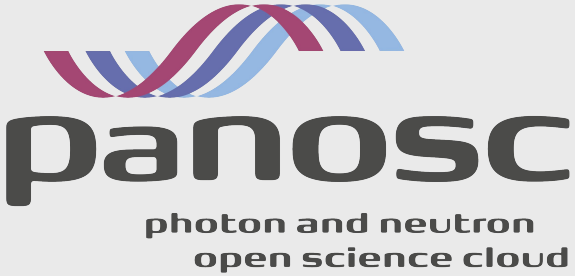

WP5 (M36-M48) Copenhagen workshop

29th November, 2021

Juncheng E, Mads Bertelsen, Shervin Nourbakhsh, Mousumi Upadhyay Kahaly, Aljosa Hafner, Nagy Gergely, Manuel Sanchez Del Rio, Juan Reyes Herrera, Stella dAmbrumenil, Carsten Fortmann-Grote

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Deliverables

No.	Title	Due	Verification	Status	Who is working on this?
D5.1	Prototype simulation data formats as openPMD domain specific extensions including example datasets	M12	Written report	Done	
D5.2	Release of documented simulation APIs	M24	Software	Done	
D5.3	Repository of documented jupyter notebooks and Oasys canvases showcasing simulation tasks executable via JupyterHub or remote desktop.	M42 (31.05.2022)	Software	Working on	Carsten, Juncheng, Mads, Aljosa, Shervin, Juan, Manuel
D5.4	VINYL software tested, documented, and released, including integration into interactive data analysis workflow with feedback loop.	M48 (30.11.2022)	Written report + Software	Start after integration	All WP5 members and WP4

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Milestones

No.	Title	Due	Verification	Status	Who is working on this?
MS5.1	Simulation codes in PaNData Software Catalog	M6	PaNData software catalog website	Done	
MS5.2	Demonstration of simulation services	M24	Written report	Done	
MS5.3	VINYL software release	M42 (31.05.2022)	Software released via open source repository	Working on	Carsten, Juncheng, Mads, Shervin, Manuel, Juan
MS5.4	Validation of simulation services	M48(30.11.2022)	Written report	Working on	All WP5 members and WP4

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Outcomes

2. **Estimates for having the key outcomes achieved and maintained** (to be filled in by all WP leaders and also all partners):

#	WP	Item	Who is working / will work on that?	Achieved by	issues /concerns	Will you continue operating this service and in what form and with which resources? (for partners only)	Sustainability comments & What are the resources / financing required to make this sustainable? (WP leaders only)
1.1	2	FAIR data policy					
1.2	2	DMPs					
2.1	2	FAIR assessment					
2.2	2	Common PID framework					
3	3	Standardised metadata (Nexus/HDF5, PaN ontologies)					
4	3	Federated search API for PaN data catalogues					
5.1	3 & 4	Open Data portal					
5.2	3, 4 & 6	Downloading data from data portal					
6	6	Community AAI UmbrellaId					
7.1	4	JupyterLab notebooks					
7.2	4	HDF5/NeXus files visualisation					
8.1	4	Remote data analysis with VISA					
8.2	4	Data analysis pipelines					
9	5	VINYL Software Package (SIMEX simulation software?)	**Is working:** All WP members **Will be working on:** To be defined at each RI, has not been discussed until now.	30.11.2022		To be discussed at each RI	1/2 FTE per RI
10	8	PaN-learning platform (pan-learning.org + pan-training.org)					

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PMs estimation

4b. Estimates of how many PMs are required in the last year of project execution (From December '21 until end November '22) (to be filled by each WP leader)

WP	ESRF	ILL	European XFEL	ESS	ELI	CERIC-ERIC	EGI	Comments
WP1 – Management								
WP2 – Data Policy								
WP3 – Data Catalog Services								
WP4 – Data Analysis Services								
WP5 – Vinyl			13.2					
WP6 – EOSC Integration								
WP7 – Sustainability								
WP8 – Training								
WP9 - Communication								

Need input from other partners to estimate how many PMs they need to achieve the the final goals according to the future plan.

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The M36-M48 plan

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Tasks for each partner

https://panosc-vinyl.github.io/tools/

1	1	Review
2	1.5	Alijosa
	1.5.1.1	Prepare PR to openPMD standard
	1.2.1	Docker image
	1.5.3.3	Internal Review Implementation
	1.5.2.3	Internal Review Implementation
	1.3.2	Oasys schools material uploaded to PAN learning
	1.5.1.3	Submission to openPMD
	1.5.1.4	follow up till integration
	1.5.4.2	Internal Review Implementation

CERIC-ERIC

6	1.6	Mousumi
	1.1.1	In-silico neutron diffraction from Boro-carbon systems
	1.5.3.3	Internal Review Implementation
	1.5.2.3	Internal Review Implementation
	1.5.4.2	Internal Review Implementation

ELI

5	1.2	Mads
	1.6.4	McStasScript using libPyVinyl
	1.5.1.2	Interal review
	1.5.3.3	Internal Review Implementation
	1.5.2.3	Internal Review Implementation
	1.6.8	Instrument database API (load, diff) [0/2]
	1.5.4.2	Internal Review Implementation

ESS

8	1.4	Shervin
	1.5.3.1	Implementation
	1.5.3.6	Remaining issues [0/2]
	1.4.1	Adding section about simulation vs simulation comparison
	1.5.5	OpenPMD raytracing to numpy conversion for ML training
	1.6.3	Support for numpy arrays in Parameter class
	1.7.3	McStas example for D22 with parameters
	1.5.3.3	Internal Review Implementation
	1.5.2.3	Internal Review Implementation
	1.5.2.4	Documentation
	1.5.2.5	Tests
	1.5.2.6	CI
	1.5.3.4	Documentation
	1.5.3.5	CI
	1.7.2	Automatic tests
	1.7.4	McStas example for Thales with parameters
	1.5.2.7	Remaining issues [0/1]
	1.5.4.1	Implementation
	1.5.4.2	Internal Review Implementation
	1.5.4.3	Documentation
	1.5.4.4	Tests
	1.5.4.5	CI

ILL

9	1.8	Manuel
	1.6.6	Shadow3 calculator and parameters
	1.5.3.3	Internal Review Implementation
	1.5.2.3	Internal Review Implementation
	1.5.4.2	Internal Review Implementation

ESRF

3	1.7	Cartsten
	1.5.1.2	Interal review
	1.4.2	Review and fixes
	1.5.4.2	Internal Review Implementation
4	1.3	Jun
	1.6.2	Integration Instrument class
	1.6.5	SimEx-lite using libPyVinyl
	1.7.1	SimEx example with parameters
	1.5.3.3	Internal Review Implementation
	1.5.2.3	Internal Review Implementation
	1.6.7	New release of libPyVinyl
	1.6.8	Instrument database API (load, diff) [0/2]
	1.3.1	Simex material
	1.5.4.2	Internal Review Implementation

EuXFEL

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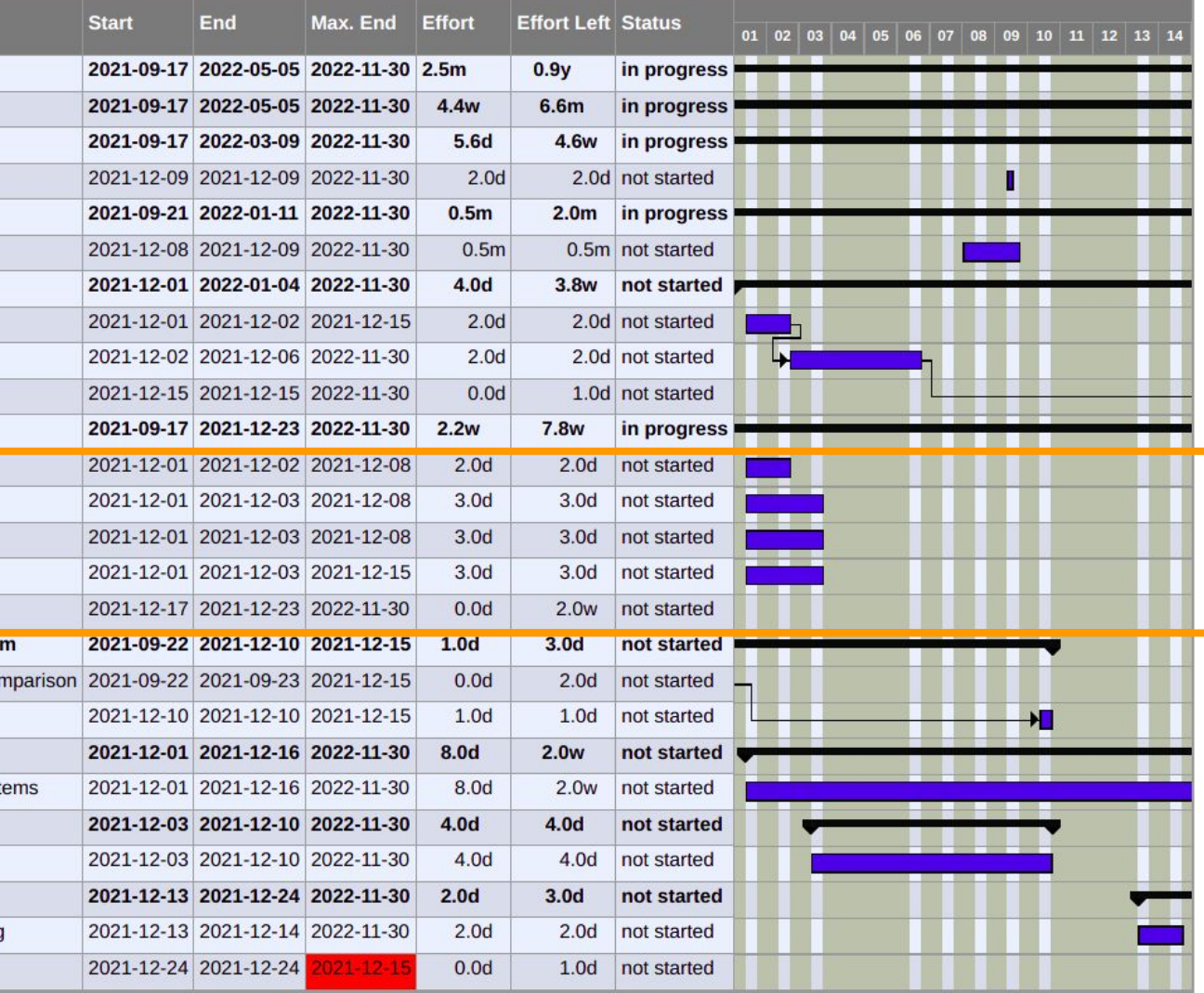
Sprint2021 Plan

BSI	Name	Start	End	Max. End	Effort	Effort Left	Status
1	**PANOSC WP5**	**2021-09-17**	**2022-05-05**	**2022-11-30**	**2.5m**	**0.9y**	**in progress**
1.5	**OpenPMD**	**2021-09-17**	**2022-05-05**	**2022-11-30**	**4.4w**	**6.6m**	**in progress**
1.5.2	**raytracing C++ API**	**2021-09-17**	**2022-03-09**	**2022-11-30**	**5.6d**	**4.6w**	**in progress**
1.5.2.3	Internal Review Implementation	2021-12-09	2021-12-09	2022-11-30	2.0d	2.0d	not started
1.5.3	**McStas openPMD I/O component**	**2021-09-21**	**2022-01-11**	**2022-11-30**	**0.5m**	**2.0m**	**in progress**
1.5.3.3	Internal Review Implementation	2021-12-08	2021-12-09	2022-11-30	0.5m	0.5m	not started
1.5.1	**raytracing extension**	**2021-12-01**	**2022-01-04**	**2022-11-30**	**4.0d**	**3.8w**	**not started**
1.5.1.1	Prepare PR to openPMD standard	2021-12-01	2021-12-02	2021-12-15	2.0d	2.0d	not started
1.5.1.2	Interal review	2021-12-02	2021-12-06	2022-11-30	2.0d	2.0d	not started
1.5.1.3	Submission to openPMD	2021-12-15	2021-12-15	2022-11-30	0.0d	1.0d	not started
1.6	**PyVinyl**	**2021-09-17**	**2021-12-23**	**2022-11-30**	**2.2w**	**7.8w**	**in progress**
1.6.3	Support for numpy arrays in Parameter class	2021-12-01	2021-12-02	2021-12-08	2.0d	2.0d	not started
1.6.4	McStasScript using libPyVinyl	2021-12-01	2021-12-03	2021-12-08	3.0d	3.0d	not started
1.6.5	SimEx-lite using libPyVinyl	2021-12-01	2021-12-03	2021-12-08	3.0d	3.0d	not started
1.6.6	Shadow3 calculator and parameters	2021-12-01	2021-12-03	2021-12-15	3.0d	3.0d	not started
1.6.8	Instrument database API (load, diff) [0/2]	2021-12-17	2021-12-23	2022-11-30	0.0d	2.0w	not started
1.4	**Protocol comparison sim vs data and sim vs sim**	**2021-09-22**	**2021-12-10**	**2021-12-15**	**1.0d**	**3.0d**	**not started**
1.4.1	Adding section about simulation vs simulation comparison	2021-09-22	2021-09-23	2021-12-15	0.0d	2.0d	not started
1.4.2	Review and fixes	2021-12-10	2021-12-10	2021-12-15	1.0d	1.0d	not started
1.1	**Papers**	**2021-12-01**	**2021-12-16**	**2022-11-30**	**8.0d**	**2.0w**	**not started**
1.1.1	In-silico neutron diffraction from Boro-carbon systems	2021-12-01	2021-12-16	2022-11-30	8.0d	2.0w	not started
1.2	**Oasys**	**2021-12-03**	**2021-12-10**	**2022-11-30**	**4.0d**	**4.0d**	**not started**
1.2.1	Docker image	2021-12-03	2021-12-10	2022-11-30	4.0d	4.0d	not started
1.3	**PAN-learning**	**2021-12-13**	**2021-12-24**	**2022-11-30**	**2.0d**	**3.0d**	**not started**
1.3.2	Oasys schools material uploaded to PAN learning	2021-12-13	2021-12-14	2022-11-30	2.0d	2.0d	not started
1.3.1	Simex material	2021-12-24	2021-12-24	2021-12-15	0.0d	1.0d	not started



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KPIs

KPIs	Title	Now (2021-11-5)	Estimate
5.1.1	Number of contributors to ViNYL	9	9
5.2.1	number of users of ViNYL services at ESRF	0	2
5.2.2	number of users of ViNYL services at ILL	0	2
5.2.3	number of users of ViNYL services at XFEL	3	4
5.2.4	number of users of ViNYL services at ESS	2	3
5.2.5	number of users of ViNYL services at ELI	0	2
5.2.6	number of users of ViNYL services at CERIC	2	4
5.3.1	Number of modules included in ViNYL service	3	3
5.4.1	Number of partner infrastructures that have used ViNYL service	3	5
5.5.1	Number of DOIs for simulated data (by counting datasets with "ViNYL" labels on open-access repositories like Zenodo).	5	10
5.6.1	Number of openPMD standard domain extensions merged into mainline openPMD repository	1	3

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Summary

- WP5 is currently in line with the plan.
- No obvious issues and concerns.
- The upcoming sprint will ensure the deliverables and milestones to be delivered on time.

- The WP5 outcome sustainability plan needs to be clarified.
- The PM estimation needs input from other partners.

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Thanks

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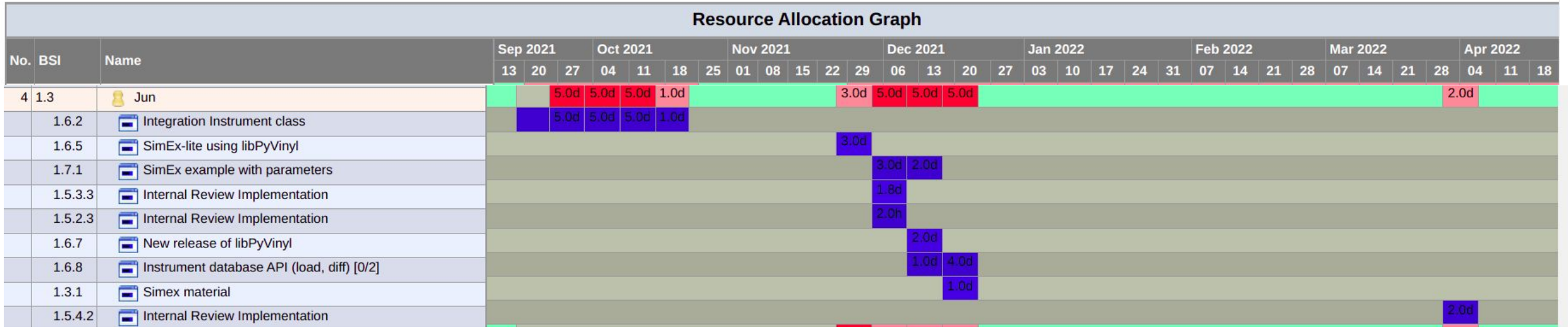
European XFEL contributions to WP5

- WP5 Management
- SIMEX platform (SimEx and SimEx-Lite)
- libpyvinyl development



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