



PRACE 18th Call for Proposals welcomes 2 new HPC systems and includes a Pilot Phase with the Fenix federated data infrastructure

The 18th Call for Proposals for PRACE Project Access received 51 eligible proposals, of which 36 were awarded a total of 1.46 billion core hours. This brings the total number of Project Access proposals awarded to 688 since 2010. Taking into account the six multi-year projects from the 14th and 16th Calls that were renewed, and the 9.2 million core hours reserved for Centres of Excellence, the total amount of computing time awarded by PRACE to date totals nearly 21 billion core hours.

The 36 awarded proposals are led by principal investigators from 13 different European countries as well as one from Australia. In addition, several of these proposals involve collaborators from Canada, China, USA and Japan.

Among the newly awarded proposals, seven scientific domains are represented: 7 proposals are linked to the fields of Biochemistry, Bioinformatics and Life Sciences; 10 to Chemical Sciences and Materials; 3 to Earth System Sciences; 4 to Engineering; 8 to Fundamental Constituents of Matter; 1 to Mathematics and Computer Sciences; and 3 to Universe Sciences.

The 18th Call for Proposals included two new HPC systems. Two proposals were allocated a total of 62 million core hours on **JUWELS@GCS@JSC, Germany** while 3 proposals were allocated a total of 77.4 million core hours on **SuperMUC-NG@GCS@LRZ, Germany**. The 18th Call also allowed applicants to access resources from the Fenix federated data Research Infrastructure, funded by the European ICEI project. This Pilot will also be included in the 19th Call for Proposals.

The largest allocation of 86 million core hours on **Marconi-KNL@CINECA, Italy** was awarded to Prof. Kalman Szabo from the Jülich Supercomputing Centre in Germany. This project, titled **STRONGSCALE – Precision Determination of a Length Scale in Simulations of the Strong Force**, will carry out simulations to determine more precise values for parameters that can be used in physics experiments and large scale lattice QCD simulations. The next largest allocation of 81.6 million core hours on **Piz Daint@ETHZurich/CSCS, Switzerland** was awarded to Dr. Gabriele Tocci from the University of Zurich in Switzerland. This project, titled **Ab Initio Molecular Dynamics for Nanoscale Osmotic Energy Conversion**, will investigate the role of the electronic structure of materials on ionic transport by performing accelerated ab initio molecular dynamics simulations and computing transport properties using hydrodynamic theory.

Two proposals that aim to carry out simulations to assist in the design of anticancer drugs were awarded. **High Performance Computing assists Drug Design in the Discovery of Innovative Anticancer Drug Candidates as Ligands of the Shelterin Protein TPP1** will be led by Prof. Vittorio Limongelli from Università della Svizzera Italiana in Switzerland and was awarded 16.5 million core hours on **Joliot Curie-SKL@GENCI@CEA, France**. **COMPUNANOBIO SOL – Computational Nanobiosolutions: In Silico Drug Design of Efficient Metal Complexes and Polyoxometalates for Cancer Treatments and Antibiotic Resistance** will be led by Dr. Adrià Gil-Mestres from CIC-nanoGUNE in Spain and was awarded 72.6 million core hours on **Marconi-KNL@CINECA, Italy**.

Overall, the 18th PRACE Call for Proposals for Project Access awarded resources to Principal Investigators whose work is funded by the following: ERC Advanced Grant (3), ERC Starting Grant (2), ERC Consolidator Grant (1), COST Action (2), and Marie Skłodowska Curie Fellowship (4). In addition, resources were also awarded to Principal Investigators involved in H2020 (3), and the EUROfusion (1) and Human Brain (1) projects.



All information and the abstracts of the projects awarded under the 18th PRACE Call for Proposals can be found here: www.prace-ri.eu/prace-18th-project-call/

The **18th Call** for Proposals for PRACE Project Access (Tier-0) was open from 04 September 2018 until 30 October 2018. Selected proposals will receive allocations to PRACE resources from 02 April 2019 to 01 April 2020. The **19th Call** for Proposals for PRACE Project Access (Tier-0) is open from 05 March 2019 to 30 April 2019, 10:00 CEST, see here: www.prace-ri.eu/prace-project-access/

About PRACE

The Partnership for Advanced Computing in Europe (PRACE) is an international non-profit association with its seat in Brussels. The PRACE Research Infrastructure provides a persistent world-class high performance computing service for scientists and researchers from academia and industry in Europe. The computer systems and their operations accessible through PRACE are provided by 5 PRACE members (BSC representing Spain, CINECA representing Italy, ETH Zurich/CSCS representing Switzerland, GCS representing Germany and GENCI representing France). The Implementation Phase of PRACE receives funding from the EU's Horizon 2020 Research and Innovation Programme (2014-2020) under grant agreement 730913. For more information, see www.prace-ri.eu

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