ICSC
Centro Nazionale HPC, Big Data e Quantum Computing

Spoke 3, Astrophysics and Cosmos Observations
Presentation of WP2
Pierluigi Monaco, UniTS (+INAF, INFN, IFPU)

Kick-off meeting, INAF Roma, 27-28 October 2022

WP2: design of innovative algorithms, methodologies and codes towards exascale and beyond

Scope: This WP identifies innovative algorithms and methodologies upgrading their capability to exploit, and scale on, the exascale and post exascale architectures, reintegrating the resulting improved features in codes, workflows and pipelines. The energy impact will also be specifically considered. Leader: UniTS; Participants: INAF, SISSA, SNS, UniTS, UniCT, UniTo, UniTOV, INFN

T2.1: **Science cases definition**, algorithms **identification**, parallelism level assessment and profiling

T2.2: **Algorithms co-design** and methodologies to scale-up the capabilities of the algorithms and to find new innovative solutions

T2.3: Design of **new architectural solutions** aimed at the exploitation of post-exascale infrastructures (GPUs, FPGAs, Vector accelerators, NVM, HBM, ARM)

T2.4: Algorithms and methodologies **integration** into new big-data analysis applications

WP2: participants

Partner	Task	Personale partecipante	PM A1	PM A2	PM A3	PM
UniTS	T2.1, T2.2, T2.4	Pierluigi Monaco, Stefano Borgani, Alexandro Saro, Matteo Costanzi, Francesco Longo	16.25	16,25	16,25	**48,75**
INAF	T2.1, T2.2, T2.3, T2.4	Giuliano Taffoni, Andrea Possenti, Aldo Bonomo…	11	19	14	**44**
SISSA	T2.1, T2.3	Matteo Viel, Mario Spera	11	18	18	**47**
UniTO	T2.1, T2.2, T2.3, T2.4	Andrea Mignone, Susanna Terracini	14	8	8	**30**
UniCT	T2.1, T2.2, T2.4	Alessandro Lanzafame, Loreto Di Donato, Letizia Pumo	14,5	15,8	16,5	**46,8**
INFN	T2.1	Giovanni Signorelli, Massimiliano Lattanzi, Martina Gerbino	6,5	6,5	0	**13**
SNS	T2.1, T2.3, T2.4	Andrea Pallottini, Julien Bloino	17	16	16	**49**
RomaTOV	T2.1, T2.2, T2.3	Giuseppe Puglisi, Pasquale Mazzotta, Francesco Tombesi, Herve' Bourdin, Francesco Berrilli, Giancarlo De Gasperis, Giuseppe Bono	26	28	30	**84**

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Total: 362,6 PM

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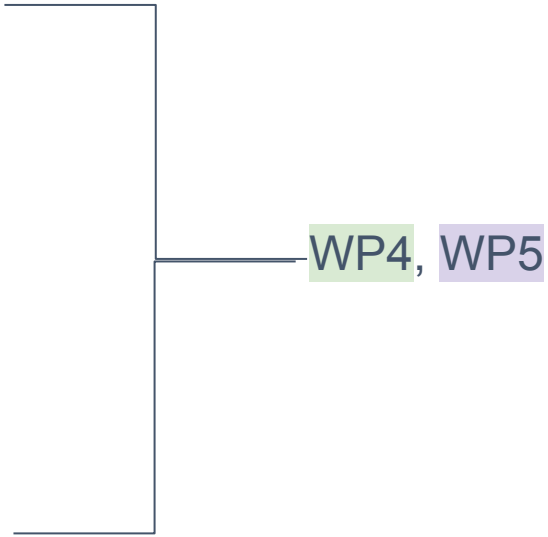
Total: 362,6 PM

no interest from industrial partners

Proposed working groups

1. Eulerian Codes (WP1, WP2)
2. Lagrangian Codes (WP1, WP2)
3. Time series (WP1, WP2, WP3)
4. Feature extraction (WP3)
5. Bayesian inference(WP2 , WP3)
6. Deep learning (WP1,WP3)
7. Visualization (WP3)
8. Data-reduction & imaging (WP1, WP2)
9. Semi-numerical codes (WP1, WP2)
10. Web-tools (WP4, WP5)
11. Platforms (WP4, WP5)
12. Data-model (WP1, WP2, WP3 ,WP4, WP5)



WP2: topics of interest (to be completed and homogeneized)

Partner	Codes / algorithms	Recruited personnel
UniTS	OpenGadget (WG2), Pinocchio (WG2)	1 PhD, 1 RTDA
INAF	*N-body EXASCALE simulations; galaxy formation with reinforcement learning; direct-summation N-body simulations of stellar systems in the realm of galactic nuclei through advanced Exascale-ready codes; optimization of gravity solvers; [other scientific activities]*	
SISSA	OpenGadget (WG2), GALAPY (WG5), SCAMPY (WG9), SEVN (WG9), TSUNAMI (WG2), ISTEDDAS (WG2)	2 AdR
UniTO	PLUTO (WG1), Symorb/Norbit (WG9), Dashboard (WG11)	1 PhD, 1 AdR, 1 RTDA
UniCT	MCMC inference algorithms (WG5)	1 PhD
INFN	COSMICA (WG9), PLUTO (WG1), data analysis for LiteBIRD (WG9), Boltzmann codes (WG9)	2 PhD, 1 tecnologo
SNS	*Pipeline development for observational, experimental and synthetic data analysis; implementation of coding solutions for ARM-based clusters coupled with traditional HPC machines*	
RomaTOV	TOAST (WG9), *MHD code for planet formation (WG1), fitting multi-temporal and multi-frequency signals (WG3)*	2 PhD, 1 AdR, 1 tecnologo

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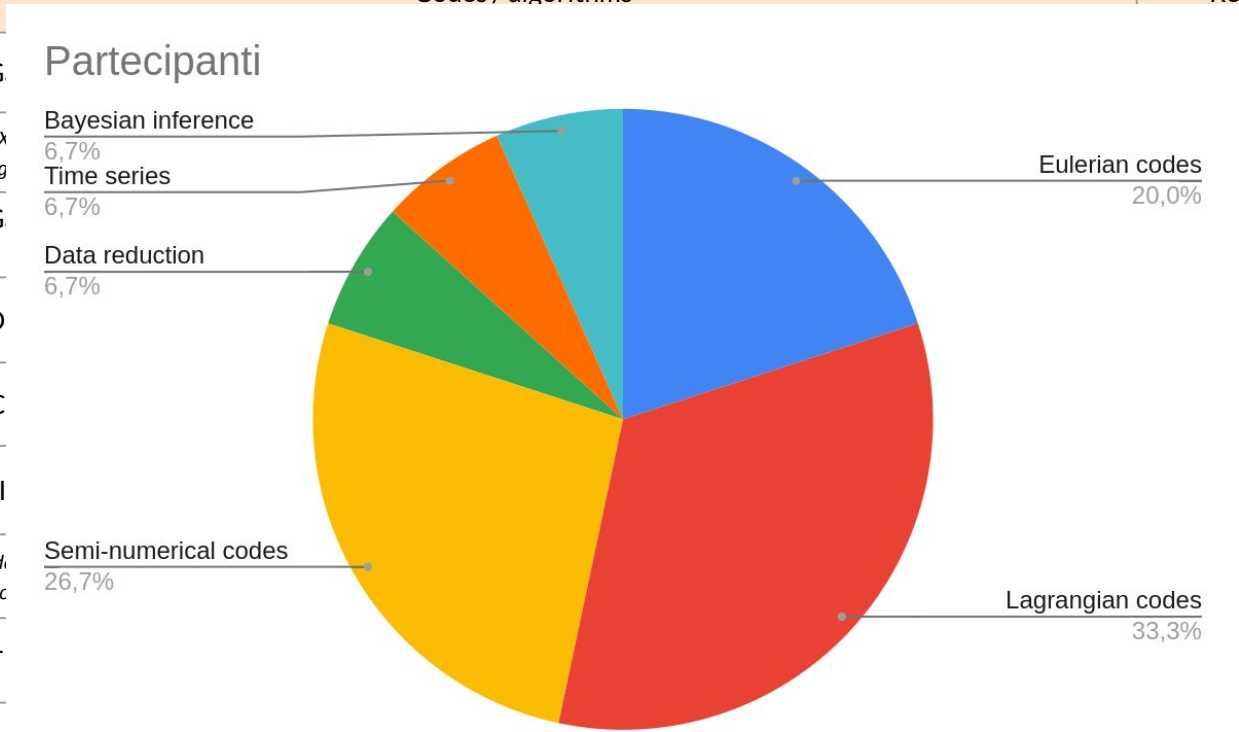
INAF	*N-body EX realm of g*	
SISSA	OpenG (WG2)	
UniTO	PLUTO	. AdR, 1 RTDA
UniCT	MCMC	
INFN	COSMI	. tecnologo
SNS	*Pipeline d clusters co*	
RomaTOV	TOAST	. AdR, 1 tecnologo



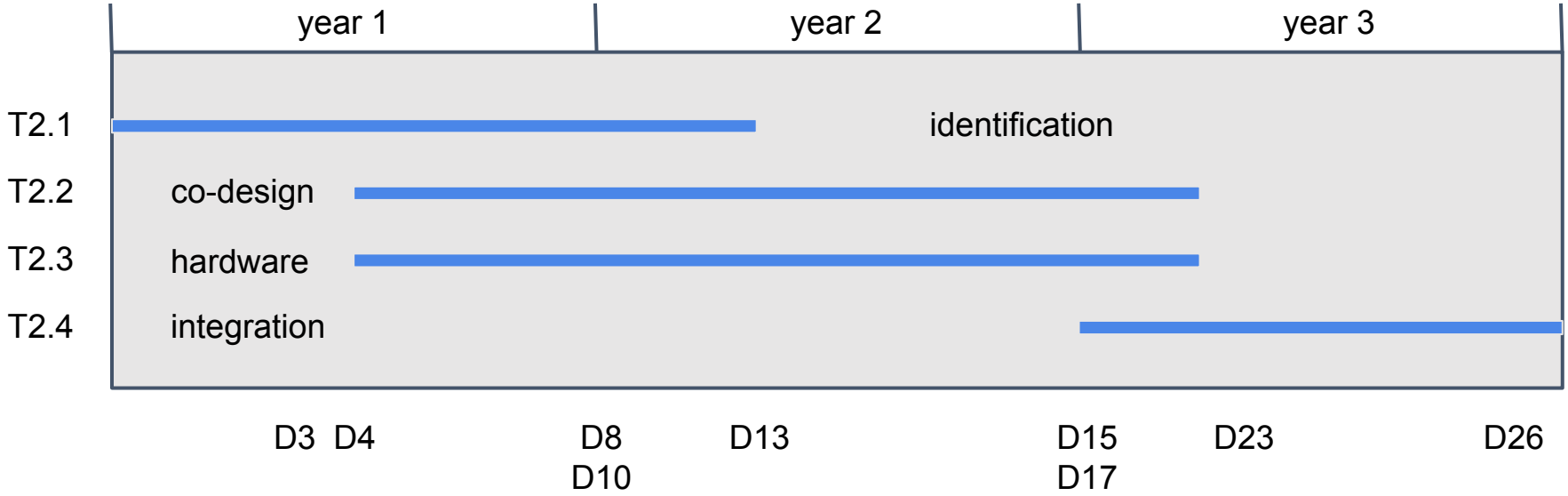
WP2: participants

	PM in 3 years	Involvement	Topics (from Tabella Riassuntiva of WP partners efforts)
INAF	44,0	10 %	Co-desing, energy, innovative algorithms, parallel algorithms, numerical simulations
INFN	13,0	15 %	Development of advanced models in CMB analysis pipeline with a focus on the inclusion of systematic effects due to cosmic rays
ROMATOV	84,0	29 %	Development of advanced models to be fitted to hyper-spectral and spatial resolution data. New algorithms for the identification and characterization of multi-temporal and multifrequency signals. Re-designing of simulation codes for CMB datasets to exploit GPUs.
UNITS	48,75	18 %	Co-design, including green-ization, of specific algorithms utilized in codes for cosmological simulations
UNITO	30	20 %	Sviluppo di metodi innovativi per l'implementazione di metodi ibridi fluido-particelle; Code validation / Verification; Sviluppo di nuove pipelines per la riduzione di ingenti quantità di dati osservativi (LOFAR, SKA,MUSE)
UNICT	46,8	42 %	Optimization of MCMC inference techniques on parallel/HPC architectures to include the spectroscopic inference of stellar parameters in large large astrophysical surveys; innovative approaches to data analysis and visualizations.
SNS	49	35 %	Pipeline development for observational, experimental and synthetic data analysis; implementation of coding solutions for ARM-based clusters coupled with traditional HPC machines
SISSA	47	35 %	N-body EXASCALE simulations; galaxy formation with reinforcement learning; direct-summation N-body simulations of stellar systems in the realm of galactic nuclei through advanced Exascale-ready codes; optimization of gravity solvers; [other scientific activities]
TOTAL	**362,6**		

WP2: deliverables (as in the proposal)

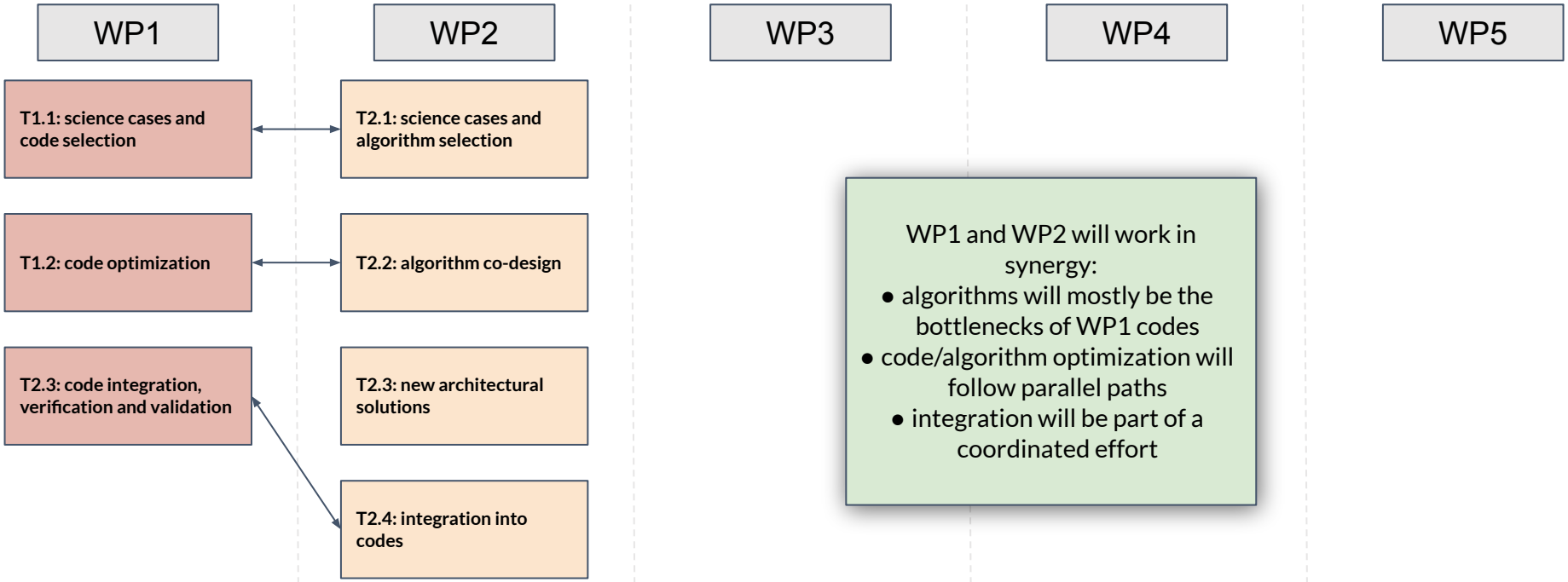
#ID	Deliverable name	Short description	Type	Dissem. level	Delivery date (months)
D3	Spoke Project Plan (M4.2)	This will be written by all WPs	Report	Public	M4
D4	Activity status report (M6.1)	Science cases/requirements definition activity status report	Report	Public	M6
D8	Activity status report (M12.2)	Spoke's first year activity status report, written by all WPs	Report	Public	M12
D10	Requirements definition document (M12.4)	Spoke requirement definition document: science cases, algorithms and technologies definitions	Report	Public	M12, M16
D13	Requirements definition document (M12.4)	Algorithms identification, extraction and profiling definitions	Report	Public	M16
D15	Activity status report (M24.2)	Spoke's second year activity status report, written by all WPs	Report	Public	M24
D17	Performances (M24.4)	Report on performances, scaling and profiling of selected algorithms	Report	Public	M24
D23	Best analysis strategies (M28.2)	Report on best analysis strategies and profiling on HPC infrastructures for astrophysical cases	Report	Public	M28
D26	Final activity report (M36.3)	Spoke's final activity status report, written by all WPs	Report	Public	M36

WP2: timeline (as in the proposal)



Note: deliverables are very generic, we need to identify a number of flagship algorithms to deliver, algorithm selection must take into account project feasibility, for the given resources

WP2: interactions with other WPs



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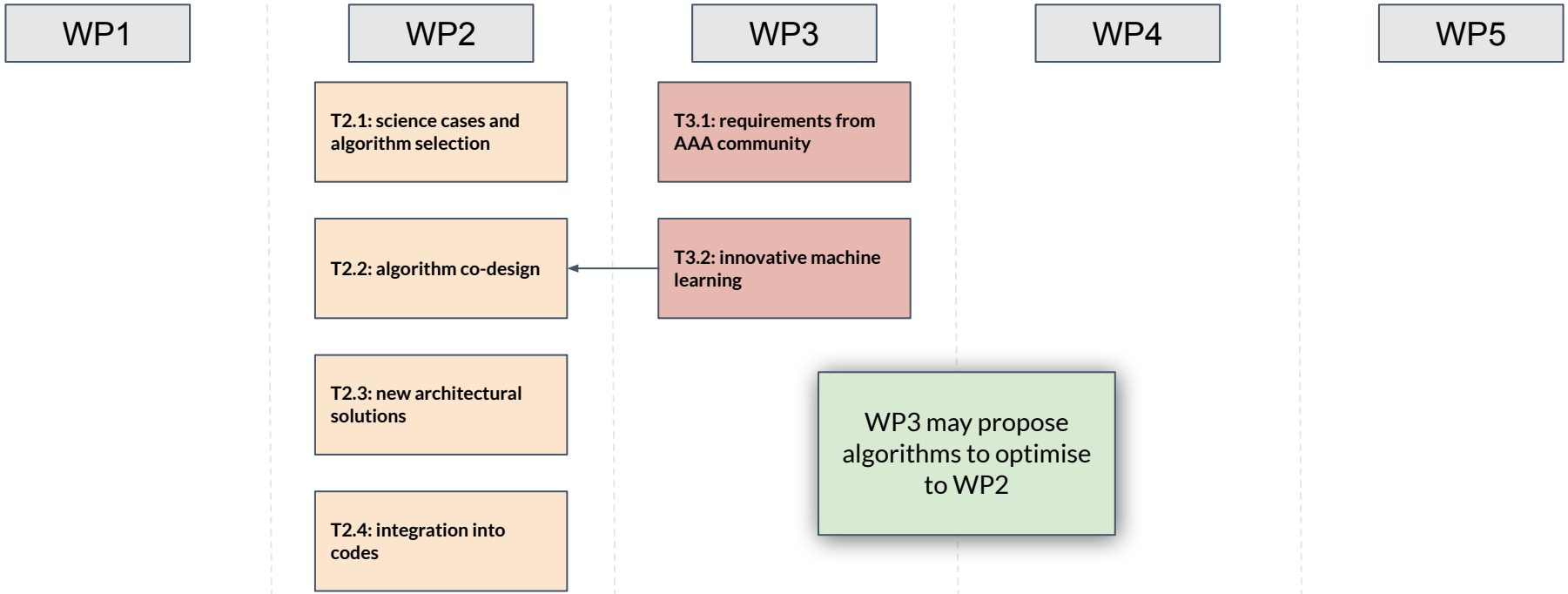

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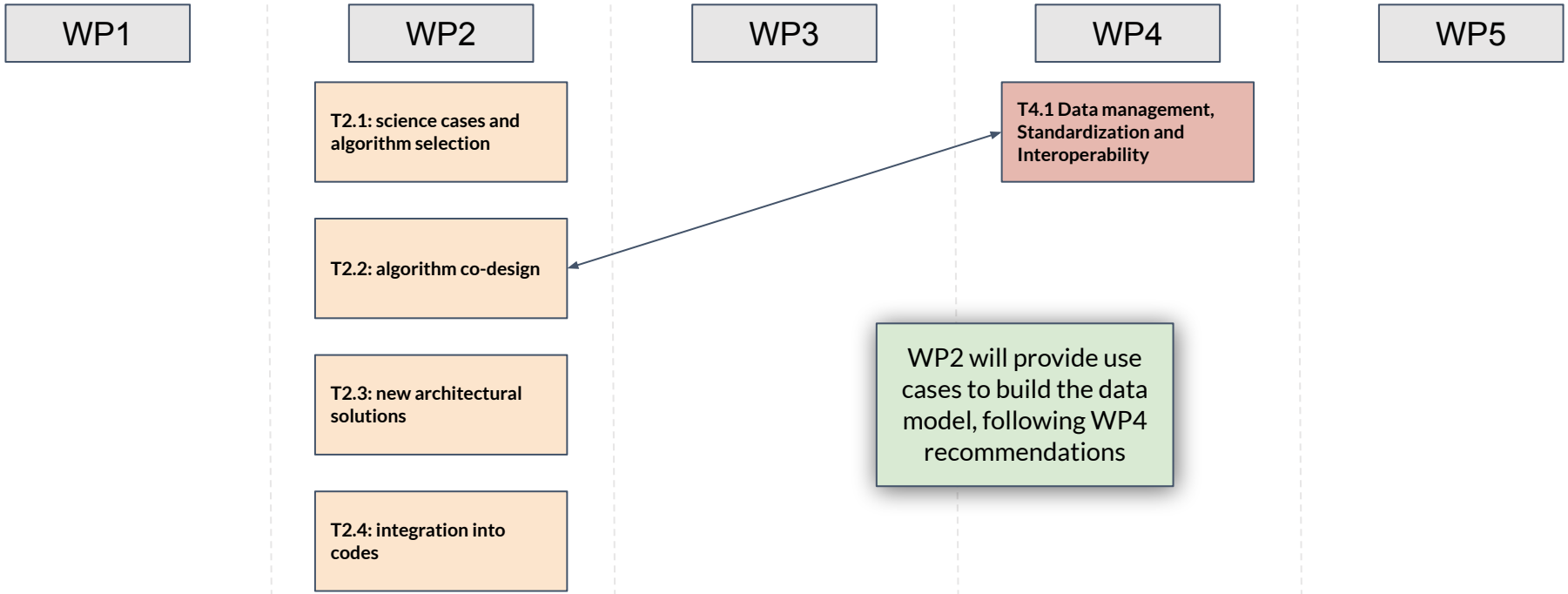

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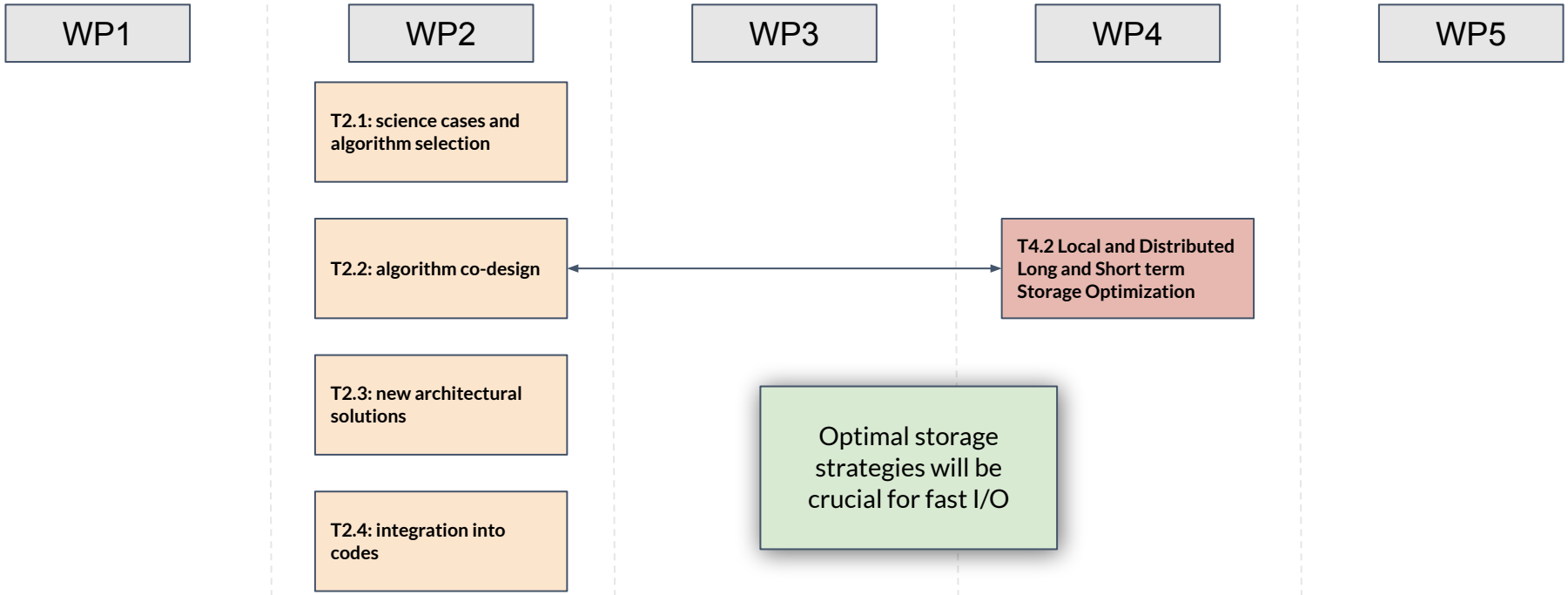

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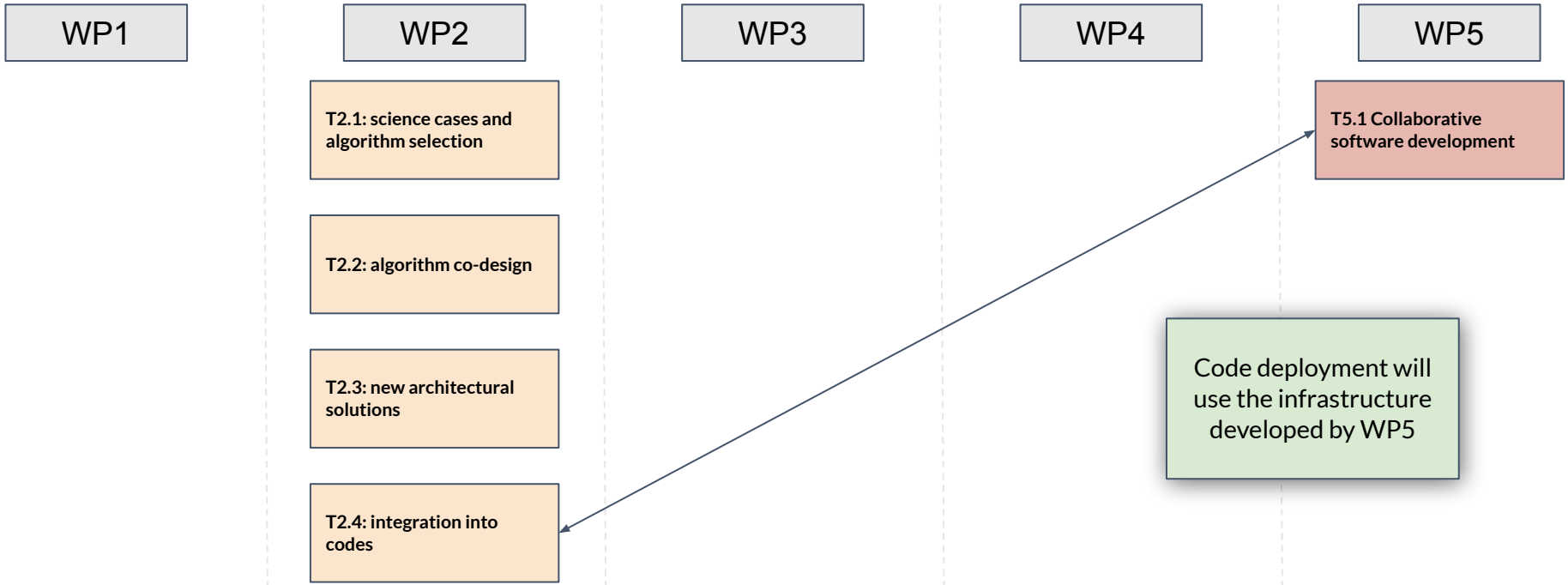

WP2: risks

Risk	Likelihood	Severity
Our recruitment campaign fails	medium	high
We fail to produce and deliver improved codes/algorithms	high	low (with priorities)
We fail in creating synergies among WPs and WGs	medium	high
Project purpose and needs are not well defined	high	high
Software/code/services clash with the chosen architecture	high	high
We replicate the same effort in different Spokes	high	medium
…		

WP2 Conclusions: what we need to do

WP1 and WP2 should be considered as parts of the same work:

- re-engineering a code for better performance is WP1,
- extreme optimization on a part of a code is WP2.

By december 2022 we need a **draft workplan**, that details WG structure, deliverables, milestones.

Deliverables **must be delivered** to have access to the next chunk of funds, so we need to be very careful in specifying what we are going to do. We need to prioritise our plans, e.g.:

- **P1**: algorithms that are critical to the success of the project,
- **P2**: algorithms that will plausibly be delivered,
- **P3**: algorithms that we wish to improve, but success depends on extra resources.

Task 2.1: with WP1 we are surveying our participants to decide which codes/algorithms we select for the three priority classes, splitting the work into WP1 and WP2 (also a-posteriori). We can use open calls to

People joining the effort will be divided into two classes:

- **developers**,
- **consultants**.

Once algorithms are selected, we need to provide **use cases to WP4** for the DMP, and receive recommendations for good practices of data management.

Thanks for the attention, pierluigi.monaco@inaf.it, cn1-spoke3-wp2@inaf.it