TSVV #7 requests for ACH support

Support of Advanced Computer Hubs (ACH) for "Theory, Simulation, Validation and Verification" (TSVV) Task 7 "Plasma-Wall Interaction in DEMO" is requested on two levels corresponding to the following categories as defined in the call, Ref. PMU/1740:

Cat.1 – High Performance Computing (in particular, code parallelization & performance optimization, GPU-enabling)

Cat.2 – Integrated Modelling and Control (in particular, code adaptation to IMAS)

The requested ACH support is estimated at 9 ppy in total, or 1.8 ppy/y in average over 5 years of the project duration.

The codes listed below currently have no or only rudimental IMAS compatibility.
ALL of the listed codes will need ACH4 (IPPLM) support estimated in total at 5 ppy (1 ppy/y).

The HPC related support (Cat.1) is summarized in the following table:

Code name	Code description	Tasks required to ACH	ACH name	PPY estimate
BIT-1D BIT-3D	PIC-MC codes for plasma, neutral and impurity dynamics in the scrape-off layer, including their non-linear interaction	The codes have already been optimized by the HLST. Currently no further support is requested but not excluded in the future.	ACH-MPG or other of Cat.1	0.0 ppy
SPICE-2D SPICE-3D	PIC codes for sheath modelling	Upscaling from cluster-parallel to HPC-parallel, some optimization has been already done by the HLST	ACH-MPG or other of Cat.1	0.5 ppy
ERO2.0	3D Monte-Carlo code for impurity tracing and plasma-wall interaction	Improved parallelization, such as e.g. compiler optimization and GPU, some work initiated via HLST	ACH-MPG or other of Cat.1	0.5 ppy
SDTrimSP-1D SDTrimSP-3D	Monte-Carlo codes for transport of ions in matter	Upscaling from cluster-parallel to HPC-parallel	ACH-MPG or other of Cat.1	0.3 ppy

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MEMOS-U	Melting and melt layer motion. Solves incompressible resistive thermoelectric magneto-hydrodynamic equations in the magneto-static limit and the heat convection-diffusion equation.	Improvement of the code architecture and modularity, in particular in terms of reduction of memory usage	Any of Cat.1	0.5 ppy
MIGRAINe	A coupled system of equations describing charging, heating, motion and mass ablation of spherical dust particles in 3D plasma environment.	Ensure HPC compatibility of the effective parallelization of serial simulations achieved by splitting the simulated trajectories into batches	Any of Cat.1	0.2 ppy
RAVETIME	Parallel finite-volume 3D transport code designed to take advantage of developments within the European Exascale computing project VECMA on UQ methods	Upscaling from cluster-parallel to HPC-parallel and GPU-enabling	ACH-MPG or other of Cat.1	0.5 ppy
EasyVVUQ	Meta-code for UQ of other codes	Currently no support requested		0.0 ppy
Interatomic potential development	Molecular Dynamics Simulations and/or Gaussian Approximation Potential (GAP) machine learning formalism	Optimization and GPU-enabling	ACH-VTT (local for respective modelling group) or any of Cat.1	0.5 ppy
Retention codes	Reaction-diffusion and FEM codes that are partly using commercial software and so far run on local machines	A framework for effective parallelization will be considered at a later stage of the project	Any of Cat.1	0.5 ppy

Total: 4.0 ppy (0.8 ppy/y)