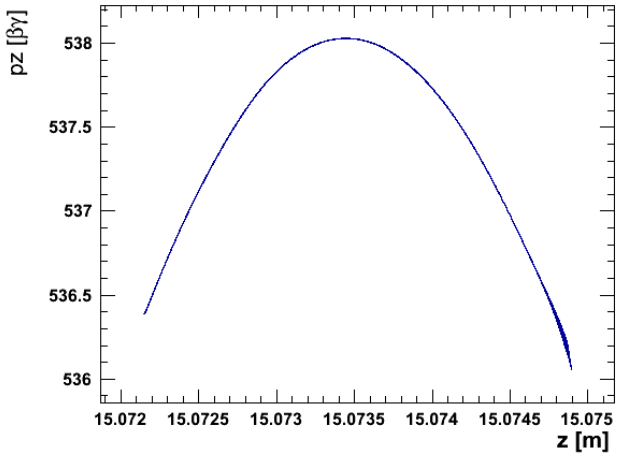
*A. Adelmann, et. al., ***The Opal (Object oriented Parallel Accelerator Library) Framework***, Paul Scherrer Institut, PSI-PR-08-02.

Current injector beam properties at ~250 MeV

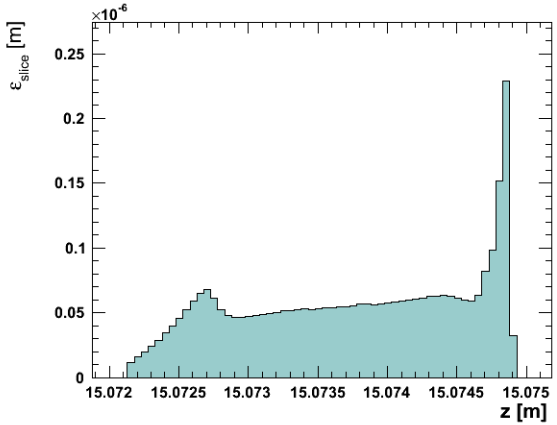
Transverse Phase Space



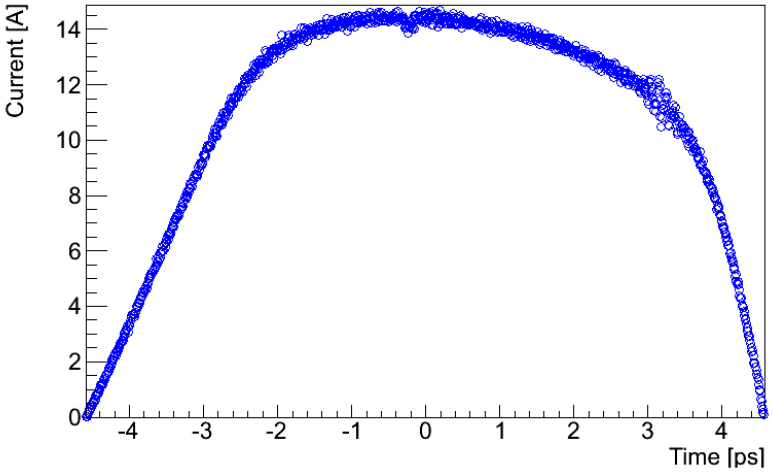
Longitudinal Phase Space



Transverse Slice Emittance



Beam Current



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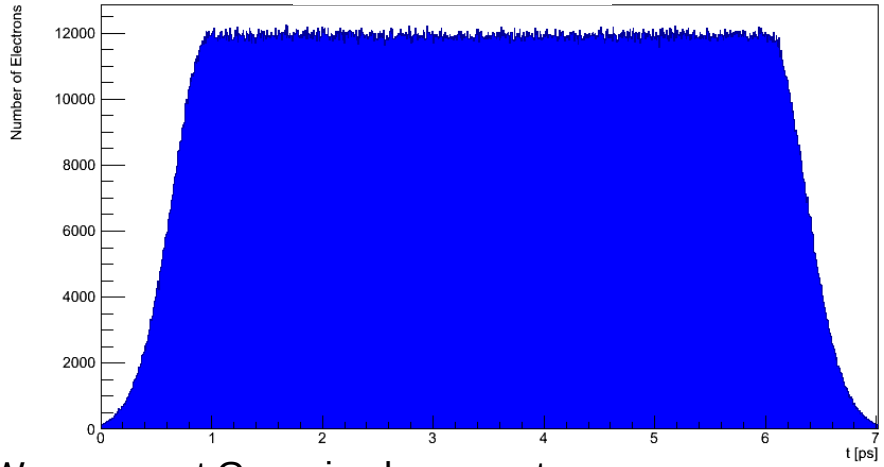
Initial beam/laser distribution and final beam parameters from injector

Initial Laser Spot Properties

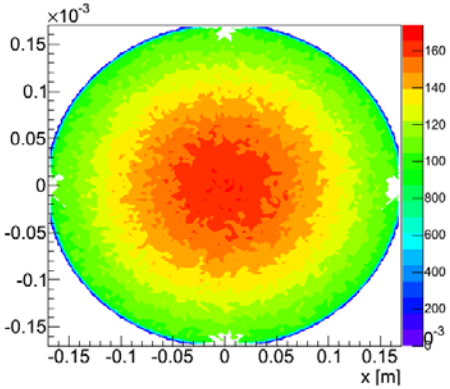
Time Profile



We use a cut Gaussian laser spot:

$\sigma_r = 0.17$ mm
$r_{max} = 0.17$ mm

Cut Gaussian Laser Spot



F. Zhou et. al., ***Impact of the spatial laser distribution on photocathode gun operation***, *Phys. Rev. STAB*, **15**, p. 090701 (2012)

Final Electron Beam Properties at ~250 MeV

Property	Value
Transverse ε_n	65 nm
Thermal ε_n (atomically clean copper*)	44 nm
Residual ε_n	48 nm
RMS Length	2.1 ps
RMS Energy Spread	0.08%

*D. H. Dowell and J. F. Schmerge, ***Quantum efficiency and thermal emittance of metal photocathodes***, *Phys. Rev. STAB*, **12**, p. 0764201 (2009).

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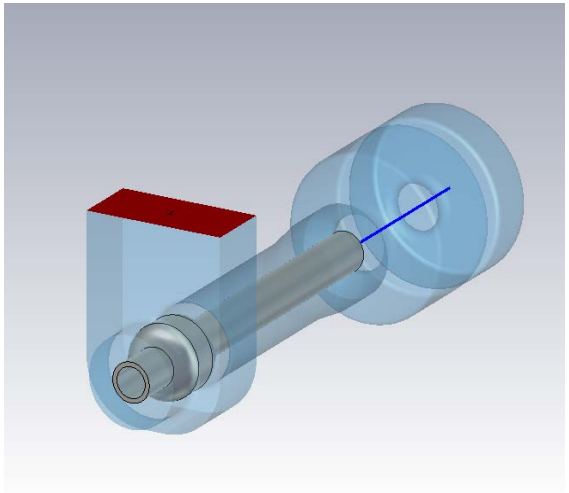
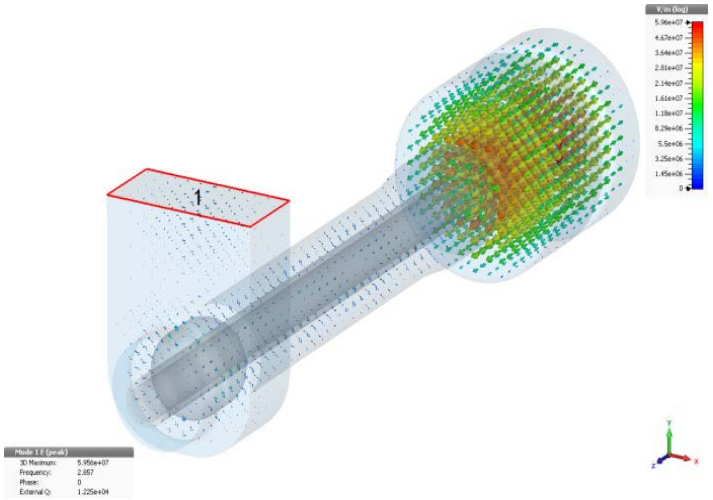
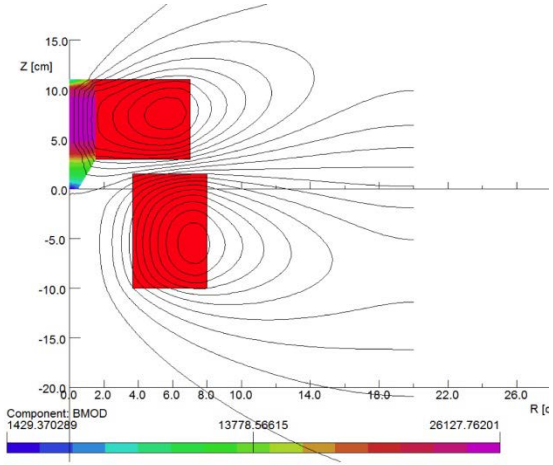
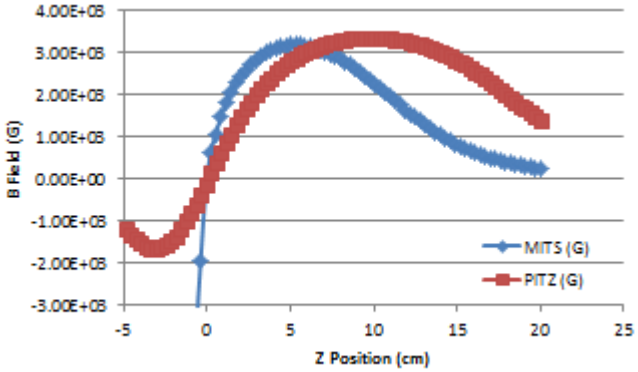
We have started the RF photoinjector design and are developing a realistic bucking coil design









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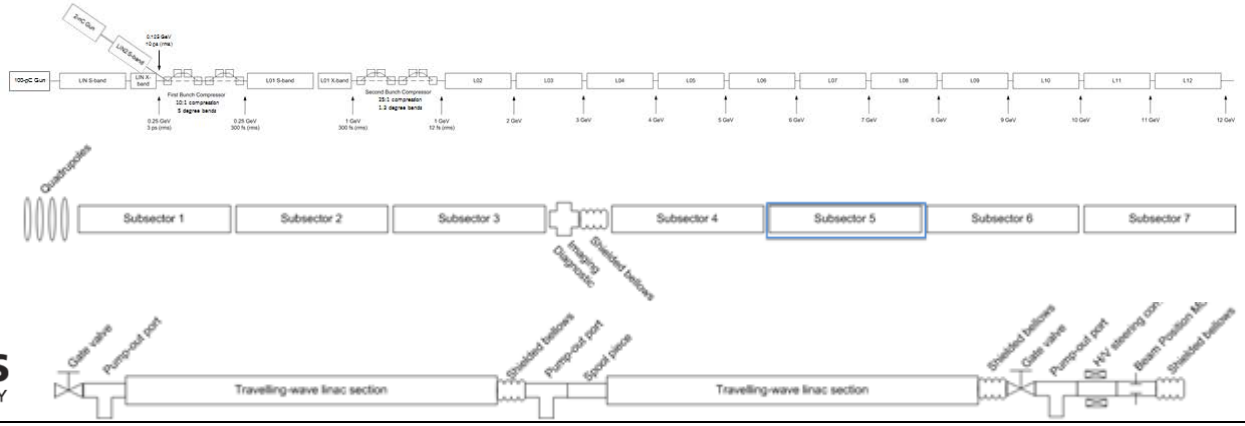
We have an initial start-to-end (S2E) simulation to 12 GeV (John Lewellen)

Section	Energy (MeV)	RMS Bunch Length (fs)	Primary Code
Injector	0 ➔ 250	~2400	OPAL
BC1	250	2400 ➔ 300	Elegant/OPAL
L01	250 ➔ 1000	300	Elegant
BC2	1000	300 ➔12	Elegant
L02 – L12	1000 ➔12,000	12	Elegant



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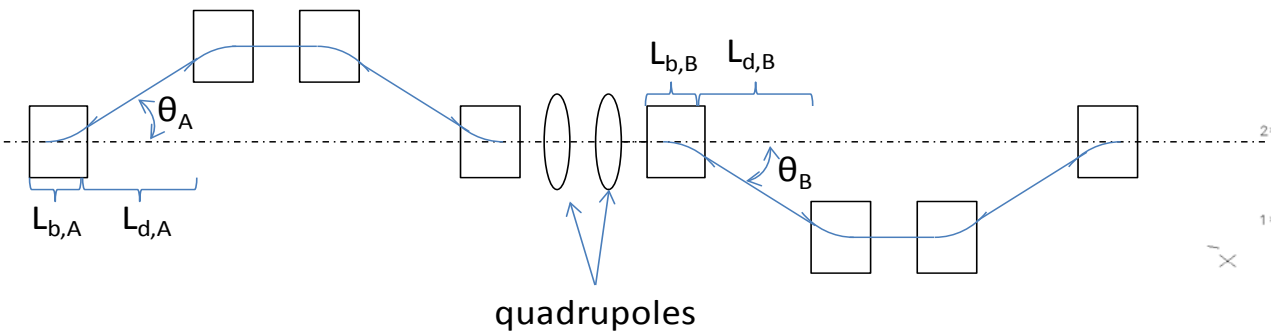
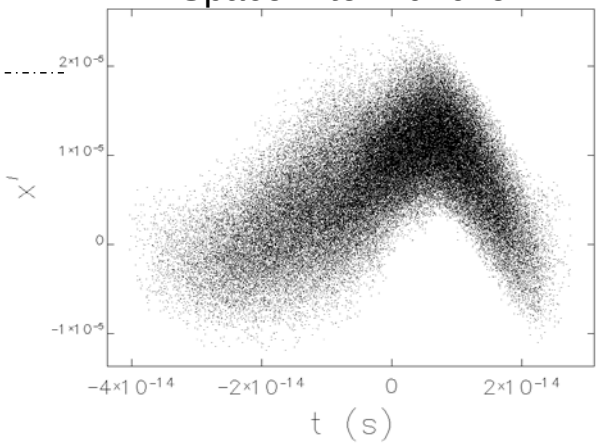
Novel chicane-based BC2 design (John Lewellen)



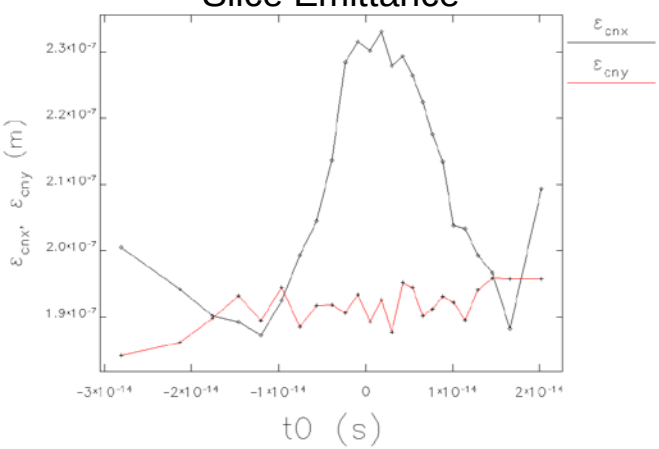
Bend Plane Phase Space After Buncher



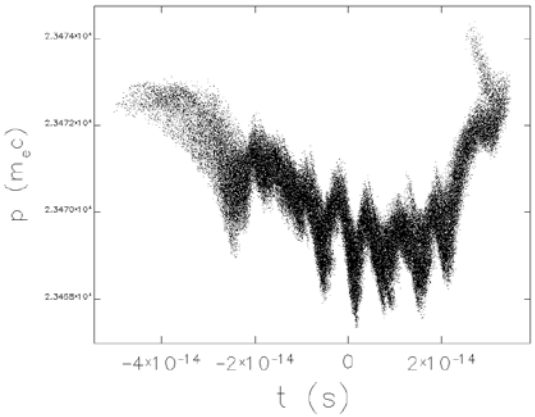
Double chicane is used to reduce CSR effects (5.8:1 and 4.3:1 for a total of 25:1 compression, or 300 fs to 12 fs)

- Initial emittances: 0.2 μm (100 pC)
- Final bend plane emittance: 0.56 μm RMS, 0.23 μm slice

Slice Emittance



Some micro-bunching out of BC2 portends issue when using actual injector distribution instead of smooth ellipse . *(A laser heater will turn off the XFEL, so LCLS solution will not work for us.)*



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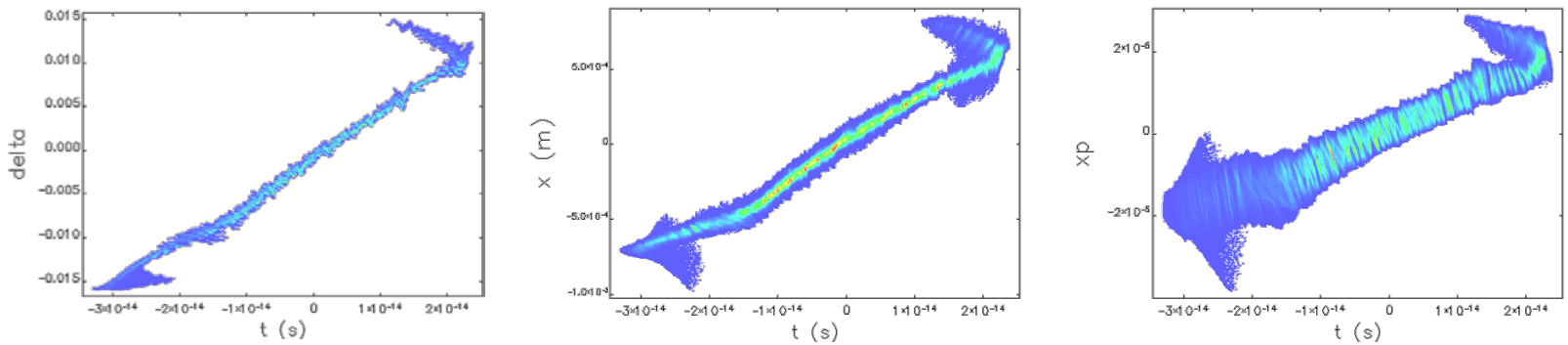
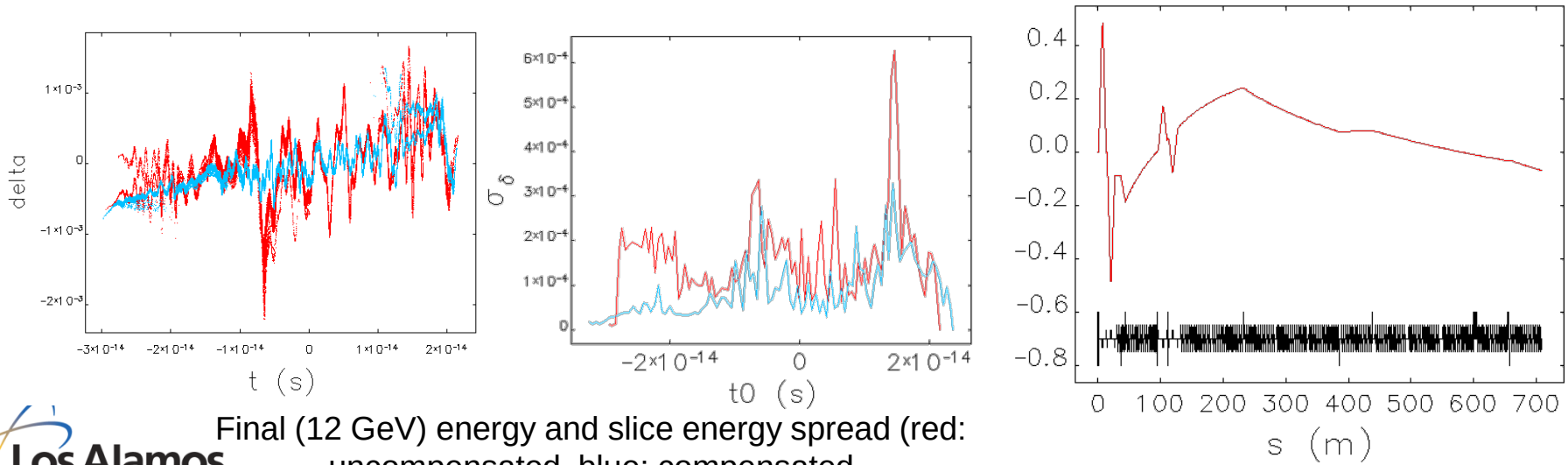
We use residual dispersion to suppress MBI (Ji); slice emittance is about 0.1 μm at the undulator



Energy, horizontal position and horizontal divergence after BC2

Use large energy slew and low R56 to help suppress MBI



Final (12 GeV) energy and slice energy spread (red: uncompensated, blue: compensated

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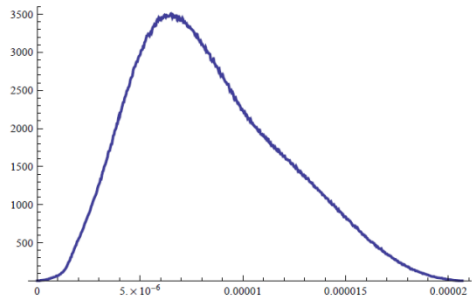
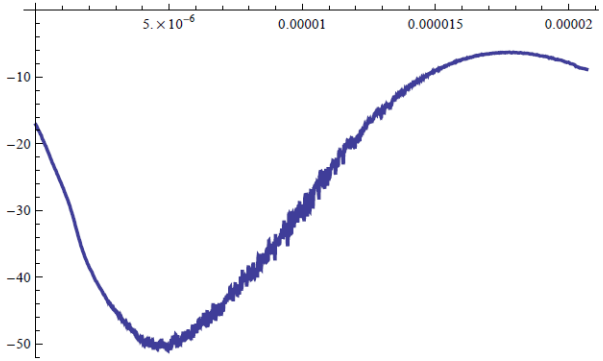
GENESIS simulations using the beam from our S2E results include undulator resistive wall wake (Q. Marksteiner, P. Anisimov)

SASE start to finish simulations: undulator without gaps, 80 wavelength per slice; 20μm window for current bunch in IDL; tapered to compensate energy loss due to wake fields

- **Current in the bunch I(A) vs Z_1(m) is**



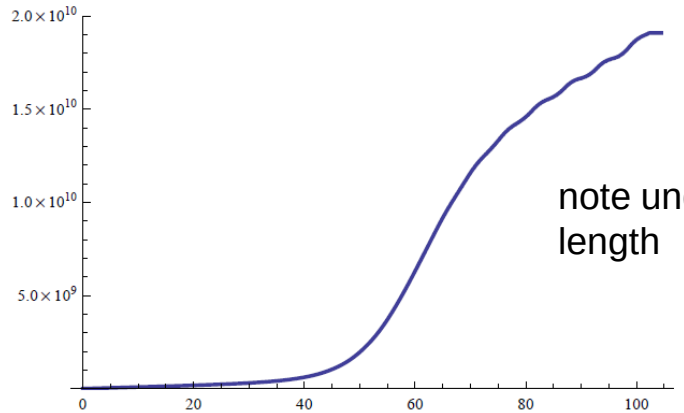
- **Energy distribution in the bunch vs Z_1(m) along the bunch**



It demonstrate effect of the wake field. Generation takes place in the hairy part

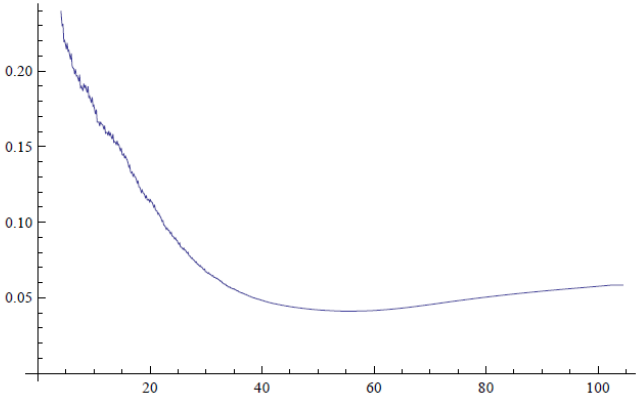
This corresponds to $n_{ph} = 1.91\times10^{10}$ photons at $\lambda = 2.93\times10^{-11}\ m$

- **Photon number has the following dependence alnog the undulator n_{ps} vs Z(m)**



note undulator length

- **Bandwidth dependence is vs Z(m)**



It correspond to 4.2×10^{-4} relative RMS badwidth at 50m point.

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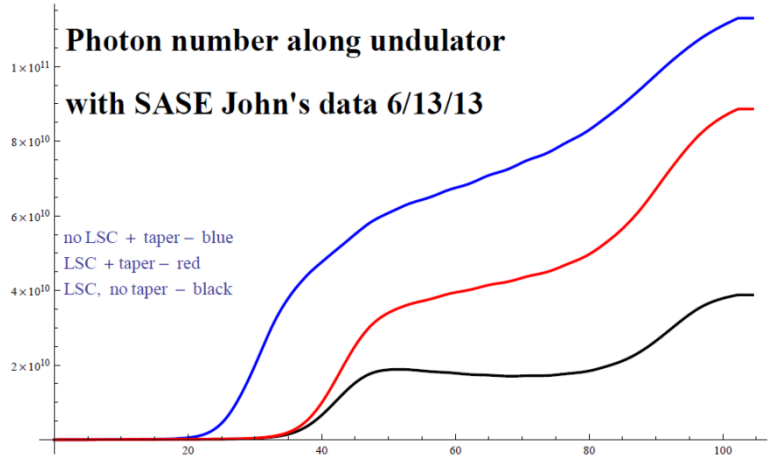
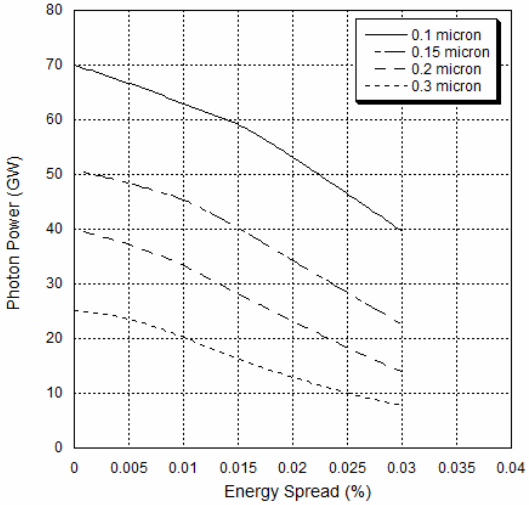
Genesis simulations using the beam from our S2E results shows we get over 2 x 10^{10} photons (Q. Marksteiner, P. Anisimov)





Comparison between 3-D and slice GENESIS simulations. 60 GW (0.1 μm and 0.015% energy spread) is 1.5 10^{11} X-rays for a 100 pC bunch; with undulator resistive wall wake and other real effects we predict about 4 10^{10} X-rays (factor of 2 > requirement)

We have worked on an alternative eSASE scheme where we bunch the beam with a 1 μm wavelength.

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Our S2E simulations are still pretty rough

- Need to move beamline simulations from ELEGANT to OPAL (beam is always in the space-charge dominated regime).
- We still need to develop a realistic photoinjector design and use it for S2E modeling.
- We need to meet the bandwidth requirement.
- There is a lot of physics still to add, including transverse wakes, misalignments, tolerances, etc.
- We need to consider 3rd harmonic 6 GeV design with iSASE and tapering to regain 42 keV photon flux.
- We need to compare baseline to eSASE scheme.