Introduction to breakout session B1 (hard X-ray beamlines)

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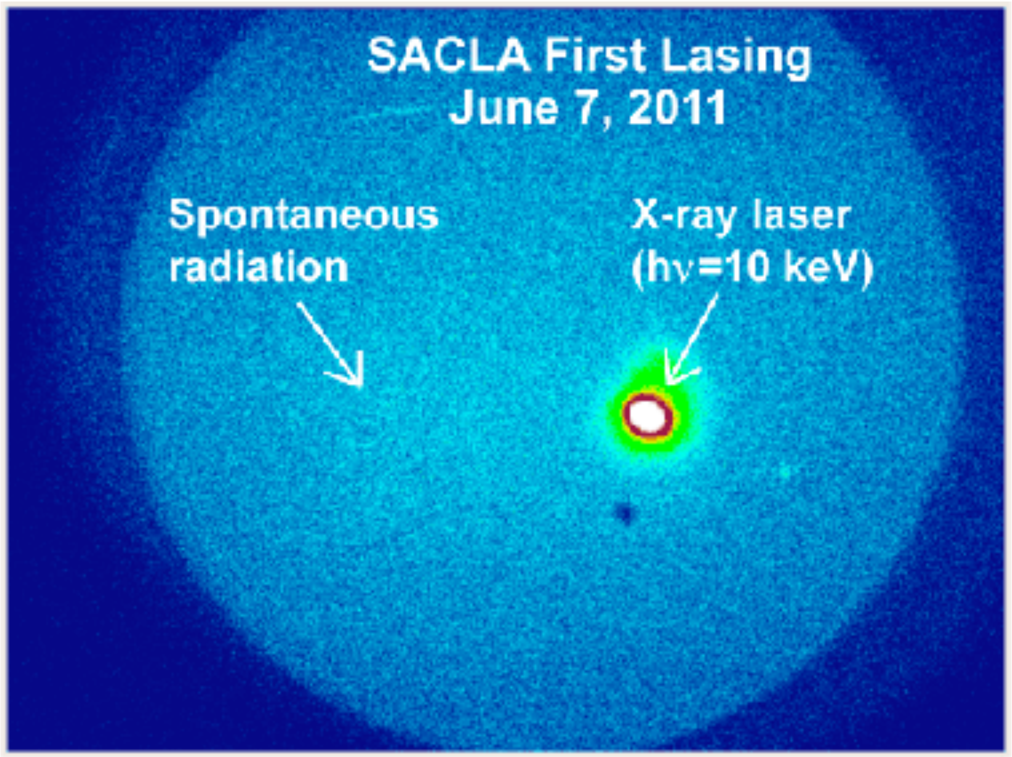
This year: 10-year anniversary of hard XFELs at SACLA

Birth of the first hard X-ray laser
at SACLA (June 7, 2011)




LETTERS
PUBLISHED ONLINE: 24 JUNE 2012 | DOI: 10.1038/NPHOTON.2012.141
nature photonics

A compact X-ray free-electron laser emitting in the sub-ångström region

Hitoshi Tanaka and Makina Yabashi *et al.**

# of citation > 1400

Thanks for your continuous support!!

It is truly disappointing that we can not celebrate this memorial year in person, but…

First user experiment (March 7, 2012)

Prof. Shen's group of Okayama U.

Next year is also a memorial year

2022: 10-year anniversary of *user operation*

SACLA performance exceeded our expectations

Technical design report (Feb., 2010)

Target values:

Wavelength (nm) ※4	0.13
Photon energy (keV)	9.9
Bandwidth	9.2e-4
Source size (um, rms)	33
Angular divergence (urad, rms)	0.73
Peak power (GW)	29
Pulse energy (mJ)	0.78
Photons per pulse (phs/pls)	5.0e11
Pulse width (fs, FWHM)	30

(http://xfel.riken.jp/eng/pdf/XFEL_BL-TDRver1.05.pdf)

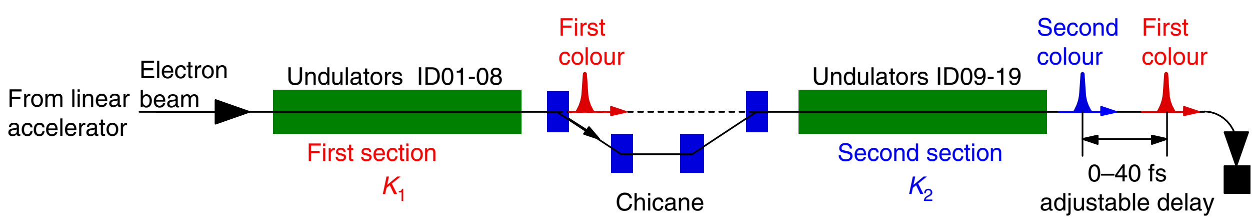
Routinely achieved!!

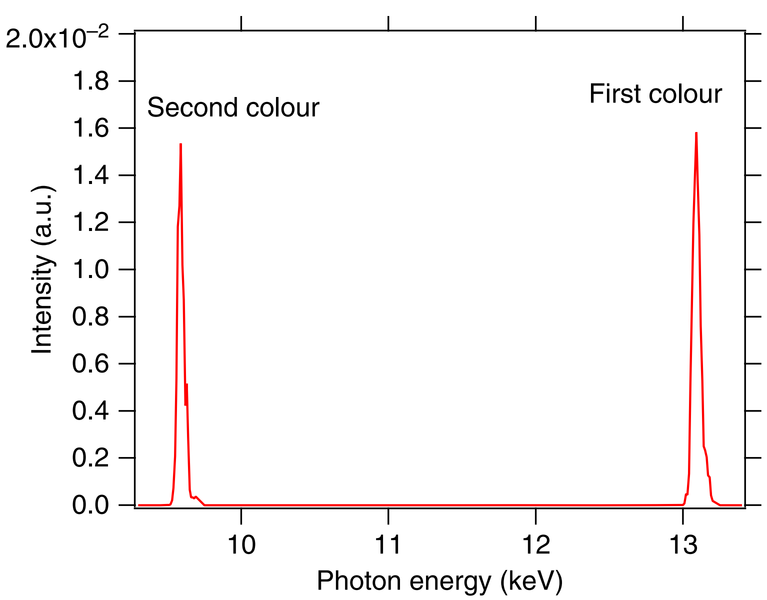
Typical pulse duration: ~6 fs

Peak brilliance is 5 times greater than the expected value!!

New capabilities we did not imagine in the designing phase

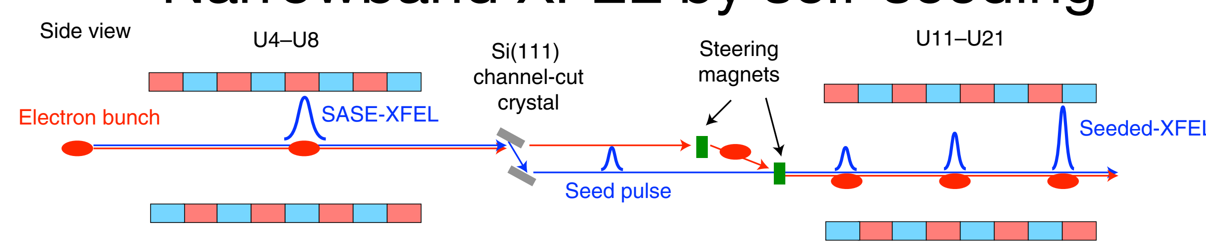
2-color FEL by splitting undulator

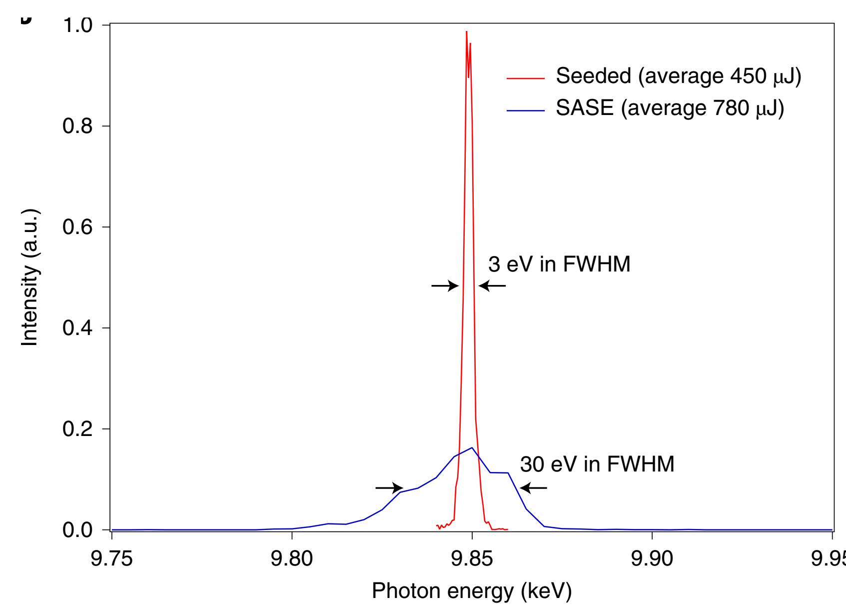


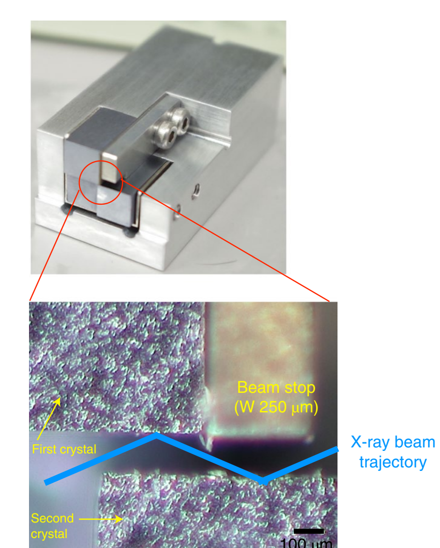


T. Hara *et al.*, *Nature Commun*. 4, 2919 (2013).

Narrowband XFEL by self-seeding







I. Inoue *et al*., *Nature Photon*. 13, 319 (2019).

Early results (within 3 years after the start of user operation)

Damage-free PX

-> Talk by Prof. Iwata (Kyoto U) on Mar. 11

Determination of damage-free crystal structure of an X-ray–sensitive protein using an XFEL

Kunio Hirata[1,2,9], Kyoko Shinzawa-Itoh[3,9], Naomine Yano[2,3], Shuhei Takemura[3], Koji Kato[3,8], Miki Hatanaka[3], Kazumasa Muramoto[3], Takako Kawahara[3], Tomitake Tsukihara[2–4], Eiki Yamashita[4], Kensuke Tono[5], Go Ueno[1], Takaaki Hikima[1], Hironori Murakami[1], Yuichi Inubushi[1], Makina Yabashi[1], Tetsuya Ishikawa[1], Masaki Yamamoto[1], Takashi Ogura[6], Hiroshi Sugimoto[1], Jian-Ren Shen[7], Shinya Yoshikawa[3] & Hideo Ago[1]

Grease matrix as a versatile carrier of proteins for serial crystallography

Michihiro Sugahara[1], Eiichi Mizohata[2], Eriko Nango[1], Mamoru Suzuki[1,3], Tomoyuki Tanaka[1], Tetsuya Masuda[1,4], Rie Tanaka[1], Tatsuro Shimamura[5], Yoshiki Tanaka[5], Chiyo Suno[5], Kentaro Ihara[5], Dongqing Pan[6], Keisuke Kakinouchi[7], Shigeru Sugiyama[7], Michio Murata[7], Tsuyoshi Inoue[2], Kensuke Tono[8], Changyong Song[1], Jaehyun Park[1], Takashi Kameshima[8], Takaki Hatsui[1], Yasumasa Joti[8], Makina Yabashi[1] & So Iwata[1,5]

K. Hirata, *Nat. Methods* 11, 734 (2014).
M. Sugahara, *Nat. Methods 12, 61* (2015).

LETTER

doi:10.1038/nature13991

Native structure of photosystem II at 1.95 Å resolution viewed by femtosecond X-ray pulses

Michihiro Suga[1]*, Fusamichi Akita[1]*, Kunio Hirata[2,3], Go Ueno[2], Hironori Murakami[2], Yoshiki Nakajima[1], Tetsuya Shimizu[1], Keitaro Yamashita[2], Masaki Yamamoto[2], Hideo Ago[2] & Jian-Ren Shen[1]

Ultrafast pump-probe

-> Talk by Prof. Ihee (KAIST) on Mar. 11

LETTER

doi:10.1038/nature14163

Direct observation of bond formation in solution with femtosecond X-ray scattering

Kyung Hwan Kim[1,2]*, Jong Goo Kim[1,2]*, Shunsuke Nozawa[3]*, Tokushi Sato[3]†*, Key Young Oang[1,2], Tae Wu Kim[1,2], Hosung Ki[1,2], Junbeom Jo[1,2], Sungjun Park[1,2], Changyong Song[4], Takahiro Sato[4]†, Kanade Ogawa[4]†, Tadashi Togashi[5], Kensuke Tono[5], Makina Yabashi[4], Tetsuya Ishikawa[4], Joonghan Kim[6], Ryong Ryoo[1,2], Jeongho Kim[7], Hyotcherl Ihee[1,2] & Shin-ichi Adachi[3,8]

Nonlinear X-ray interactions with matter

LETTER

doi:10.1038/nature14894

Atomic inner-shell laser at 1.5-ångström wavelength pumped by an X-ray free-electron laser

Hitoki Yoneda[1,2], Yuichi Inubushi[2,3], Kazunori Nagamine[1], Yurina Michine[1], Haruhiko Ohashi[2,3], Hirokatsu Yumoto[3], Kazuto Yamauchi[2,4], Hidekazu Mimura[2,5], Hikaru Kitamura[6], Tetsuo Katayama[3], Tetsuya Ishikawa[2] & Makina Yabashi[2]

nature photonics | LETTERS
PUBLISHED ONLINE: 16 FEBRUARY 2014 | DOI: 10.1038/NPHOTON.2014.10

X-ray two-photon absorption competing against single and sequential multiphoton processes

Kenji Tamasaku[1]*, Eiji Shigemasa[2], Yuichi Inubushi[1], Tetsuo Katayama[3], Kei Sawada[1], Hirokatsu Yumoto[3], Haruhiko Ohashi[3], Hidekazu Mimura[4], Makina Yabashi[1], Kazuto Yamauchi[5,6] and Tetsuya Ishikawa[1]

Received 5 Apr 2014 | Accepted 27 Aug 2014 | Published 1 Oct 2014 DOI: 10.1038/ncomms6080

Saturable absorption of intense hard X-rays in iron

Hitoki Yoneda[1,2], Yuichi Inubushi[2,3], Makina Yabashi[2], Tetsuo Katayama[2,3], Tetsuya Ishikawa[2], Haruhiko Ohashi[2,3], Hirokatsu Yumoto[3], Kazuto Yamauchi[2,4], Hidekazu Mimura[2,5] & Hikaru Kitamura[6]

163901 (2014) PHYSICAL REVIEW LETTERS

X-Ray Second Harmonic Generation

S. Shwartz,[1,2,*] M. Fuchs,[3,4] J. B. Hastings,[5] Y. Inubushi,[6] T. Ishikawa,[6] T. Katayama,[7] D. A. Reis, T. Sato,[6] K. Tono,[7] M. Yabashi,[6] S. Yudovich,[1] and S. E. Harris[2]

L 111, 043001 (2013) PHYSICAL REVIEW LETTERS week ending 26 JULY 2013

Double Core-Hole Creation by Sequential Attosecond Photoionization

Kenji Tamasaku,[1,*] Mitsuru Nagasono,[1,†] Hiroshi Iwayama,[2] Eiji Shigemasa,[2] Yuichi Inubushi,[1] Takashi Tanaka,[1] Kensuke Tono,[3] Tadashi Togashi,[3] Takahiro Sato,[1] Tetsuo Katayama,[3] Takashi Kameshima,[3] Takaki Hatsui,[1] Makina Yabashi,[1] and Tetsuya Ishikawa[1]

110, 173005 (2013) PHYSICAL REVIEW LETTERS week ending 26 APRIL

Deep Inner-Shell Multiphoton Ionization by Intense X-Ray Free-Electron Laser Pulses

H. Fukuzawa,[1,2] S.-K. Son,[3] K. Motomura,[1] S. Mondal,[1] K. Nagaya,[2,4] S. Wada,[2,5] X.-J. Liu,[6] R. Feifel,[7] T. Tachibana,[1] Y. Ito,[1] M. Kimura,[1] T. Sakai,[4] K. Matsunami,[4] H. Hayashita,[5] J. Kajikawa,[5] P. Johnsson,[8] M. Siano,[9] E. Kukk,[10] B. Rudek,[11,12] B. Erk,[11,12] L. Foucar,[11,13] E. Robert,[6] C. Miron,[6] K. Tono,[14] Y. Inubushi,[2] T. Hatsui,[2] M. Yabashi,[2] M. Yao,[4] R. Santra,[3,15,*] and K. Ueda[1,2,†]

50 papers/year -> 1 paper / 1 experiment !!

Similar to early days of X-ray crystallography ??

> *"It was a wonderful time. Like discovering a new goldfield where nuggets could be picked up on the ground, with thrilling new results every week".*

by W. L. Bragg

XFELs are becoming popular tools like synchrotron X-ray sources

- XFEL experiments are gradually maturing.

  e.g. some kinds of experiments are standardized (SFX, pump-probe).

- Currently, most researchers are trying to reveal unexplored information about the samples, rather than carry out the principle-of-proof experiments.

➡ Improving qualities of XFELs should be a key for maximizing scientific outputs

Now that SACLA team is almost done with initial R&D for the machine and standardization of experimental set-up.

It's a good timing to discuss about what direction we should go for next 10 years.

Photon parameters compared to other XFEL facilities

	Photon energy (fundamental)	Pulse energy	Duration (FWHM)	Rep. rate	Unique modes
SACLA	4-22 keV	up to 1 mJ	~6 fs (fixed)	BL2+BL3: 60 Hz in total	•Two-color •Self-seeding
LCLS	0.25-12.8 keV (up to 25 keV@ LCLS-II HE)	~4 mJ for 30 … (proportional to pulse duration)	Variable (nominally … fs)	120 Hz (1 MHz @LCLS-II HE)	•Two-color •Self-seeding •Attosecond
European XFEL	5-24 keV	0.5-4 mJ	20-60 fs	2.7 kHz (4.5 MHz for intra-train)	Under commissioning (two-color, self-seed)
PAUL SCHERRER INSTITUT PSI	2-12 keV	~0.5 mJ for 120 fs pulse (proportional to pulse duration)	Variable (nominally, 120 fs)	100 Hz	•Two-color •Large bandwidth •Attosecond
PAL POHANG ACCELERATOR LABORATORY	2-15 keV	~1 mJ	•Variable (10-40 fs)	60 Hz	•Two-color •Self-seeding

•Enhance strong points?
•Overcome weak points?

Moving SACLA forward: short- and long-term development plans

Short-term (2021~2023)

Maximize performance of *existing machine*

Software development

-> This talk

•Machine learning-based accelerator tuning

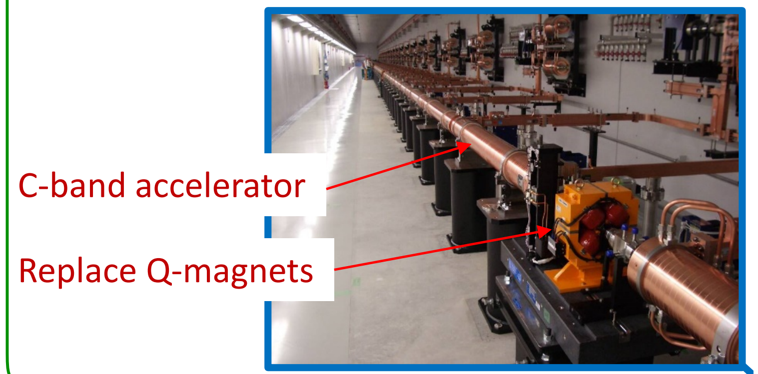
Long-term (5-10 years from now)

Upgrade machine to make breakthroughes in photon qualities

Hardware (accelerator) development

-> presented by Takahiro

•Pulsed quadrupole(Q) magnets



"Completely decoupling BL2 and BL3 operations"

Candidates/ideas for future upgrades

•New electron gun (pulse energy↑)
•THz acceleration (photon energy↑)
•Slotted foil (short pulse)
•Dielectric assisted cavity (high rep rate)
etc…

Short-term development: maximizing machine performance

Issues in present FELs

- **Photon parameters are not reproducible.**
  → change from beam time to beam time
- **Parameters sometimes drift with time, especially for unique operation modes**

↑

☑ Small changes in electron conditions cause big differences in photon qualities.

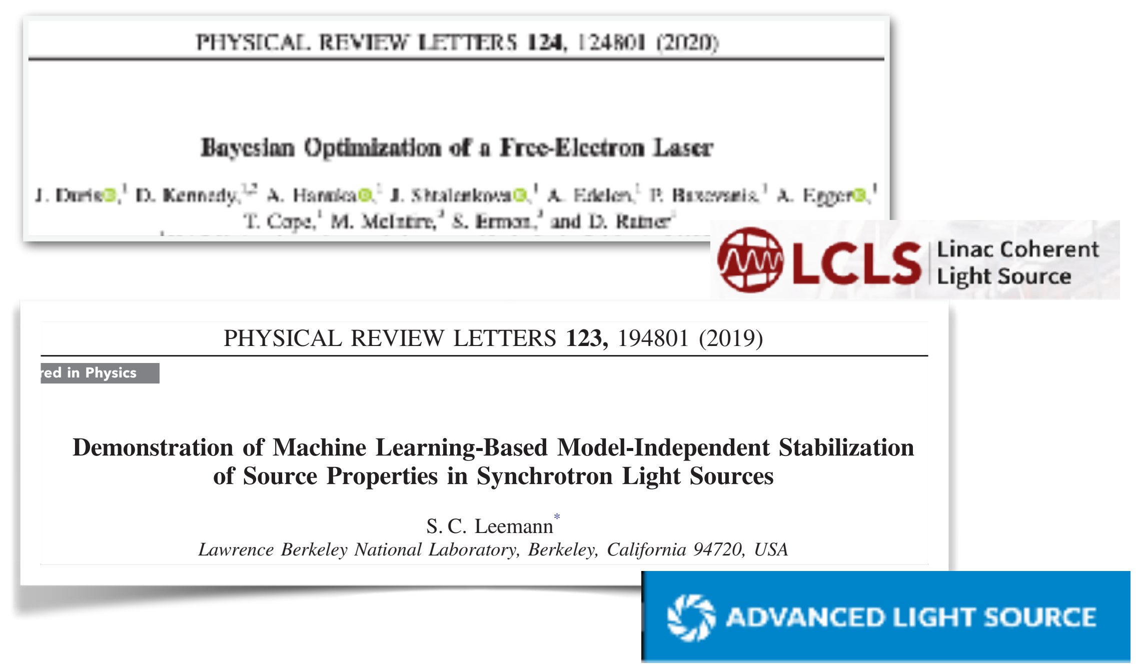
☑ Most parts of machine tuning rely on operators' experiences, although number of accelerator components is huge. Machine optimization is sometimes inadequate.

Facility activities

Implemented machine learning (ML) optimizer for maximize the pulse energy

(Bayesian approach using Gaussian processes)

cf. ML optimization at large-scale X-ray facilities


PHYSICAL REVIEW LETTERS 124, 124801 (2020)

Bayesian Optimization of a Free-Electron Laser

J. Duris,[1] D. Kennedy,[1,2] A. Hanuka,[1] J. Shtalenkova,[1] A. Edelen,[1] P. Baxevanis,[1] A. Egger,[1] T. Cope,[1] M. McIntire,[2] S. Ermon,[2] and D. Ratner[1]

PHYSICAL REVIEW LETTERS 123, 194801 (2019)

Demonstration of Machine Learning-Based Model-Independent Stabilization of Source Properties in Synchrotron Light Sources

S. C. Leemann*

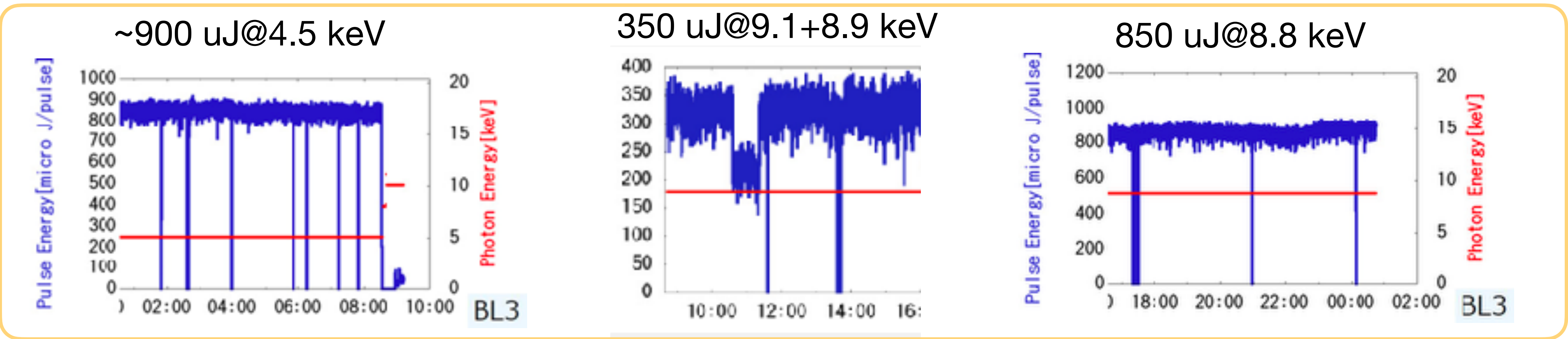
Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

Machine learning based-tuning (optimizing pulse energy)

Project led by E. Iwai (SACLA)

- R&D started in the middle of 2020.
- From 2020 winter, developed optimizers are used for daily machine tuning.
- Already as good as best human operators.

Significant results in 2021: pulse energy reached all-time high!



As a next step, we are expanding ML technique to more complicated optimization problems (multiple parameters, beam profile) towards realizing tailor-made XFELs.

Concept of tailor-made XFELs

Tunable Parameters

1. Pulse energy
2. Spectral width
3. Beam size
4. Pointing stability
5. Output of beamline instruments (e.g. Photo diode signal, MPCCD signal)
6. Functions using 1-5
   e.g. spectral density=(1)÷(2)

Optimize single parameter

Boost spectral density!

Maximize pulse energy!

Optimize multiple parameters

I have target values for all parameters (1-4)

maximize pulse energy, while keeping <50 eV bandwidth

10 mJ,
10 atto-seconds…

You cannot request unrealistic parameters…

Almost ready to release!

Under development

(will be released soon)

Questions from facility

- Any other parameters we should optimize?
- Are there critical photon parameters in each science case?

Tailor-made XFELs for more demanding users/experiments

Option 1.

Facility provides virtual data set of XFEL pulses (pulse energy, spectrum, profile) prior to the experiment.

→ Users define which pulses are acceptable.

→ Facility staffs make an evaluation function (via neural network). The accelerator is tuned using the function.

Option 2. (for extremely demeaning users/experiments)

Users evaluate XFEL pulses (acceptable or not) during the beam time.

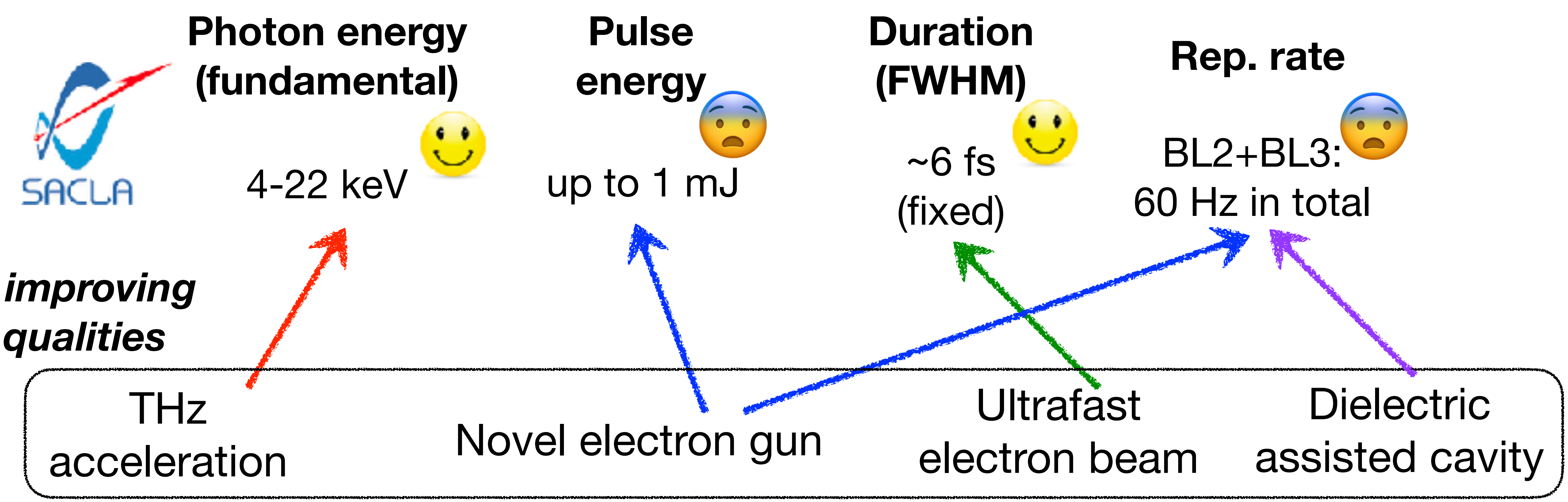
→ Facility staffs update evaluation function.

→ Accelerator tuning.

iteration loop

R&D of these schemes for tailor-made XFELs is on-going.

Long-term development plan (machine upgrade)



Ideas for improving photon qualities

•How long will it take for implementing these technologies to SACLA?
•How much the photon qualities will be improved?

-> Takahiro's talk

Questions from facility

•Which improvement(s) will be a game changer for your scientific field?

•What is the target values for respective parameters?

Note:

- Due to the limited budget and man power, simultaneous development of all technologies is not realistic. We need to define the priority.