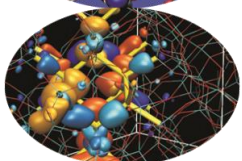
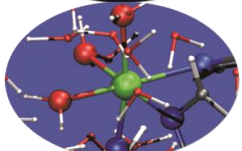
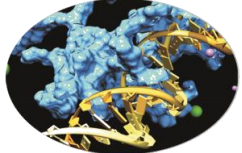
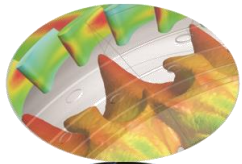


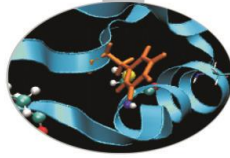


# How to obtain HPC resources

A. Emerson, HPC, Cineca.

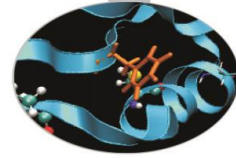


# How do I get access to a supercomputer?



- With the exception of commercial agreements, virtually all access to HPC systems is via peer-reviewed calls to national or international resource providers.
- Depending on the call and provider, usually necessary to write a project proposal detailing the scientific case, how the CPU hours will be used and the application codes which will be run.
- Projects are then evaluated scientifically (for high quality research) and technically (for feasibility).
- In Europe, the principal provider of computer time is PRACE.

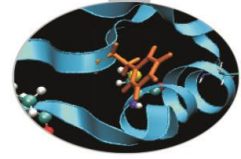
# PRACE



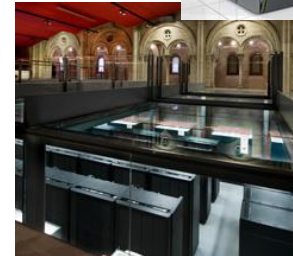
- Partnership for Advanced Computing in Europe
- <http://www.prace-ri.eu/>
- The mission of PRACE is to enable high impact scientific discovery and engineering research and development across all disciplines to enhance European competitiveness for the benefit of society.
- PRACE seeks to realize this mission through world class computing and data management resources and services through a peer review process.
- PRACE is established as an international non-profit association with its seat in Brussels. It has 25 member countries .
- Five Hosting Members (France, Germany, Italy and Spain, Switzerland) provide Multi-PFlop/s Tier-0 Systems.



# PRACE Tier-0 Systems (10<sup>th</sup> Call, 2017)

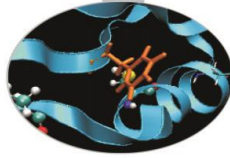


- **Marconi** A1, A2 (Cineca, Broadwell/KNL partition)
- **MareNostrum** (BSC, SandyBridge/SKL)
- **Piz Daint** (CSCS, Cray P100 GPU)
- **Hazel Hen** (HRLS, SuperMUC Broadwell, Sandybridge)
- **Curie** (CINES, SandyBridge)



***Next Call open September 2017***

# PRACE Tier-0 calls



PRACE offers 3 different forms of access to Tier-0 resources:

- **Project Regular Access calls**

Calls for Proposals are issued twice a year and are evaluated by leading scientists and engineers in a peer-review process. Tier-0 proposals typically request many millions of core hours and must demonstrate high parallel scalability.

- **Multi-Year Project Access**

It is available to major projects or infrastructures that can benefit from PRACE resources and for which more than a single year of access is needed.

- **Preparatory Access**

It is a simplified form of access for limited resources for the preparation of resource requests in response to Project Access Calls for Proposals.

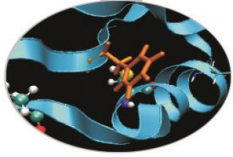
Type **A** (scalability tests)

Type **B** (Enabling + Scalability tests)

Type **C** (Enabling + Scalability tests with PRACE involvement)

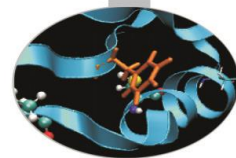
Type **D** (Tier1 for Tier0, Start on Tier1 with the aim of moving to Tier0)

# How to apply for Tier-0 project access - procedure



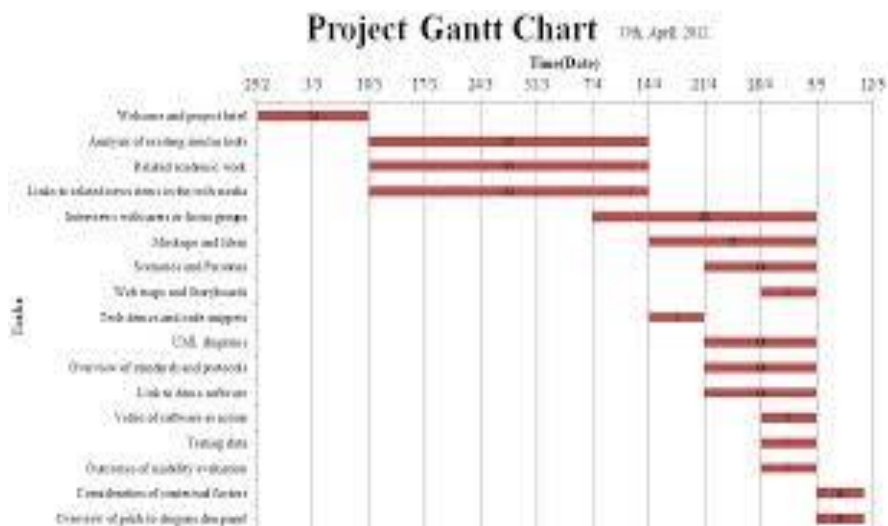
- Consult the application guide from the PRACE website. (<http://www.prace-ri.eu/application-guide/>)
- Register to obtain username+password for the application portal.
- Fill in the on-line application including abstract and technical details.
- Prepare and attach separate project document according to template.
- Submit before deadline (possible to save preliminary versions and even un-submit before final deadline).
- *For Italian applicants (i.e. based in Italy) we strongly recommend you contact us (i.e. Cineca) first before preparing the application.*
- Researchers based in other countries may try contacting their national representative. PRACE staff can also be contacted.

# How to apply for Tier-0 project access –some advice



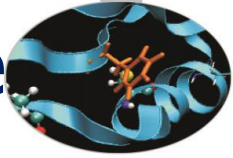
You will have to provide a **Workplan** where you justify the budget you are asking for and how the simulations will be performed in the timescale of the project. Thus in the project document you should include:

- A GANTT chart detailing the activities during the project duration.
- A table demonstrating how you arrive at the requested budget



Simulation type	#cores/run	#runs	Walltime/run (h)	Core hours
Simple MD APoa1	2048	10	1000	20M
MD complex	4096	5	1000	20M
MD complex 2	2048	1	100	2M
			TOTAL	42M

# How to apply for Tier-0 project access – some advice

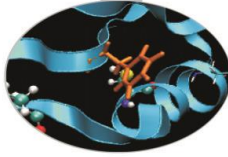


You **must** demonstrate adequate parallel scaling on the chosen computer system.

- Ideally, you will have benchmark results of the proposed input systems (or similar) from a preparatory access or other project on the chosen computer.
- If you don't have such data find scaling data which matches as closely as possible what you wish to do considering hardware, software and input. For classical molecular dynamics, always cite clearly the **number of atoms** in the input – this gives the reviewers a clue as to the scalability (typically max performance at 100-150 atoms/core)
- If possible, consider the use of MPI/OpenMP versions of the applications to save on memory/core and make use of multithreaded hardware.
- Be careful with Replica-Exchange and biased MD-algorithms
  - In NAMD 2.9 (2.10?), Targeted and Steered MD scale poorly because of rank 0 communication.
- NAMD on KNL works only for very large systems. In most cases ask for Marconi/Broadwell.



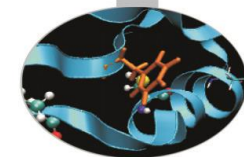
# How to apply for Tier-0 project access – some advice



For classical MD projects other sections in the form are not critical:

- Memory requirements are usually low.
- For most MD simulations I/O is almost negligible so no need to mention MPI/IO, HDF5, etc. Also number of files needed is low.
- Archival of trajectories should be within guidelines (mistake anyway to generate large trajectories)
- All MD codes allow checkpoints (restarts) and so job walltimes < 24h.
- Typical allocations are ~20M core hrs. For <5M hrs you must justify Tier-0 resources.

# Features of PRACE 10<sup>th</sup> Call



## Technical requirements for call 10

[https://prace-peer-review.cines.fr/proposal/PRACE\\_Technical\\_Guidelines\\_for\\_Applicant\\_CALL10.pdf](https://prace-peer-review.cines.fr/proposal/PRACE_Technical_Guidelines_for_Applicant_CALL10.pdf)

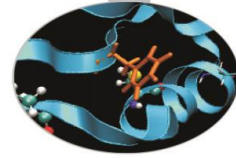
Computer System	Minimum Parallel Scaling	Max memory/core (Gb)
Curie	Fat Nodes 128	4
	Thin Nodes 512	4
	Hybrid 32	3
Fermi	2048 (but typically $\geq 4096$ )	1
SuperMUC	512 ( typically $\geq 2048$ )	*
Hornet	2048	*
Mare Nostrum	1024	2Gb

Other requirements include:

- max no. of files
- storage and archive space
- checkpoint frequency
- simultaneous jobs

\* should use a substantial fraction of available memory

# Typical PRACE Tier-0 call life cycle (project access)



Example CALL 10

10th Sept 2014

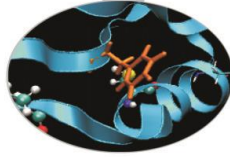
22nd Oct 2014

15-21 Jan 2015

10th March 2015

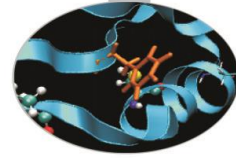
9th March 2016

# Preparatory Access Calls



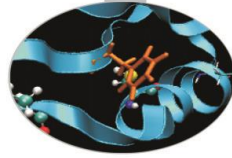
- Designed for code optimisation and benchmarking, possibly with PRACE staff.
- Three types:
  - **Type A** (scalability tests)
  - **Type B** (Enabling + Scalability tests)
  - **Type C** (Enabling + Scalability tests with PRACE involvement)
  - *(Type D [Tier1 for Tier 0] Small allocation on Tier1 machines in Europe.)*
- Calls every quarter (March; July; September; December). Start date 2 months after submission (if successful).
- Allocation periods normally 2 months (Type A) and 6 months (Types B and C).
- Budget allocations depend on type and computer and partition (GPU, MIC, etc). For example, 100K (Type A) and 250K core hours (Type B,C) for BG/Q, between 50K-200K core hours for other computers.
- Proposals evaluated using a “lightweight” evaluation procedure. Applications should include description of issues preventing scalability.

# National Resources - Italy



- For Italy-based researchers, Cineca provides computer time via the **ISCRA** calls. <http://www.hpc.cineca.it/services/iscra>
- Two types of call (B and C) available for accessing Marconi:
  - B KNL: 200K- 4M hrs, BROADWELL: 200K- 2M core hours
  - C KNL: <400K core hours, BROADWELL: <200K core hours.
- For type B two calls/year, type C continuous submission and reviewed once/month.
- Applications must be submitted in English and are evaluated both scientifically and technically.

# HPC Europa-3

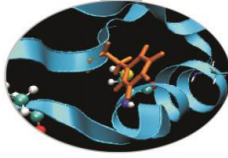


## *Trans-national Access for researchers*

- The project is based on a **program of visit**, in the form of traditional transnational access, with researchers visiting HPC centres and/or scientific hosts who will mentor them scientifically and technically for the best exploitation of the HPC resources in their research. **The visitors will be funded for travel, accommodation and subsistence, and provided with an amount of computing time suitable for the approved project.**
- The **calls for applications are issued 4 times per year** and published online on the HPC-Europa3 website.

Next call expected around early December 2017.

# Final comments



***Do not neglect the technical description of the project!***

- Like experimental work it is important before submitting any application to understand what resources are needed, particularly CPU time but also memory, disk, accelerators, etc.
- For any call, important to have good estimates of the performance at the parallelism you need (i.e. number of cores) so you can plan the simulations and know how long they are likely to take. If you don't know, you can try PRACE preparatory access or ISCRA-C. ***At the very least include the number of atoms in the project description*** (but not sufficient for PRACE T0).
- Include also MD-specific optimisations or algorithms – time step, implicit/explicit solvent, SHAKE, REMD, metadynamics, etc.
- In case of doubt for any of these calls feel free to contact us.