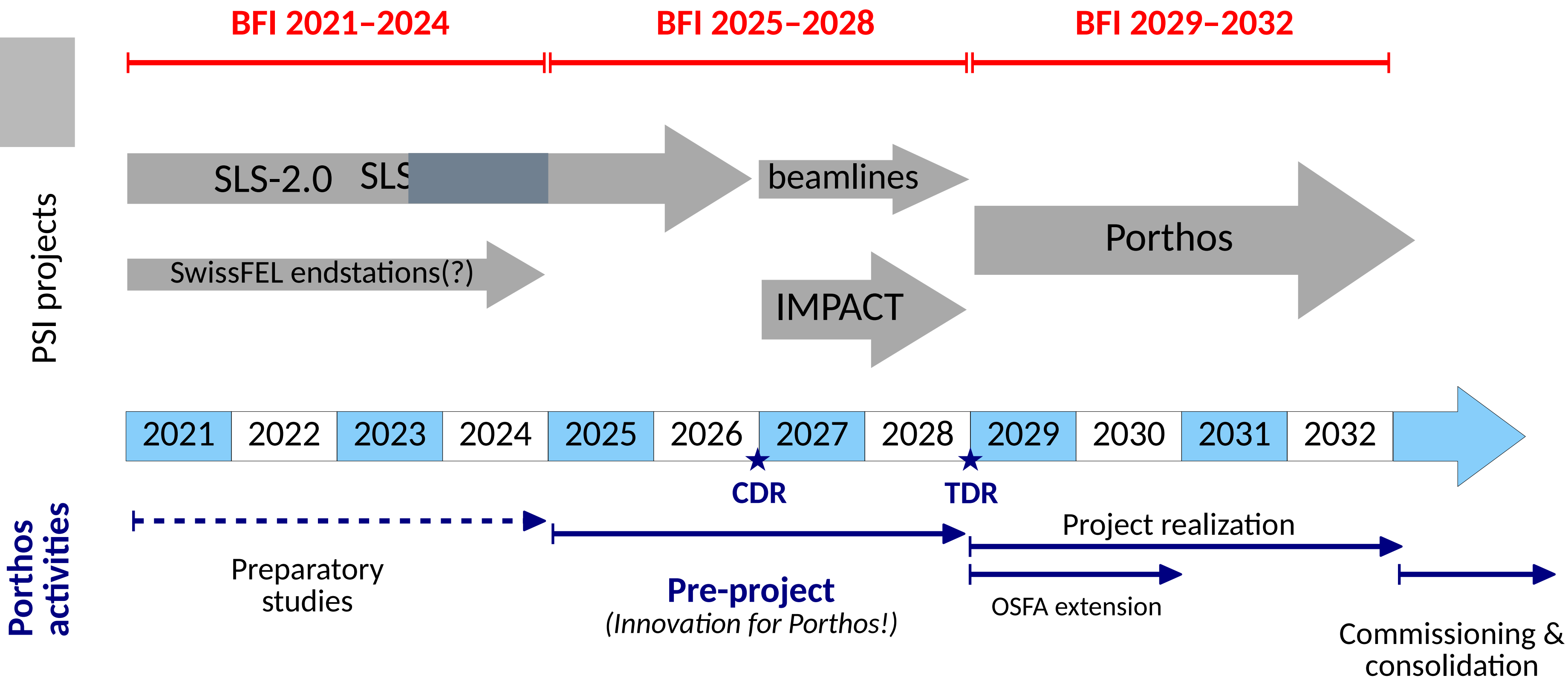
PAUL SCHERRER INSTITUT

Thomas Schietinger :: Paul Scherrer Institut

Porthos preproject options: status and outlook

Porthos Working Group, 19 September 2022

Reminder: Porthos timeline



PAUL SCHERRER INSTITUT

"Pre-announcement" for Roadmap 2027 submitted to ETH Board

ETH BOARD

Strategic Planning 2025-2028 of the ETH Board for the ETH Domain
Proposal for a Research Infrastructure --- PRE-ANNOUNCEMENT FOR ROADMAP 2027

Name of the Research Infrastructure: ***Porthos – An advanced hard X-ray waveform generator***
Responsible Institution(s): ***Paul Scherrer Institut***
New research infrastructure ☐ / substantial upgrade of existing research infrastructure ☒

1. Summary

The ability to visualize the structure of matter and functioning of biological, chemical, and physical processes has been a fundamental driver of science and the resulting technological innovations. In the past decades, the frontier has moved towards ultrafast processes on the femto- to attosecond time scale, imaging structures with atomic resolution and following reactions with sensitivity to individual chemical elements. PSI has successfully set into user operation the hard X-ray branch Aramis at SwissFEL, with two running experimental stations and a third one being implemented while the soft X-ray branch Athos has been recently installed and first pilot experiments are scheduled. Knowledge gained during the design and realization of Aramis and Athos in combination with innovative accelerator concepts have paved the road to **the extension of SwissFEL to its third branch, Porthos, which will be unique in its conception as an advanced hard X-ray waveform generator with an expected paradigm-shifting impact** like that brought about by analogous optical and microwave signal generators. In fact, Porthos will produce sequences of very bright, hard coherent X-ray pulses (as short as 10^{-16} seconds) at a repetition rate of 100 Hz with full polarization control up to the Mössbauer gamma line (14.4 keV) and beyond. The increase of the electron beam energy will allow pushing the X-ray wavelength below 0.5 Å, i.e., half of the atomic radius, and will double the achievable energy range compared to Aramis (!), i.e., to the point where thicker experimental systems, including samples as well as their containers for *operando* studies, particularly relevant for the sustainability agenda, become accessible.

2. Strategic relevance

With the recently commissioned SwissFEL, delivering femtosecond pulses of soft, tender and hard X-rays at a repetition rate of 100 Hz, Switzerland has leveraged opportunities from the ultrafast community and the unique power of X-ray investigations for a broad range of scientific applications. Porthos will accomplish SwissFEL's original design concept, i.e., the provision of 9 world-class FEL endstations for science, medicine and engineering (corresponding to a 50% capacity increase compared to what Aramis and Athos can provide using the same linear accelerator), thereby strengthening Switzerland's leadership role as a worldwide key player in the field.

2.1. Scientific rationale and challenges

Porthos will significantly contribute addressing the grand challenges facing our society, from the development of smart/new materials and mitigation of climate change to fundamental aspects in infectious diseases and atomically resolved biochemical structures and processes. Applications will cover all science and engineering disciplines, from semiconductors for electronics, catalysis for chemical reactions, to lead molecules for drug development. Examples of key experiments are:

- <u>Life Sciences:</u> Structure determination through truly radiation-damage-free diffraction-before-destruction time-resolved crystallography, exploiting the envisaged short-pulse/high-power (SPHP) operation mode at very short wavelengths. This will be particularly appealing for tiny crystals, to better map rapid diffusion of small molecule ligands.
- <u>Novel materials for future technologies:</u> Non-linear operando X-ray spectroscopy at K-edges of several 4d transition metals via stimulated emission studies with chemical sensitivity and nonlinear transient grating X-ray spectroscopy, enabling new ways in inorganic chemistry, catalysis, and materials science, for example to measure momentum-dependent ultrafast demagnetization processes (spintronics) of key importance in the field of quantum and neuromorphic computing.
- <u>Quantum Technologies:</u> Time-domain interferometry in the hard X-ray regime, exploiting the expected tunability of the phase difference and relative amplitudes of two adjacent pulses provided by Porthos Mode-Locked Lasing (MLL) capabilities, resulting in the coherent control and readout of quantum states, as well as highly precise and efficient measurements of electronic transition linewidths. Moreover, the q-range accessible with hard X-rays will allow the investigation of ultrafast charge and spin fluctuations on atomic length scales in novel quantum nanodevices.
- <u>Imaging</u>: Single-shot full-field and ptychographic imaging of ultrafast non-repeatable phenomena with single-digit nanometer spatial resolution in complex, operando conditions, perfectly complementing the imaging portfolio offered by SLS2.0.

2.2. Advantages for science and society

Porthos will enrich Switzerland's scientific landscape of tomorrow and will enable paradigm-shifting scientific progress. The first SwissFEL user publications reported on pioneering, high-impact experiments elucidating, among other things, the behaviour of ferric/ferrous heme proteins that play an important role in the respiratory function of hemoglobin, the dynamics of active transport across bio-membranes, and the functionality of organic light emitting diodes (LED). As described above, Porthos will produce harder X-rays with tailored pulses and expand the range of operation to be much closer to direct applications in all sectors. Moreover, the track records of the SLS and SwissFEL show that many technical innovations required to realize and continually advance cutting-edge facilities such as Porthos bear a large potential for commercial applications outside the project itself, and thereby become important innovation boosters for the ETH Domain and Switzerland.

2.3 Contribution to unique features of the ETH Domain

a) *Organisational embedding*

The project will be designed, constructed and operated by the PSD, GFA and LOG divisions of PSI following the matrix paradigm used also for the Athos undulator branch of SwissFEL and the upgrade SLS 2.0 of the Swiss Light Source. The execution of large-scale high-tech engineering projects for leading edge science is a feature of the ETH Domain shared by only a very small handful of international academic competitors such as Stanford (with SLAC) and the University of California (with the Lawrence Berkeley Laboratory). Strong links within the "campus" communities of ETHZ and EPFL as well as other national laboratories will be provided through joint faculty/staff appointments, shared studentships and other training programmes as well as collaborative user-driven research.

b) *Institutions involved*

The ETH Domain, Swiss academic units and Universities of Applied Sciences as well as major pharmaceutical companies and numerous SMEs will all benefit and capitalize on the new capabilities offered by Porthos. International organizations such as European XFEL and CERN are our long-term partners and will remain key collaborators during the upcoming decade.

3. Financial requirements (estimate) *** indicates PSI costs*

The current budget estimation foresees 100 MCHF investments for the machine and two endstations. In addition, construction costs of 40 MCHF have been estimated for extending the building in order to accommodate the new experimental areas. A first tranche of 10 MCHF will be borne by PSI in the 2025-2028 funding period to finance a "Pre-project" phase for the technical machine design as well as the advanced conceptual design for the endstations and the planning of the civil construction. The remaining 130 MCHF are requested for the 2029-2032 funding period and dedicated to the realization of the project.

Costs (MCHF)	2021-2024	**2025-2028**	2029-2032
Investment costs		10**	90
Operating costs			
Construction costs			40
Total costs		10**	130

Date: 6 April 2021

"Pre-announcement" for Roadmap 2027 submitted to ETH Board

Porthos preproject 2025–2028

Costs (MCHF)	2021-2024	**2025-2028**	2029-2032
Investment costs		10**	90
Operating costs			
Construction costs			40
Total costs		10**	130

ETH BOARD

Strategic Planning 2025-2028 of the ETH Board for the ETH Domain
Proposal for a Research Infrastructure --- PRE-ANNOUNCEMENT FOR ROADMAP 2027

Name of the Research Infrastructure: ***Porthos – An advanced hard X-ray waveform generator***
Responsible Institution(s): ***Paul Scherrer Institut***
New research infrastructure ☐ / substantial upgrade of existing research infrastructure ☒

1. Summary

The ability to visualize the structure of matter and functioning of biological, chemical, and physical processes has been a fundamental driver of science and the resulting technological innovations. In the past decades, the frontier has moved towards ultrafast processes on the femto- to attosecond time scale, imaging structures with atomic resolution and following reactions with sensitivity to individual chemical elements. PSI has successfully set into user operation the hard X-ray branch Aramis at SwissFEL, with two running experimental stations and a third one being implemented while the soft X-ray branch Athos has been recently installed and first pilot experiments are scheduled. Knowledge gained during the design and realization of Aramis and Athos in combination with innovative accelerator concepts have paved the road to **the extension of SwissFEL to its third branch, Porthos, which will be unique in its conception as an advanced hard X-ray waveform generator with an expected paradigm-shifting impact** like that brought about by analogous optical and microwave signal generators. In fact, Porthos will produce sequences of very bright, hard coherent X-ray pulses (as short as 10^{-16} seconds) at a repetition rate of 100 Hz with full polarization control up to the Mössbauer gamma line (14.4 keV) and beyond. The increase of the electron beam energy will allow pushing the X-ray wavelength below 0.5 Å, i.e., half of the atomic radius, and will double the achievable energy range compared to Aramis (I), i.e., to the point where thicker experimental systems, including samples as well as their containers for *operando* studies, particularly relevant for the sustainability agenda, become accessible.

2. Strategic relevance

With the recently commissioned SwissFEL, delivering femtosecond pulses of soft, tender and hard X-rays at a repetition rate of 100 Hz, Switzerland has leveraged opportunities from the ultrafast community and the unique power of X-ray investigations for a broad range of scientific applications. Porthos will accomplish SwissFEL's original design concept, i.e., the provision of 9 world-class FEL endstations for science, medicine and engineering (corresponding to a 50% capacity increase compared to what Aramis and Athos can provide using the same linear accelerator), thereby strengthening Switzerland's leadership role as a worldwide key player in the field.

2.1. Scientific rationale and challenges

Porthos will significantly contribute addressing the grand challenges facing our society, from the development of smart/new materials and mitigation of climate change to fundamental aspects in infectious diseases and atomically resolved biochemical structures and processes. Applications will cover all science and engineering disciplines, from semiconductors for electronics, catalysis for chemical reactions, to lead molecules for drug development. Examples of key experiments are listed:

- Life Sciences: Structure determination through truly radiation-damage-free diffraction-before-destruction time-resolved crystallography, exploiting the envisaged short-pulse/high-power (SPHP) operation mode at very short wavelengths. This will be particularly appealing for tiny crystals, to better map rapid diffusion of small molecule ligands.
- Novel materials for future technologies: Non-linear operando X-ray spectroscopy at K-edges of several 4d transition metals via stimulated emission studies with chemical sensitivity and nonlinear transient grating X-ray spectroscopy, enabling new ways in inorganic chemistry, catalysis, and materials science, for example to measure momentum-dependent ultrafast demagnetization processes (spintronics) of key importance in the field of quantum and neuromorphic computing.
- Quantum Technologies: Time-domain interferometry in the hard X-ray regime, exploiting the expected tunability of the phase difference and relative amplitudes of two adjacent pulses provided by Porthos Mode-Locked Lasing (MLL) capabilities, resulting in the coherent control and readout of

quantum states, as well as highly precise and efficient measurements of electronic transition linewidths. Moreover, the q-range accessible with hard X-rays will allow the investigation of ultrafast charge and spin fluctuations on atomic [illegible] quantum nanodevices.

- Imaging: Single-shot full-field and ptycho[illegible] ultrafast non-repeatable phenomena with single-digit nanometer spatial resolution in complex, operando conditions, perfectly complementing the imaging portf[illegible]

2.2. Advantages for science and society

Porthos will enrich Switzerland's s[illegible] will enable paradigm-shifting scientific progress. The first SwissFE[illegible]ering, high-impact experiments elucidating, among other things, the behaviour of ferric/ferrous heme proteins that play an important role in the respiratory function of hemoglobin, the dynamics of active transport across bio-membranes, and the functionality of organic light emitting diodes (LED). As described above, Porthos will produce harder X-rays with tailored pulses and expand the range of operation to be much closer to direct applications in all sectors. Moreover, the track records of the SLS and SwissFEL show that many technical innovations required to realize and continually advance cutting-edge facilities such as Porthos bear a large potential [illegible] commercial applications outside the project itself, and thereby become important innovation boosters for the ETH Domain and Switzerland.

2.3 Contribution to unique features of the ETH Domain

a) Organisational embedding

The project will be designed, constructed and operated by the PSD, GFA and LOG divisions of PSI following the matrix paradigm used also for the Athos undulator branch of SwissFEL and the upgrade SLS 2.0 of the Swiss Light Source. The execution of large-scale high-tech engineering projects for leading edge science is a feature of the ETH Domain shared by only a very small handful of international academic competitors such as Stanford (with SLAC) and the University of California (with the Lawrence Berkeley Laboratory). Strong links within the "campus" communities of ETHZ and EPFL as well as other national laboratories will be provided through joint faculty/staff appointments, shared studentships and other training programmes as well as collaborative user-driven research.

b) Institutions involved

The ETH Domain, Swiss academic units and Universities of Applied Sciences as well as major pharmaceutical companies and numerous SMEs will all benefit and capitalize on the new capabilities offered by Porthos. International organizations such as European XFEL and CERN are our long-term partners and will remain key collaborators during the upcoming decade.

3. Financial requirements (estimate) *** indicates PSI costs*

The current budget estimation foresees 100 MCHF investments for the machine and two endstations. In addition, construction costs of 40 MCHF have been estimated for extending the building in order to accommodate the new experimental areas. A first tranche of 10 MCHF will be borne by PSI in the 2025-2028 funding period to finance a "Pre-project" phase for the technical machine design as well as the advanced conceptual design for the endstations and the planning of the civil construction. The remaining 130 MCHF are requested for the 2029-2032 funding period and dedicated to the realization of the project.

Costs (MCHF)	2021-2024	2025-2028	2029-2032
Investment costs		10**	90
Operating costs			
Construction costs			40
Total costs		10**	130

Date: 6 April 2021

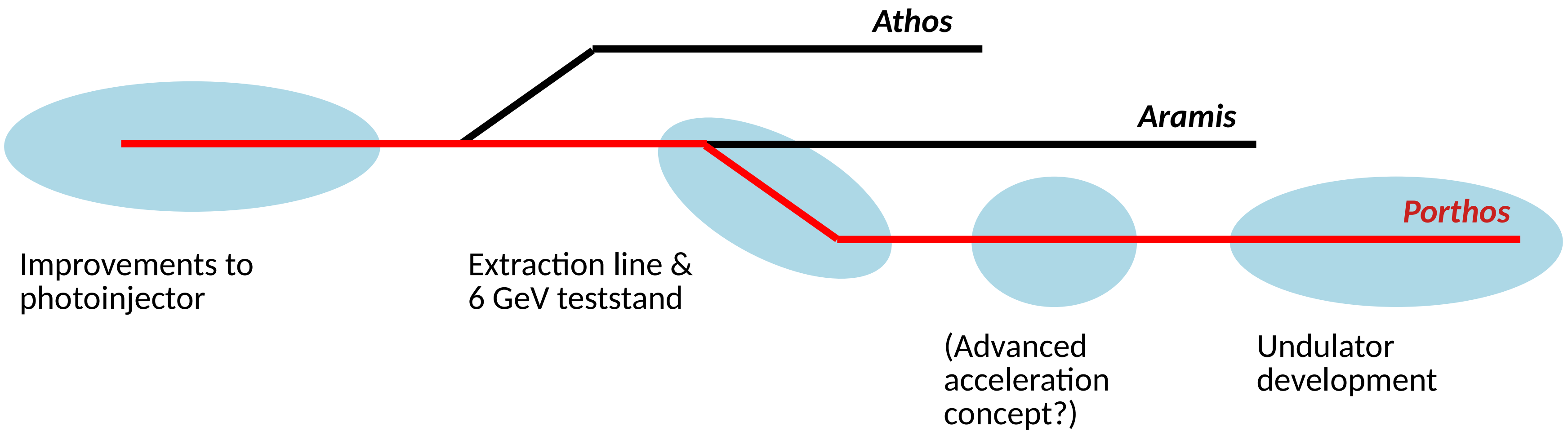
How to spend the 10 MCHF?

- After discussion at SSB, PSAC and elsewhere, high-level agreement to pursue 3–4 main directions during the pre-project (with emphasis on *innovation!*)
  - **Improvements of photoinjector**
  - **Extraction line with 6-GeV test stand**
  - **Undulator development**
  - (Advanced acceleration concepts)

- Other important directions, not directly listed in the preproject, but important to push (emphasis on *feasibility*):
  - Resonant kicker development (21 ns, possibly 14 ns)
  - Additional gun laser system and infrastructure
  - LLRF scheme to handle 21 ns (or less)
  - Diagnostics readout to handle 21 ns (or less)
  - Building annex for experiments

How to spend the 10 MCHF?

After discussion at SSB, PSAC and elsewhere, high-level agreement to pursue four main directions during the pre-project (emphasis on *innovation!*)



Preproject 1: Improvements to photoinjector

- Preproject objectives:
  - (Technical) Design for a new injector complex (gun, LH, BC1)
  - Beam test stand for SwissFEL gun developments (WLHA)
  - Installations in SwissFEL as far as financial and time resources allow
- Status:
  - Gun RF teststand in preparation, new C-Band TW gun in design (I.FAST)
  - Basic model to include IBS and MBI effects in injector simulation available
- Financial needs:
  - Extension of RF gun test stand to a full beam test stand. Details to be defined (3 MCHF?)
  - Installations in SwissFEL (2 MCHF?)

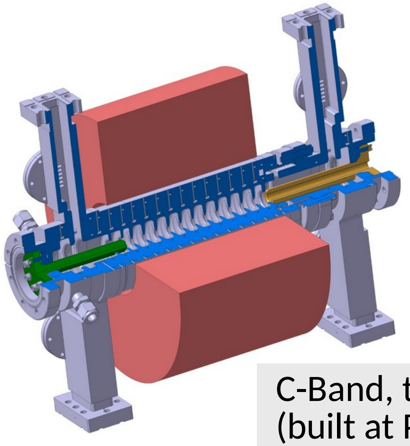
- Synergies with other PSI projects:
  - C-band TW gun development (I.FAST)
- International collaborations:
  - I.FAST
  - Other labs may be interested in photo-injector improvements...

- Task list / work packages (before pre-project):
  - Comparison of different injector layouts (simulation):
    - RF frequencies (S-band vs. C-band gun and booster)
    - Bunch compression scheme (incl. linearization)
  - Baseline design for new injector → new locations for RF stations (important for modulator upgrade)
  - Preliminary design of beam test stand in WLHA (incl. instrumentation)

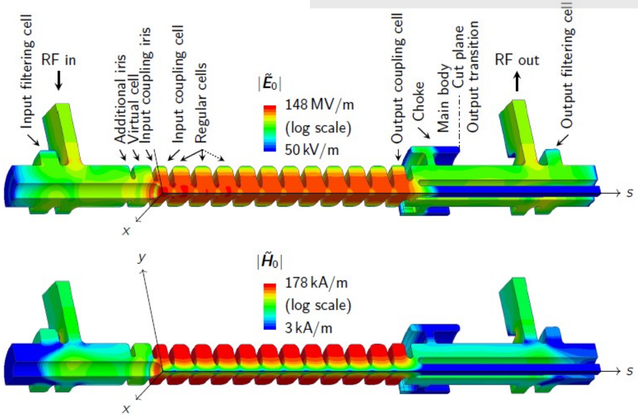
Preproject 1: Improvements to photoinjector

T. Lucas, GFA accelerator seminar, 29 Nov. 2022

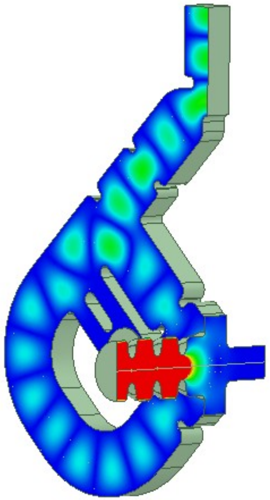
New gun concepts

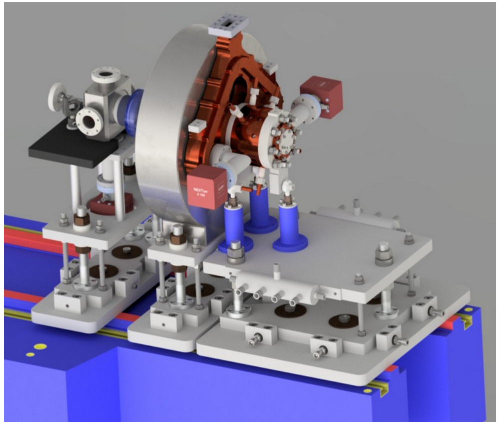


C-Band, travelling wave
(built at PSI)



C-Band, standing wave
(built at LNFN Frascati)



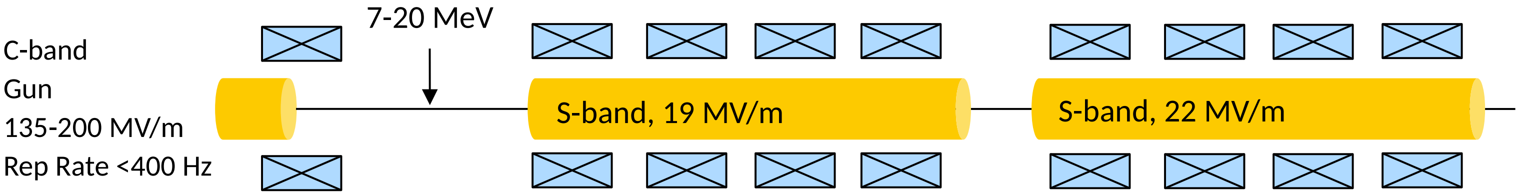


Preproject 1: Improvements to photoinjector

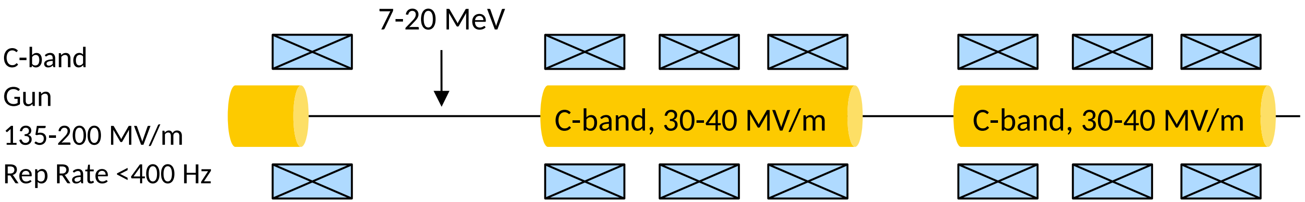
Injector RF configurations

T. Lucas, GFA accelerator seminar, 29 Nov. 2022

C-band gun → S-band booster (20 MV/m or 30 MV/m with new FERMI-type structures)



C-band gun → C-band booster

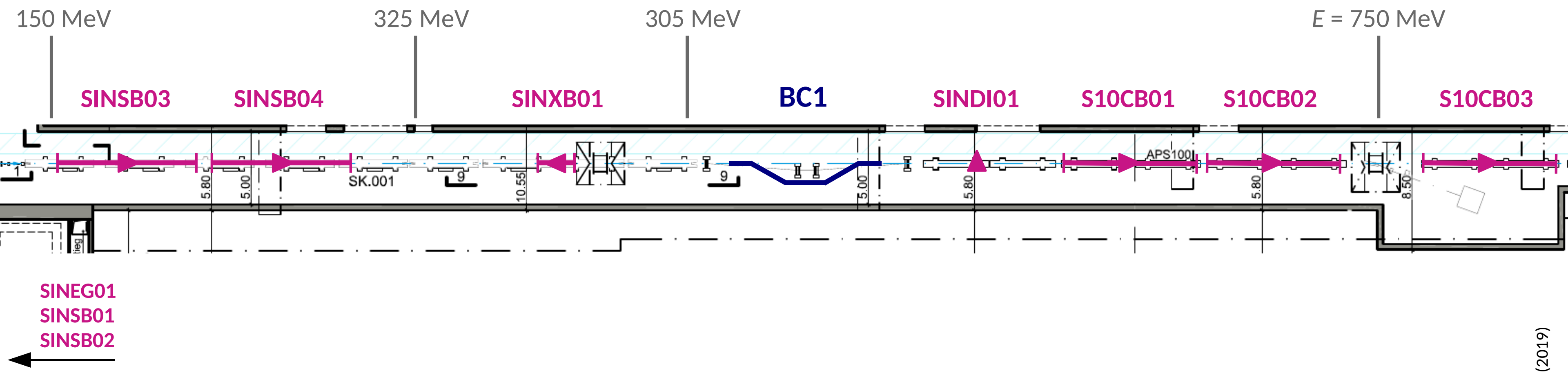


Do we still have the flexibility to go to an all C-band injector?

Preproject 1: Improvements to photoinjector

Bunch compression scheme

Current layout: BC1 at 305 MeV

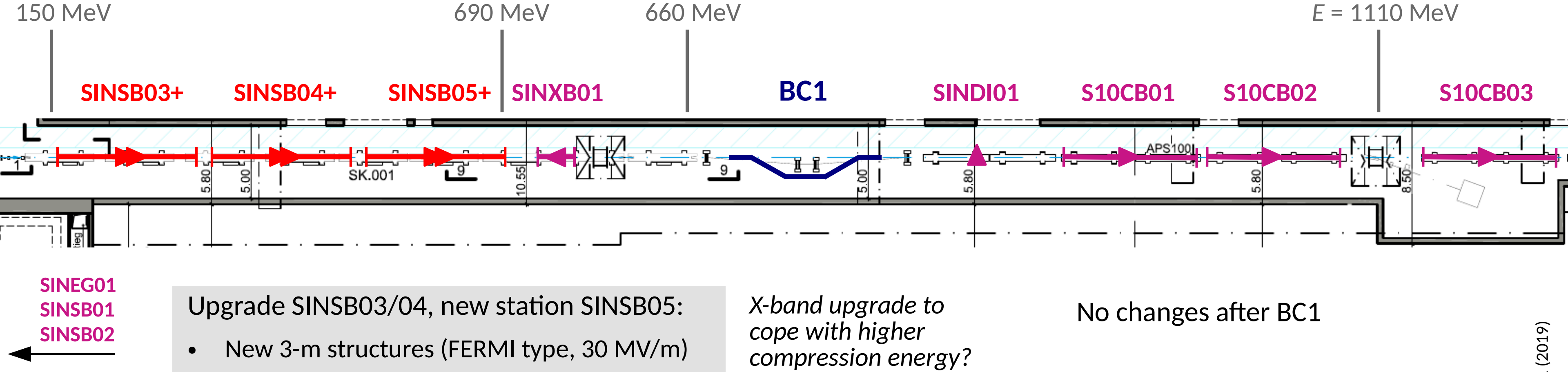


PSI drawing
No. 2R-393601 (2019)

Preproject 1: Improvements to photoinjector

Bunch compression scheme

Option S-band upgrade only: BC1 at 660 MeV



Upgrade SINSB03/04, new station SINSB05:

- New 3-m structures (FERMI type, 30 MV/m)
- S-band BOCs
- 180 MeV per S-band station
  (1 HV modulator/klystron serving two structures)

X-band upgrade to cope with higher compression energy?
⇒ BD simulations needed...

No changes after BC1

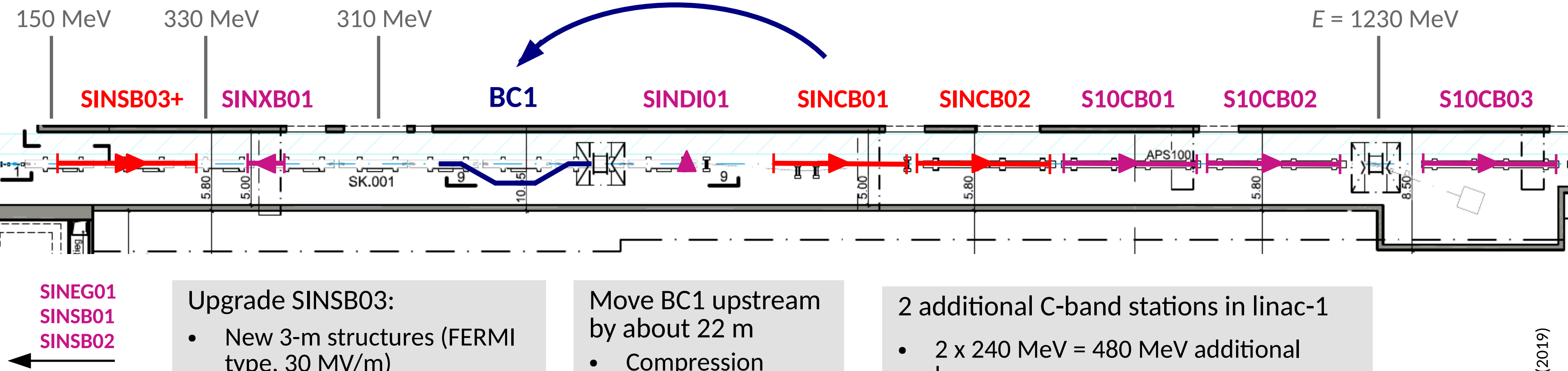
Option needs further study!...

PSI drawing
No. 2R-393601 (2019)

Preproject 1: Improvements to photoinjector

Bunch compression scheme

Option S-band & C-band upgrade: BC1 at 310 MeV



Upgrade SINSB03:

- New 3-m structures (FERMI type, 30 MV/m)
- S-band BOCs
- 180 MeV from a single S-band station (1 HV modulator/klystron serving two structures)

Move BC1 upstream by about 22 m

- Compression energy stays at ~300 MeV
- No X-band upgrade necessary
- **Long shutdown!**

2 additional C-band stations in linac-1

- 2 x 240 MeV = 480 MeV additional beam energy
- Stay at current acc. gradient for klystron stability (30 MV/m)

Option needs further study!...

PSI drawing No. 2R-393601 (2019)

Preproject 2: Extraction line and 6 GeV teststand

- Preproject objectives:
  - Complete (simplified) extraction line
  - Multi-purpose 6 GeV test stand
- Status:
  - Extraction line design done (Sven Reiche), presented at FEL'2022 (WEP09)
  - Rough installation plan (for P^3) by D. Hauenstein – under scrutiny (overlap with SLS dark time)
- Financial needs:
  - Components for extraction line (1 MCHF)
  - Infrastructure test stand (0.5 MCHF?)

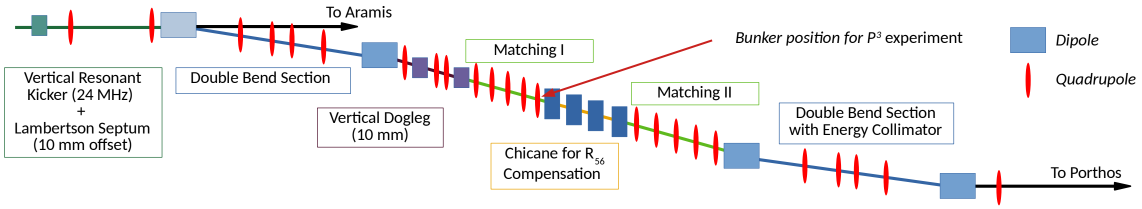
- Synergies with other PSI projects:
  - Positron Production at PSI (P^3) (FCC study, CERN)
  - Possibly LTP (detector test stand)
- Additional support
  - Possible support from SNF through R'Equip proposal

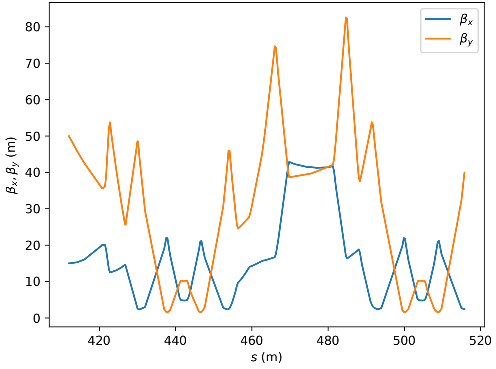
- Task list / work packages (before pre-project):
  - Secure early financing before preproject phase: GFA management, R'Equip proposal,…
  - Survey of potential users of test stand (SwissFEL and other) → required for R'Equip proposal
  - Ideas / design for a multi-purpose 6 GeV test stand with instrumentation

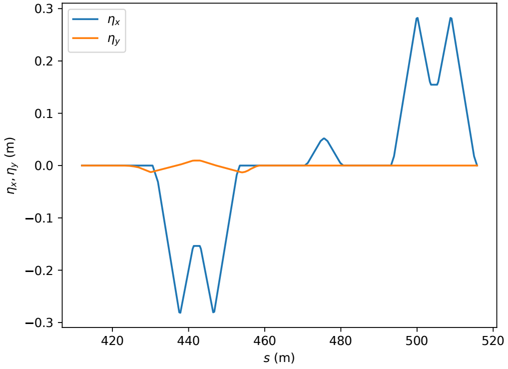
Preproject 2: Extraction line and 6 GeV teststand

S. Reiche, FEL2022, WEP09

Layout simplified extraction line (no kicker, no vertical offset)







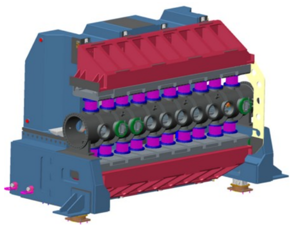
Preproject 3: Undulator development

- Preproject objectives:
  - Selection of optimal undulator type for Porthos.
  - Demonstration of a viable undulator design by assembling and testing a prototype.
- Status:
  - Two main undulator technologies in evaluation: cryogenic APPLE-X and SCAPE
  - Some simulations performed for various undulator configurations.
- Financial needs:
  - Undulator prototype with appropriate infrastructure (~3 MCHF)

- Synergies with other PSI projects:
  - Possibly SLS-2.0 undulator technology
- International collaboration:
  - Depending on undulator design: Soleil and HZB (cryo-APPLE-X) or EuXFEL and Argonne (SCAPE)
- Additional support:
  - CHART funding requested (seed funds for 2025)

- Task list / work packages (before pre-project):
  - More detailed assessment of technological potential and risks of undulator types under consideration
  - Systematic evaluation of different undulator concepts (entire Porthos line) with respect to user requirements.

Preproject 3: Undulator development

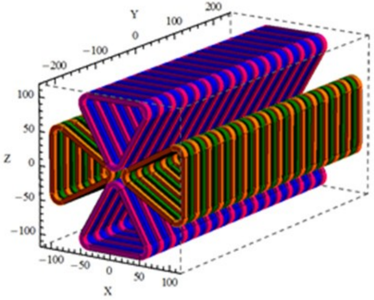


Undulator types

K. Zhang, M. Calvi, Supercond. Sci. Technol. ***35,*** *093001 (2022)*

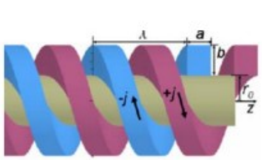
Cryo-Apple-X

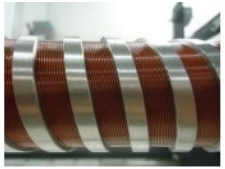
- Full polarization control, linear-α and elliptical
- Cryogenics: LN2 (77 K)
- Controls: gap and shift drive system (like Athos, but more involved)
- Nobody working on this configuration, but synergies with **cryo-Apple-II/III** at HZB and SOLEIL (Rial/Valleau)
- Synergy with HZB and SOLEIL (but no ready design yet)



SCAPE: Superconducting Arbitrarily Polarizing Emitter

- Cryogenics: LHe (4.2 K)
- Controls: power supply – easy!
- Synergy with Argonne and EuXFEL (Kesgin/Casalbuoni)
- Concept could be upscaled to full polarization control



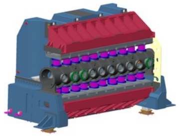


Superconducting Helical Undulator

- Cryogenics: LHe (4.2 K)
- Controls: power supply – easy!
- Originally developed for polarized positron sources (e.g. CLIC gun)
- Limited to helical polarization, combining C+/C- can give ~85% lin. pol. ("crossed undulator" scheme)
- Synergy with Daresbury/Rutherford Lab (Shepherd)

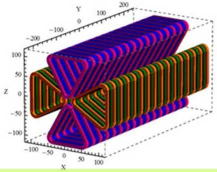
Preproject 3: Undulator development

1) **Cryogenic APPLE-X** (current baseline)



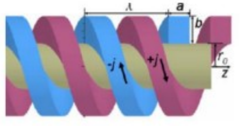
Undulator configurations

2) **SCAPE**



new baseline?

3) **Helical SCU**, linear polarization option by:



3a) Polarizer / waveplate

3b) C+ and C– combined ("crossed undulator" scheme)

3c) SCAPE afterburner (could be an upgrade to Porthos), suppression of initial polarization by beam separation or reverse tapering

For all scenarios assume:

- E.g. 2 × 10 identical modules
- Small interundulator chicanes (CHIC)
- One large central chicane (self-seeding, two-color)

- **These undulator options / configurations to be compared systematically in view of Porthos!**
- Evaluation in terms of:
  - Final FEL performance and flexibility
  - Technical feasibility
  - Operational aspects (e.g. change of K values)

(Preproject 4: Advanced acceleration)

- Preproject objectives:
  -
  -
- Status:
  -
  -
- Financial needs:
  -
  -

- Synergies with other PSI projects:
  -
- International collaboration:
  -

- Task list / work packages (before pre-project):
  -
  -

(Preproject 4: Advanced acceleration)

- Preproject objectives:
  - Demonstrate viability of wakefield acceleration with pilot bunch and dechirper to extend energy reach of Porthos.
- Status:
  - Tests with existing dechirper planned.
  - Generation and transport of two closely spaced bunches demonstrated (for two-color generation with emittance spoiling, PRAB 24, 060703)
- Financial needs:
  - Dechirper development? (Expect only little funding required.)

- Synergies with other PSI projects:
  - Experience from routine use of standard dechirpers in SwissFEL.
- International collaboration:
  - UCLA (Musumeci group)
  - Potentially interest from other groups/labs…

- Task list / work packages (before pre-project):
  - Demonstration of wakefield acceleration with existing dechirper.
  - Assessment of suitability of accelerated bunch for lasing.

Compact task list (homework!)

- **Photoinjector improvements**
  - Agree on RF boundary conditions (S-band, C-band,…) (RF)
  - Simulations for new injector layout (assuming different gun types) (BD)
  - Preliminary design of beam test stand in WLHA (Laser, RF, BD, construction,…)
  - Evaluation of gun type (S-band vs. C-band, SW vs. TW) (RF & BD)
- **Extraction line and 6 GeV teststand**
  - R'Equip proposal including survey of potential users (RF & BD)
  - Prepare funding packages (200–300 kCHF) to be submitted to GFA finance workshops (RF)
- **Undulator development**
  - Preliminary performance figures for the considered undulator types (ID group)
  - Systematic comparison of options for undulator lines (BD)

Timeframe: R'Equip proposal *spring 2023*,
injector and undulator studies ready for PSI internal circulation be *fall 2023*

Next Porthos Meetings: 4 Nov. (preliminary exchange), 9 Dec. (intermediate results)

Thank you