

## **Atto di affidamento per l'utilizzo delle soluzioni CINECA**

### **e dei servizi di assistenza connessi**

#### **CONDIZIONI DI DETTAGLIO**

L'Istituto Nazionale di Oceanografia e di Geofisica Sperimentale - OGS (di seguito anche OGS o "il RICHIEDENTE"), con sede legale in Borgo Grotta Gigante, 42/C, 34010 Trieste, Codice Fiscale e Partita IVA 00055590327, nella persona del Presidente Prof. Nicola Casagli, il quale dichiara di essere munito di tutti i necessari poteri per la sottoscrizione del presente atto nell'ambito dei rapporti consortili, ha richiesto e affidato a CINECA lo svolgimento delle attività di seguito indicate, tenuto conto di quanto definito nel documento "*Atto di affidamento per l'utilizzo delle Soluzioni Cineca e dei servizi connessi - Premesse e condizioni generali*" e nella documentazione tecnica, nella versione corrente al momento della sottoscrizione dell'atto, consultabili nello spazio wiki <http://documentazione.cineca.it>, cui il presente atto fa riferimento.

#### **PREMESSO CHE**

- grazie alla collaborazione tra 25 Paesi europei ed al supporto dalla Commissione Europea è stata creata una infrastruttura di ricerca nel campo dell'High Performance Computing, denominata PRACE, giuridicamente configurata quale associazione internazionale con finalità di facilitare l'accesso alle più avanzate risorse di calcolo e servizi di data management ai ricercatori europei per applicazioni scientifiche e ingegneristiche. Lo statuto e la struttura governativa di PRACE sono fase di ridefinizione (entro il 2023);
- la European High Performance Computing Joint Undertaking (EuroHPC JU) è un'entità legale e finanziaria, creata il 28 settembre 2018 e con sede in Lussemburgo con lo scopo di guidare il supercalcolo europeo; EuroHPC JU consente all'Unione Europea e ai paesi partecipanti all'iniziativa di coordinare i loro sforzi e mettere in comune le proprie risorse per fare dell'Europa un leader mondiale nel supercalcolo, rafforzando l'eccellenza scientifica e la forza industriale dell'Europa, e sostenendo la trasformazione digitale della sua economia garantendone al tempo stesso la sovranità tecnologica.

- L'OGS è un Ente di ricerca a carattere multidisciplinare nel campo delle Scienze della Terra che, in coerenza con la propria storica tradizione di eccellenza scientifica e con lo scopo di diffondere le conoscenze e la cultura, opera e sviluppa la propria missione nell'ERA (Area Europea della Ricerca) e in ambito internazionale con prioritario riferimento ai settori della ricerca in Oceanografia (fisica, chimica, biologica e geologica), Geofisica sperimentale e di esplorazione, Sismologia e sismologia applicata all'ingegneria.
- L'OGS promuove e realizza, anche interagendo a livello nazionale ed internazionale con analoghi soggetti, la relativa ricerca scientifica e tecnologica avvalendosi tra l'altro di navi da ricerca oceanografiche globali e di infrastrutture di ricerca strategiche e di eccellenza nei campi di competenza.
- L'OGS ha una lunga e consolidata esperienza nell'utilizzo di calcolo avanzato e nelle attività di sperimentazione di sistemi avanzati per il calcolo e l'elaborazione dei dati nell'ambito delle Scienze della Terra, attività che vede l'OGS impegnato sia mediante investimenti economici, sia mediante l'impegno di numerosi ricercatori;
- nell'ambito dei propri fini istituzionali l'OGS ha inteso promuovere la propria partecipazione al progetto di ricerca PRACE ed ha ricevuto, a tal fine, dal Ministero dell'Università, dell'Istruzione e della Ricerca (MIUR) (oggi MUR) un contributo straordinario denominato PRACE-Italy ("Contributo straordinario MUR relativo al FOE per la partecipazione dell'Italia alle attività relative all'infrastruttura internazionale PRACE – The Partnership for Advanced Computing in Europe");
- CINECA è un consorzio interuniversitario costituito per le finalità meglio definite nel citato documento *"Atto di affidamento per l'utilizzo delle Soluzioni Cineca e dei servizi connessi - Premesse e condizioni generali"*;
- CINECA ha ricevuto mandato dall'allora MIUR per ospitare il sistema di calcolo di livello Tier-0 italiano;
- CINECA ha ottenuto nell'ambito del programma PRACE un co-finanziamento per istruire una iniziativa di "Pre-Commercial Procurement" per un sistema di calcolo con caratteristiche di prototipo di produzione che è stato installato nella seconda metà del 2017;

- CINECA, essendo uno dei membri fondatori di PRACE e rappresentando l'Italia in ambito PRACE su mandato del Ministero dell'Istruzione, dell'Università e della Ricerca ed in qualità di uno dei 5 Hosting Members di sistemi PRACE HPC di classe Tier-0, ha messo a disposizione della comunità scientifica italiana ed europea il supercalcolatore MARCONI100, la nuova partizione Marconi accelerata disponibile da aprile 2020 sino a marzo 2023. Si tratta di un sistema IBM equipaggiato con NVIDIA Volta V100 GPU e capace di una potenza di picco di 21,6 PFlops, che lo pone attualmente al 11° posto assoluto e al 3° in Europa nella classifica dei 500 calcolatori più potenti al mondo ([www.top500.org](http://www.top500.org), novembre 2020). MARCONI100 è dotato di 980 server di calcolo, ognuno equipaggiato da due processori IBM Power9 e 4 GPU NVIDIA Volta V100. I server di calcolo sono interconnessi tramite rete ad alte prestazioni (alta banda e bassa latenza) di tipo Mellanox EDR InfiniBand a 100 Gbs. Il sistema dispone di un totale di 31.360 core di calcolo, 3.920 dispositivi di accelerazione GPU, oltre 250 TB di memoria RAM e uno spazio di archiviazione di tipo hot-storage di 8 PB;
- CINECA ha installato un sistema di supercalcolo Lenovo, basato su microprocessori e rete Intel di ultima generazione. La configurazione attuale è costituita da Marconi-A3 con SkyLake (in produzione da agosto 2017, aggiornato a gennaio 2018 e completato a novembre 2018);
- CINECA ha partecipato al progetto europeo ICEI (Interactive Computing e-Infrastructure) per la creazione di una infrastruttura di supercalcolo a supporto dei workflow interattivi (Interactive Supercomputing), data intensive (BigData) e virtualizzati (HPC-Cloud). Questo nuovo sistema, denominato GALILEO100 progettato da DELL, è disponibile per il pubblico italiano e per i ricercatori industriali da settembre 2021.
- Recentemente CINECA, insieme all'Istituto Nazionale di Fisica Nucleare (INFN), ha ricevuto fondi dal MIUR per costruire un nuovo datacenter che è situato al Tecnopolo di Bologna, nello stesso polo tecnologico in cui è stato realizzato il nuovo centro per il Centro Meteo Europeo ECMWF. A luglio 2022 è stata completata una prima parte del data center, cioè il white space che ospita il supercalcolatore Leonardo realizzando

una struttura sisma-resistente a tre livelli, il gray space che ospita 4 centrali frigorifere per il raffreddamento del supercalcolatore, 4 tunnel tecnologici che collegano il white space e il gray space. Il datacenter verrà completato nell'estate del 2023.

- Il 24 novembre 2022 è stato inaugurato il sistema Leonardo pre-exascale nel nuovo datacenter del Cineca presso il Tecnopolo di Bologna. Leonardo è il risultato di una proposta presentata dal CINECA in rappresentanza dell'Italia in accordo con il MUR, INFN e la Scuola Internazionale Superiore di Studi Avanzati (SISSA) e approvato dalla Joint Undertaking Europea EuroHPC. E' stato progettato da Cineca e combina i componenti di calcolo più avanzati per essere in grado di affrontare anche i flussi di lavoro computazionali più complessi, eventualmente coinvolgendo applicazioni HPC, AI, high-throughput e di visualizzazione. Con una prestazione High-Performance Linpack (HPL) misurata di 174,7 petaflop, il supercomputer Leonardo ha raggiunto la quarta posizione nell'ultima edizione della classifica Top500 dei supercomputer più veloci al mondo.
- CINECA collabora con l'OGS dagli anni '90 nell'ambito delle applicazioni numeriche per le scienze della terra (modellistica oceanografica accoppiata alla biogeochimica e modellistica sismica per la propagazione di onde sismiche in mezzi eterogenei 3D). Tale collaborazione è stata fondamentale per condurre le ricerche finanziate da progetti europei e nazionali in questi ambiti;
- l'OGS e il CINECA hanno stipulato un accordo per la realizzazione di un programma di formazione nel campo del calcolo ad alte prestazioni (High Performance Computing - HPC) per applicazioni in Scienze della Terra, denominato "High Performance Computing Training and Research for Earth Sciences" (HPC-TRES), co-finanziato dal MUR tramite il contributo straordinario PRACE-Italy. Gli obiettivi principali del programma sono il capacity building, la valorizzazione del capitale umano e la formazione avanzata nei campi della modellistica del Sistema Terra e dei metodi numerici, questi ultimi considerati componente trasversale strategica per la modellistica. Tali obiettivi verranno perseguiti attraverso l'utilizzo delle infrastrutture e dei servizi HPC nazionali ed europei in ambito PRACE e EuroHPC, l'ottimizzazione di algoritmi e codici di calcolo,

la gestione di grandi moli di dati e le tecniche di visualizzazione grafica per applicazioni multidisciplinari nelle Scienze della Terra;

- I'OGS e il CINECA sono partner in 3 progetti strategici del Piano Nazionale di Ripresa e Resilienza (PNRR): due centri nazionali (il Centro Nazionale di Ricerca in High Performance Computing, Big Data e Quantum, il National Biodiversity Future Centre), e il progetto infrastrutturale Terabit network for Research and Academic Big data in ITaly (TeRABIT).

#### **PREMESSO INOLTRE CHE**

- tra gli scopi propri del CINECA è presente quello di promuovere l'utilizzo dei più avanzati sistemi di elaborazione dell'informazione a sostegno della ricerca scientifica e tecnologica e quello di favorire il trasferimento tecnologico nel campo dell'informatica, anche sviluppando ricerche per l'utilizzo più efficace delle potenzialità disponibili;
- l'art. 3 del rinnovato Statuto consortile del CINECA dispone, tra l'altro, che *"Scopo primario del Consorzio è la realizzazione di servizi informatici innovativi per i Consorziati, al fine di renderli più efficienti e moderni, nella maniera economicamente più vantaggiosa mediante la valorizzazione di tecnologie e la condivisione degli obiettivi di sviluppo. Gli obiettivi sono realizzati mediante la produzione di servizi ad alta potenzialità ed efficienza e il trasferimento applicativo di tecnologie per lo sviluppo e l'eccellenza del sistema nazionale dell'istruzione superiore ed ella ricerca"*;
- Il supporto alle attività di ricerca della comunità scientifica tramite il supercalcolo e le sue applicazioni fa parte della missione istituzionale del CINECA, che può contribuire con un ambiente di calcolo ai massimi livelli delle architetture e delle tecnologie disponibili. Un aspetto fondamentale è il supporto offerto dal suo personale specializzato altamente qualificato, che affianca i ricercatori nell'utilizzo dell'infrastruttura tecnologica.
- Le competenze acquisite da CINECA negli ultimi decenni nel campo degli strumenti più avanzati per l'utilizzo dei sistemi di supercalcolo – sia per lo sfruttamento dell'hardware che per la progettazione e analisi

degli applicativi software sono messe a disposizione degli utenti tramite un'ampia offerta di servizi di consulenza e formazione specialistica. CINECA organizza mensilmente corsi di aggiornamento e addestramento sia per facilitare l'accesso ai servizi e alle tecnologie disponibili, che per rispondere alla crescente richiesta di figure professionali altamente qualificate nell'ambito del calcolo tecnico-scientifico e dell'Information Technology. L'esperienza formativa e la professionalità del personale docente del CINECA consentono inoltre di gestire specifiche richieste di formazione, adattando la struttura e i contenuti dei corsi al profilo e alle esigenze dei richiedenti. Questo aspetto è di fondamentale importanza in prospettiva delle applicazioni computazionali di classe exascale in grado di sfruttare i sistemi pre-exascale come Leonardo. Da questo punto di vista, CINECA offre alla comunità scientifica un'opportunità unica, garantendo una continuità tecnologica iniziata con MARCONI100 e che prosegue con il sistema accelerato Leonardo fino al 2027. In questa finestra temporale, la comunità scientifica potrà adattare e migliorare gli applicativi per i sistemi di supercalcolo accelerati, ed effettuare uno scale-up delle risorse computazionali - da MARCONI100 a Leonardo - per poter affrontare le principali sfide scientifiche computazionali. Inoltre, CINECA è uno dei PRACE Advanced Training Centres (PATCs), voluti da PRACE per fornire formazione ad altissimo livello ai ricercatori europei sui diversi temi dell'HPC e delle scienze computazionali.

- L'accesso alle risorse computazionali è reso possibile attraverso i bandi di ricerca per progetti ISCRA (Italian Super Computing Resource Allocation, <http://iscra.cineca.it/>) e quelli per i progetti EuroHPC ([https://eurohpc-ju.europa.eu/eurohpc-ju-call-proposals-extreme-scale-access-mode\\_en](https://eurohpc-ju.europa.eu/eurohpc-ju-call-proposals-extreme-scale-access-mode_en)), oltre a convenzioni specifiche con Istituti di ricerca.
- CINECA è oggi il centro di supercalcolo di riferimento per l'Italia, in grado di rafforzare l'impegno italiano per lo sviluppo di e-infrastructure in Italia ed in Europa per HPC, tecnologie HPC, archiviazione e amministrazione di dati scientifici, cloud computing per industrie e amministrazioni pubbliche, sviluppo di metodologie computing-intensive e data-intensive per la ricerca scientifica e ingegneristica. L'investimento

di risorse umane nel campo della modellistica (per quanto riguarda OGS: oceanografica, biogeochimica, sismica, etc.) non può prescindere da un aggiornamento continuo delle infrastrutture di calcolo, accompagnato da un supporto tecnico-informatico di altissimo livello che sia in grado di mantenere le risorse computazionali al passo con l'avanzamento tecnologico. Per raggiungere gli obiettivi prefissati nei progetti di ricerca europei dei programmi Horizon Europe, EuroHPC e Digital Europe, un ritardo nell'evoluzione delle infrastrutture di calcolo diventerebbe un gap difficilmente recuperabile, con il rischio di avere a disposizione risorse umane di valore ma l'incapacità di produrre scienza computazionale di alto livello.

- l'OGS è membro effettivo del Consorzio CINECA;

#### **VISTI**

- la Legge 6 agosto 2015, n. 125;
- gli artt. 5 e 192 del D.Lgs. 50/2016;

#### **SI CONVIENE E SI STIPULA QUANTO SEGUE**

##### **1) Prestazione richiesta**

In conformità a quanto stabilito nelle premesse (le premesse e gli atti in essa citati formano parte integrante e sostanziale del presente atto), l'affidamento da parte dell'OGS nei confronti del CINECA ha ad oggetto lo svolgimento delle attività inerenti allo sviluppo ed all'elaborazione di simulazioni numeriche e lo sviluppo di algoritmi e applicazioni nell'ambito dei domini della geofisica e oceanografia nell'ambito di PRACE-Italy.

La descrizione delle attività che dovranno essere svolte da CINECA è riportata nell'allegato tecnico al presente atto di affidamento. Qualora si verificassero ritardi nella realizzazione di parte delle attività così definite verrà valutata, da parte dell'OGS, una eventuale rimodulazione dei tempi previsti, dandone tempestiva comunicazione al CINECA in forma scritta.

## **2) Oneri economici**

Al fine di sostenere i costi delle attività svolte da CINECA, l'OGS si impegna a versare a CINECA, a valere sui fondi assegnati dal MUR, un importo massimo di € 200.819,67 per il 2023 e di € 230.000,00 per il 2024 (fatta salva la conferma del contributo da parte MUR per il 2024) a titolo di corrispettivo.

Tutti gli importi sopra specificati sono al netto dell'IVA di legge.

## **3) Fatturazione**

Gli importi saranno liquidati entro 30 (trenta) giorni dall'emissione di apposite fatture, che potranno essere ammesse successivamente alla stipula del presente atto di affidamento, previa emissione, da parte dell'OGS, del certificato di regolare esecuzione della prestazione eseguita da CINECA.

Le fatture dovranno riportare il Codice CUP assegnato al progetto. Il pagamento verrà effettuato, ai sensi della Legge 136/2010 e s.m.i, sul seguente conto corrente dedicato all'esecuzione del servizio:

Conto di Tesoreria: BANCA POPOLARE di SONDRIO, Filiale di Bologna via Riva di Reno, n.58/b – 40122 Bologna

IBAN IT14X0569602400000030000X43 Bank Swift POSOIT22.

Gli enti in tesoreria speciale possono effettuare il girofondo sul conto di Banca d'Italia

Conto Bankit (attuazione art. 35 commi 8-13 D.L. 24/01/2012 n.1): 0151884

IBAN: IT22Z0100003245240300151884

e che le generalità ed il codice fiscale delle persone delegate ad operare sul conto dedicato sopra indicato sono le seguenti: Maurizio Tani nato a Ferrara (FE) il 15/06/1954 c.f. TNAMRZ54H15D548E residente in Piazza Malpighi, 4, Bologna.

## **4) Estensione temporale**

Le Parti concordano sul fatto che le attività oggetto del presente atto sono state regolarmente erogate dal CINECA sin dal **01/01/2023** fino alla data di sottoscrizione da parte di CINECA del presente atto a conferma della avvenuta verifica positiva di quanto previsto dall'art. 3.2 del vigente statuto consortile e termineranno in data **31/12/2024**.



E' ammesso il rinnovo dell'affidamento per un periodo di pari durata, previa richiesta scritta da parte dell'OGS e consenso alla stessa da parte del CINECA. Ad ogni rinnovo le parti concorderanno fra loro gli oneri economici.

#### **5) Proprietà intellettuale**

Le Parti avranno la comune proprietà intellettuale delle opere di ingegno eventualmente prodotte, salvo diversi accordi.

#### **6) Obblighi derivanti dal rapporto di lavoro ed adempimenti in materia di sicurezza**

CINECA si obbliga ad ottemperare a tutti gli obblighi verso i propri dipendenti derivanti da disposizioni legislative e regolamentari vigenti in materia di lavoro, previdenza e disciplina infortunistica, assumendo a proprio carico tutti i relativi oneri.

Il personale di una parte che si rechi presso i centri o laboratori dell'altra parte o di altri soggetti coinvolti nel progetto è tenuto al rispetto dei regolamenti sanitari e di sicurezza vigenti presso la parte/soggetto ospitante.

#### **7) Riservatezza**

CINECA ha l'obbligo di mantenere riservati i dati e le informazioni, ivi comprese quelle che transitano per le apparecchiature di elaborazione dati, di cui venga in possesso o, comunque, a conoscenza per effetto delle attività contrattuali.

CINECA assume in ogni caso l'obbligo di non divulgarli in alcun modo e in qualsiasi forma e di non farne oggetto di utilizzazione a qualsiasi titolo per scopi diversi da quelli strettamente necessari all'esecuzione del presente accordo.

L'obbligo di cui al comma precedente sussiste, altresì, relativamente a tutto il materiale originario o predisposto in esecuzione del presente accordo di collaborazione.

#### **8) Referenti dell'attività**

Le Parti concordano sulla necessità di individuare, ciascuno per la sua parte, dei Referenti dell'attività in argomento, aventi il compito di verificare lo svolgimento dell'attività medesima in corso d'opera:

- Per OGS il Dott. Stefano Salon

- Per CINECA il Dott. Mirko Cestari

#### **9) Registrazione**

Il presente atto è sottoscritto in forma digitale. Il presente atto, avendo ad oggetto prestazioni soggette all'IVA, è soggetto a registrazione solo in caso d'uso. Le spese di registrazione sono a carico della parte richiedente. L'imposta di bollo sul presente atto verrà assolta con modalità virtuale tramite l'autorizzazione n. 2016/12144 del 01/03/2016 rilasciata al Consorzio dall'Agenzia delle Entrate di Bologna.

#### **10) Trattamento dati personali**

CINECA e OGS si prestano reciprocamente il consenso al trattamento dei dati personali necessari all'espletamento delle attività derivanti dal presente atto, ai sensi del Reg. UE 2016/679.

#### **11) Allegati**

Allegato tecnico

**Referenti CINECA:** *DEMAND, PM*

**Riferimento:** *Dott. Mirko Cestari*

**Struttura organizzativa:** *Direzione HPC*

Istituto Nazionale di Oceanografia e di Geofisica Sperimentale - OGS

#### **Presidente e Legale Rappresentante**

**Prof. Nicola Casagli**

**F.to digitalmente**

Verificato il rispetto dei principi di economicità, efficienza ed efficacia nonché di autonomia tecnica ed esecutiva, il CINECA, ai sensi dell'art. 3.2 del vigente statuto consortile, dichiara di essere tenuto all'esecuzione delle attività richieste.

#### **CINECA Consorzio Interuniversitario**

#### **Presidente e Legale Rappresentante**

**Prof. Francesco Ubertini**

**F.to digitalmente**

# Allegato Tecnico all'accordo di collaborazione tra CINECA e OGS per il biennio 2023-2024

*Nota: Il documento è redatto in lingua inglese per semplificare la possibilità di valorizzare i contenuti tecnico/scientifici frutto dell'accordo all'interno di documenti internazionali.*

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## Executive Summary

In the financial plan for year 2022 relative to the ordinary grant for research institutes (“Fondo ordinario per gli enti e le istituzioni di ricerca” - FOE), OGS received an extraordinary contribute from the Minister of University and Research ([MUR](#)) for the Italian participation to the activities related to the international infrastructure PRACE – The Partnership for Advanced Computing in Europe (<https://prace-ri.eu/>)<sup>1</sup>, also referred to as **PRACE-Italy**.

OGS, to support its increasing High Performance Computing research activities, that span different fields of the computational Earth Sciences, and to keep on contributing to the national effort in the different challenges posed by the Earth Sciences, either by increasing the knowledge and also toward practical solutions of environmental, economical and social issues in line with the National Program of Research (PNR), the strategic objectives set by the EU (with particular referral to Horizon Europe), and the National Recovery and Resilience Plan (NRRP – part of the Next Generation EU programme), decided to sign a collaboration agreement with Cineca with an endorsement based on the MUR-FOE grant. The present document constitutes the technical annex of the agreement.

In accordance with its mission at the Italian (ISCRA) and European (PRACE and EuroHPC) level, Cineca is going to review its High Performance Computing (HPC) and data infrastructure evolution plan to update the goals in light of the new initiatives coming from EU and international agreements on HPC and BigData signed by the Italian government, like EuroHPC<sup>2</sup> and IPCEI<sup>3</sup>, aimed at bridging the gap from here to the “exascale era”.

The process of architecture’s migration is by nature manifold and complex, should take into account emerging technological and scientific challenges, and must be feasible in terms of economic and environment sustainability.

To this end, Cineca forecasts that future supercomputing facilities will be based on a convergence of traditional HPC architecture toward a new integrated infrastructure capable of approaching the new emerging paradigms for advanced computational sciences: high performance data analytics (BigData), urgent or interactive supercomputing, real time data processing, cloud computing.

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<sup>1</sup> See the document from OGS Board of Directors n. 27/2022 date 21.02.2022 “Approvazione del piano di utilizzo del finanziamento per attività di ricerca a valenza internazionale connessa all’infrastruttura PRACE (FOE 2022) (CUP F55F22000080001)”.

<sup>2</sup> <https://ec.europa.eu/digital-single-market/en/news/eu-ministers-commit-digitising-europe-high-performance-computing-power>

<sup>3</sup> [http://europa.eu/rapid/press-release\\_IP-14-673\\_en.htm](http://europa.eu/rapid/press-release_IP-14-673_en.htm)

In view of this multi-faceted scenario, the service model Cineca is going to adopt is a data-centric paradigm where the data, exponentially increasing in size, will not need to be moved anymore from different computing systems but integrated with them, thus offering a single solution for numerical and data analysis (DA).

All these aspects, to be effective for the scientific challenges, have to be addressed in a co-design approach with application owners, like OGS, and the best place to carry out this activity is a joint lab, where experts on application and supercomputing are “virtually” collocated together in order to afford the formidable challenges behind this scientific and technological goal.

On the other end, the tight collaboration between OGS, Cineca and other relevant national stakeholders could increase the competitiveness of Italy in HPC and the possibility to be involved into European programs dedicated to HPC. An example of such collaboration is the HPC-TRES Joint Research Unit (JRU) composed by OGS, Cineca and other Italian research institutions (ICTP, CMCC, CNR, INGV and Politecnico Torino), which is a legacy of the training and research program HPC-TRES (“HPC Training and Research in Earth Sciences”, see section 3). In the HPC-TRES JRU, formally constituted in 2021, OGS and Cineca act as promoters, while the other national partners actively collaborate in the steering activities.

It is worth noting that compared to the past, the evolution of HPC infrastructure is presently undergoing a radical paradigm shift mainly due to the reaching of the physical limits in the miniaturization of silicon-based transistors, and of a critical threshold of sustainability for energy infrastructure, which becomes even more critical in the current global geo-political situation. The performance boost coming with future exascale supercomputers requires a significant reduction of its energy consumption, and presents unique challenges both in hardware and software: these challenges are so high that only international cooperation in scientific investigation is able to address them adequately.

A strong new cross-disciplinary initiative is needed in order to exploit the full potential offered by the new HPC architectures, without which there is a real risk not only of being cut off from international competition in the field of computational science, but even of not being capable of sustaining the current production capacity. In this perspective, the planned activities of the NRRP-funded National Research Centre for High Performance Computing, Big Data e Quantum Computing, with the Cineca HPC infrastructure at its core (Leonardo was awarded as the 4<sup>th</sup> most powerful world supercomputer in November 2022), are fully aligned.

## **1. PRACE and EuroHPC JU**

The mission of PRACE (Partnership for Advanced Computing in Europe) 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 by offering world class computing and data management resources and services through a peer review process. PRACE also seeks to strengthen the European users of HPC in industry through various initiatives and has a strong interest in improving the energy efficiency of computing systems and reducing their environmental impact.

PRACE is a European infrastructure included in the ESFRI roadmap and it is established as an international not-for-profit association (AISBL) with seat in Brussels. It has 25 member countries (see <http://www.prace-ri.eu/members/>) whose representative organizations create a pan-European supercomputing infrastructure, providing access to computing and data management resources and services for large-scale scientific and engineering applications at the highest performance level. The computer systems and their operations accessible through PRACE are provided by 5 PRACE members. By mandate of the MUR, Cineca represents Italy in PRACE and is one of the five PRACE

"hosting members" providing a Tier-0 computing system. The Statute and the Governance structure of PRACE are in a transitional phase and will be defined during the course of 2023.

In 2018 the EU and the Member States took another step in this strategy, coordinating their efforts to develop a European supercomputing ecosystem towards Exascale in the European HPC Joint Undertaking (EuroHPC JU). The EuroHPC JU was established on 28 September 2018 and is currently regulated by Council Regulation (EU) 2021/1173. Its mission is to deploy world-class supercomputers across Europe and developing a full European supply chain. Italy was among the first to join EuroHPC and, together with Spain and Finland, one of the three countries to host a pre-exascale-class computer.

The EuroHPC supercomputers are made accessible to European researchers, industry and businesses, to develop new applications in areas such as earth system, artificial intelligence and personalised medicine, drug and material design, bio-engineering, weather forecasting, and combating climate change.

The European supercomputer Leonardo was funded by MUR and by EuroHPC JU. Leonardo is hosted and managed by Cineca and was installed in 2022 in the new data center located in the Technopole of Bologna. Leonardo resources will be provided to the Italian researchers through the ISCRA calls and to all scientists and researchers affiliated with European research centers and industries through the calls managed by EuroHPC JU.

The plan is for these facilities to be integrated into a European federated infrastructure, together with other supercomputers through the Fenix initiative, signed by EU's leading supercomputing centres to align their services to provide scalable computing and data services across Europe.

PRACE-Italy, led by OGS and managed by Cineca, is the RI Italian node (listed as high priority RI in the National Plan for Research Infrastructures) which implements PRACE and EuroHPC roadmaps.

## **Exascale Computing**

The concept of "exascale computing" refers to computational systems able to achieve performance of calculation of at least 1 exaflops ( $10^{18}$  operations per second), significantly increasing today HPC system computing capacity. Internationally, there are many recent examples of government investments that have funded the exascale computing for research in various scientific fields, from theoretical research base, the earth sciences, biology, materials science, in the energy field and for national security. The European Union, beside the Horizon 2020 program, with an investment of the order of 700M€ in HPC programs, has recently increased the funding through the EuroHPC initiative to keep the pace with the international competition. USA, Japan, China and India are in fact developing similar programs with comparable or larger investment. It is understood that exascale and extreme data infrastructures could enable and trigger innovations and are considered a strategic asset for the economic growth. As an example, one can consider the case of the new wave of Artificial Intelligence (AI) applications. Thanks to new algorithms, these applications can exploit the computational performance to be more and more accurate. In this case, exascale infrastructures could allow breakthroughs in many field where AI is being applied, like mobility, healthcare, forecasting, social science, etc.

The main challenge toward exascale architectures is the exponential growth of power and energy consumption. With this limit in mind, Cineca is modelling its strategy for future HPC/DA systems in order to experiment, design and deploy energy-aware supercomputing facilities. To this end, Cineca has been involved in several projects at national and EU level to take advantage of the most promising techniques for limiting the overall requirements of energy-to-solution computing workflow.

## CINECA roadmap

Regarding Cineca infrastructure evolution, the upgrade of Tier-0 system Marconi was just a first step toward a tighter integration between computing and data analysis. The new supercomputing system **MARCONI100** has been installed in the first half of 2020. It is an IBM system equipped with NVIDIA Volta V100 GPUs, with a sustained computing power of 22 petaflops, opening the way to the accelerated pre-exascale Leonardo supercomputer. It was ranked in the Top500 list of November 2020 at 11th place.

To support the huge amount of data produced with the Tier-0 system, Cineca deployed in 2021 a new Tier-1 system – **GALILEO100** – devoted to data processing and analysis. It supports scalable and interactive computing workflows thanks to computing nodes equipped with state-of-the-art technology such as Intel CascadeLake CPUs, Intel Optane non-volatile memories and NVIDIA V100 GPUs. A cloud partition based on OpenStack complements the computing partitions. The system also features a high-capacity storage system (20 PB) to host *hot* data, interconnected with the remaining HPC systems in order to provide a *data-centric* approach to the whole infrastructure. To this extent, data hosted on the storage system can in principle be processed or used as input for simulations in all HPC systems, in order to use the most effective hardware for the scope.

On 24<sup>th</sup> November 2022 the **Leonardo** pre-exascale system was inaugurated in the new datacenter of Cineca in Technopole of Bologna. The system was designed by Cineca and combines the most advanced computing components to be able to address even the most complex computational workflows, possibly involving HPC, AI, high-throughput, and visualization applications. With a measured High-Performance Linpack (HPL) performance of 174.7 petaflops, the supercomputer Leonardo reached the 4<sup>th</sup> position on the latest release of the Top500 list of the fastest supercomputers in the world<sup>4</sup>.

Leonardo is structured in two main computing modules:

- A Booster module, which purpose is to maximize the computational capacity. It was designed to satisfy the most computational-demanding requirements in terms of time-to-solution, while optimizing the energy-to-solution. This result is achieved with 3456 computing nodes, each equipped with four NVIDIA Ampere based GPUs driven by a single 32-cores Intel Ice Lake CPU. This partition module has been installed in November 2022 and is capable of nearly 240 PFlops and equipped with over 100 PB of storage capacity.
- A Data Centric module aiming to satisfy a broader range of applications. Its 1536 nodes are equipped with two Intel Sapphire Rapids CPUs, each with a core count over 50, in order to reach over 9 PFlops of sustained performance. This partition will be installed during the summer of 2023.

Leonardo is interconnected through a 200 Gb/s InfiniBand data network and provides 10 times the computational power of the current Cineca flagship system Marconi100.

EuroHPC JU has recently approved Cineca expression of interest for upgrading Leonardo supercomputer, targeting an increase of 100 PFlops of computing capacity, that will be deployed in 2024. The extension – named **LISA** in short, after the universally known portrait Mona Lisa by Leonardo da Vinci – is targeting both a considerable increase in performance and a broadening of the use cases that can be well addressed with the supercomputing system. The upgrade will rely on the modular architecture of Leonardo and aims to add two more computing modules.

EuroHPC JU in October 2022 announced the selection of the six sites that will host the first European **quantum computers**: Czechia, France, Germany, Italy, Poland and Spain. This selection is part of the EuroQCI (European Quantum Communication Infrastructure) initiative, which aims to build a secure quantum communication infrastructure across Europe, and of the Quantum Technology

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<sup>4</sup> <https://www.top500.org/lists/top500/2022/11/>

Flagship, a long-term research and innovation initiative with the aim to put the European Union at the forefront of the second quantum revolution. In Italy, Cineca will manage the new quantum computer on behalf of EuroHPC JU. The new machine will be integrated with Leonardo which, thanks to its particular and futuristic architecture, lends itself extraordinarily well to the purpose. This architecture, called **MSA (Modular Supercomputing Architecture)**, has been designed to allow to easily integrate heterogeneous computational systems, or, in other words, with architectures that are profoundly different from that of the supercomputer. Quantum computers are also among these computational systems. The quantum computer will be physically connected to Leonardo through a wired network. This type of integration, called co-localized, allows a higher speed of information exchange between the two systems compared to the localization of the QPU in the cloud, consequently allowing the development of increasingly efficient hybrid algorithms. The new quantum computers are expected to be available at the six sites above by the second half of 2023. It will also be instrumental in addressing the growing demand for quantum computing resources and will be able to solve complex problems related to important areas such as health, climate change, logistics or energy consumption.

## “Big Data”

Nowadays, HPC technological evolution cannot be disjointed from the so called *Big Data* infrastructures, particularly devoted to manage, analyze and structure huge quantities of multidisciplinary data. The production rate of new data reaches orders of Exabytes per month. HPC systems like GALILEO100 and Leonardo are used as a computing back-end of such an amount of data.

This impressive trend is due both to an increase in the number of experimental variables belonging to different fields (from the classical scientific/technological one commercial/financial one) and both to an increase of the numerical model’s resolution and complexity. Huge amount of data poses numerous problems, from transfer, to analysis, from classification to management over time.

In order to overcome these challenges, it is mandatory to invest substantial resources on:

- Multidisciplinary collaboration to assess efficient and safe data sharing (i.e., data interoperability).
- New and more efficient data analysis/data mining tools and paradigms.
- An efficient infrastructure for remote access (e.g. data visualization).
- Institutional support for huge data set maintenance/management/assessment, in the frame of the FAIR principles<sup>5</sup>.
- Training and support to increase competences and skills in old and new research communities, in particular towards the Open Science paradigm and within the European Open Science Cloud (EOSC<sup>6</sup>) environment.

Referring to Earth Sciences, numerical models are able to produce TB of output data (though the data amount can easily increase in case of ensemble modeling experiments, extremely useful to analyze different model parameterizations, to study the model sensitivity or even to compare different models), but they can become “old” very soon, due to the continue code evolution and the resolution/complexity increase. The amount of remote sensing data from satellite, necessary for Earth Observation, is also increasing at a fast pace, as well as the development of the Sentinel program from

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<sup>5</sup> <https://www.openaire.eu/how-to-make-your-data-fair>

<sup>6</sup> [https://ec.europa.eu/info/research-and-innovation/strategy/goals-research-and-innovation-policy/open-science/european-open-science-cloud-eosc\\_en](https://ec.europa.eu/info/research-and-innovation/strategy/goals-research-and-innovation-policy/open-science/european-open-science-cloud-eosc_en)

Copernicus<sup>7</sup>. On the contrary, the “in-situ” or field data are usually less demanding in term of space but are, from the historical point of view, unique and their integrity must be preserved. As an example, the National Oceanographic Data Center (NODC<sup>8</sup>), database contains data and metadata (both historical and real-time) from oceanographic expeditions from 1889 up to now.

Concerning numerical experiments, in 2009 with a 3D physical-biogeochemical simulation on the whole Mediterranean Sea at 1/8 degree of horizontal resolution OGS produced, in 24 hours, a 1-year simulation, generating about 6GB, running in parallel on 64 cores (IBM-sp6). In 2015, OGS maintained the same time-frame production of 1 year in 24 hours increasing the cores number to 160 (PICO), but at a finer resolution (1/16) and integrating the more time-consuming data assimilation scheme, finally generating 250GB of data. In 2020, the recent reanalysis simulation produced for the Copernicus Marine Service (20 years of Mediterranean Sea biogeochemistry at 1/24 with daily and monthly outputs), has exploited 648 cores of Galileo, running 24 hours to produce 1 year, corresponding to about 6TB of data.

Moreover, output from seismic data analysis is also increasing in size. A data production of 60TB for each 10-year data analysis is expected. As a matter of fact, many Earth Sciences projects are moving to produce multi-ensemble climatic simulations of hundreds of years, producing datasets that needs to be managed. To this goal, Cineca became a data node for Earth System Grid Federation (ESGF) in order to provide to OGS community the opportunity to access, analyze and extract information from data made available through this service.

On another side, the growing Internet of Thing (IoT) paradigm to disseminate the environment with active sensors that can upload stream of data directly to the cloud, could constitute a formidable research tool with an enormous quantity of live data, but could also quickly saturate the current infrastructure, with the risk of not being able to keep the pace with the flow of data.

## **2. HPC and HPDA activities in OGS**

The need of high-level computational and storage resources for institutional, national and EC-granted research activities is rapidly expanding due to the development of increasing data-intensive numerical codes used in Earth Sciences, and specifically for OGS in oceanographic, geophysical and seismological applications. Earth Sciences modelling activities are indeed oriented to increase the spatial resolution of the numerical grids, the complexity of the representation of physical phenomena in the algorithms, to reduce the uncertainty of their prediction (also by means of ensemble approaches), or to produce new multi-decadal climate scenarios or multi-centennial paleo reconstructions. In particular, the resolution refining and the increasing of realism represented in the numerical models is necessary to improve the simulations in coastal areas, with important economic and social added values, also in the framework of the European Sustainable Blue Economy strategy<sup>9</sup> and in the major actions related to a Digital Twin perspective (e.g. Destination Earth<sup>10</sup>, DITTO<sup>11</sup>, DTO<sup>12</sup>). To reduce the technological gap with the fast-evolving HPC infrastructure, some OGS research groups have already started to work in porting some test applications to hybrid or accelerated architectures, developing GPU-enabled versions of their legacy numerical models (as an example, the OGSTM-BFM model, in the frame of the ESiWACE model refactoring and porting service<sup>13</sup>). To accomplish such challenges, HPC/HPDA resources and technological support are key requirements.

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<sup>7</sup> <https://sentinels.copernicus.eu/web/sentinel/home>

<sup>8</sup> <http://www.nodc.noaa.gov>

<sup>9</sup> [https://oceans-and-fisheries.ec.europa.eu/ocean/blue-economy/sustainable-blue-economy\\_en](https://oceans-and-fisheries.ec.europa.eu/ocean/blue-economy/sustainable-blue-economy_en)

<sup>10</sup> <https://digital-strategy.ec.europa.eu/en/policies/destination-earth>

<sup>11</sup> <https://ditto-oceandecade.org/>

<sup>12</sup> <https://digitaltwinocean.mercurator-ocean.eu/>

<sup>13</sup> <https://www.esiwace.eu/services/software-support/refactoring-and-porting>



In the specific frame of the research activities related to NRRP projects where OGS is involved, planned computational resources are requested for the National Centres for HPC and Biodiversity, with a total amount of about 25 millions of CPU-hours (according to latest configurations on GALILEO100). In this scope, the targets of the OGS applications mainly cover modelling of climate multi-decadal simulations and operational services for the marine ecosystems (from the open ocean to the coastal areas), seismic risk assessment and mitigation, and analysis of experimental observations, also involving AI and ML approaches.

The OGS numerical modelling groups hold an historical cooperation with Cineca in the use of HPC environments. OGS research activities, specifically in the fields of ocean biogeochemistry and seismological modelling, have extensively exploited the computational and storage facilities of Cineca, throughout the IBM series sp4/5/6 until the recent HPC systems MARCONI, MARCONI100, GALILEO and GALILEO100. These activities have been developed in the framework of European and national projects (MFSTEP, MERSEA IP, MyOcean, Copernicus Marine Service, SESAME, OPEC, PERSEUS, MEDSEA, E-AIMS, INGV-DPC, CASHIMA, CADEAU, VENEZIA2021, SHAREMED, ICCC).

Further, OGS and Cineca are part of the Mediterranean Monitoring and Forecasting Centre (Med-MFC) of the Copernicus Marine Environment Monitoring Service (CMEMS<sup>14</sup>): in such framework, Cineca technical staff gives a professional support to the operations and management of the operational workflow that involves pre-processing, run production, post-processing, data archiving, and products dissemination linked with the CMEMS Information System for the short-term forecasts of the Mediterranean Sea at 1/24° horizontal resolution. Moreover, OGS and Cineca also collaborate in the operational downstream service for the Northern Adriatic Sea, developed within the CADEAU project.

In addition, a recent activity has involved the implementation of the data repository of EMODNet Chemistry 2 on the cloud infrastructure made available at Cineca.

OGS participated to some PRACE and ISCRA calls for research activities. These are some the most significant grants received:

- **GSensMed** (Global SENSitivity analysis of the MEDiterranean sea biogeochemical model; prop. PRACE n. 2011050813; 22 millions CPU-hours on BG/Q “FERMI”, corresponding to 9% of the total offered computational resources in the 4<sup>th</sup> call): use of numerical models for global sensitivity analysis to evaluate the reliability and uncertainty of marine biogeochemistry operational forecasts.
- **MUMEBIES** (Multi-decadal simulations of the MEDiterranean Sea BIogeochemical cycles, ISCRA Class A, code: HP10AC2U33; 5 millions CPU-hours on BG/Q “FERMI”): use of numerical models for climate studies of the biogeochemical dynamics in the Mediterranean Sea.
- **VALSER** (Validation of numerical methods for earthquake ground motion prediction; ISCRA IsB04; 700.000 CPU-hours): use of numerical models to evaluate the application of seismic waveforms deterministically computed by means of HPC methods in seismic risk estimates.
- **MED21BIO** (Scenarios for the Mediterranean Sea biogeochemistry in the 21<sup>st</sup> century, ISCRA Class B, code: HP10BA8M3Y; 1,5 million CPU-hours on MARCONI, GALILEO, GALILEO100): use of numerical models to produce climate scenarios of the Mediterranean Sea biogeochemical state in 21<sup>st</sup> century under RCP4.5 and RCP8.5.
- **ECOMED** (Ecological modelling of the Mediterranean Sea, ISCRA Class C, code: HP10C1IXMA; 1 million CPU-hours on FERMI, PLX, EURORA): use of numerical models to produce climate re-analyses of the Mediterranean Sea biogeochemical state.

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<sup>14</sup> <https://marine.copernicus.eu/about/producers/med-mfc>

- **GHOSMED** (Global Higher Order Sensitivity of the biogeochemical model of the Mediterranean Sea, IS CRA Class C, code: HP10CU63X7; 1 millions CPU-hours on FERMI, PLX, EURORA): improvement of the post-processing activities of the data set produced in GSensMed.
- **BENEATH** (impact of bathymetry changes in the Ross Sea (Antarctica) on the dynamical expansion of the past and future West Antarctic ice sheet (WAIS), IS CRA Class B, code: HP10BNAZ23; 4,8 millions CPI-hours on GALILEO, GALILEO100): use of ice sheet dynamical models to simulate past evolution of Antarctica 23 Millions ago when CO2 concentration was higher than 500 ppm and thus comparable to SSP 8.5 future scenario.
- **PALEOMIT** (Paleo-oceanographic simulations with the MITgcm in the Ross Sea (Antarctica) during the last deglaciation (21,000 years ago to present day) and the Middle Miocene (16 Million years ago), IS CRA Class B, code: HP10BGPPQ8, 1,5 CPU-hours on Marconi100): development and run of a set of spinups and transient simulations with realistic climatic, oceanic, sea level and ice sheet boundary conditions for the Last Deglaciation (21,000 years ago to present day, at 1000 years steps); Miocene simulations were not attempted after delays in obtaining bathymetric data due to COVID pandemic.
- **LOST** (LOcation of Seismic evenTs from noised signals; IS CRA Class C, 200.000 CPU-hours on FERMI): implementation of a HPC procedure to identify and localize micro-seismicity events from noised signals registered from a seismic monitoring network.
- **SCAF** (Implementation of a SCALable Fourier pseudo-spectral method, prop. IS CRA Class C, 1.000.000 CPUhours on FERMI): implementation of a code for the simulation of seismic wave propagation based on Fourier pseudo-spectral method with scalability up to a high number of processors.

Many IS CRA C projects have been awarded in the frame of biogeochemical modelling studies on the Mediterranean Sea, along different temporal and spatial scales: ECOMED2 (code HP10C3FZCK), BIOSURF (code HP10CAYKIE), BIOMEDCO (code HP10CPBEJO), MYMEDBIO (code HP10C8HYKJ), MEDCOAST (code HP10CIWBYO), BIOMEDXT (code HP10C5FMRK), MEDOPT (code HP10CXLYZ9), BLOMEDXT (code HP10COFIJC), TESB (code HP10CVBUE9), VIMEDBIO (code HP10CRWG5Z), TIMBIOM (code HP10CUD292), RESM4NAD (code HP10C0GWIC), RESM4NA2 (code HP10CJ0777), BIOSURF (code HP10CAYKIE), MEDCOAT (code HP10CIWBYO), CADRI (code HP10C6X2WZ), MEDICC (code HP10CS42BK). Recent IS CRA C projects on paleoclimate research topics on polar areas were: ANTCAL (code HP10CXDWSZ), AMITAS (code HP10CJV0V4), GLAROSS (code HP10C3S6VC), DEGLAMIT (code HP10CLL9R5).

In addition to such established modelling activities, already well-framed in the previous mentioned projects, other OGS groups are designing, proposing and developing new research lines that are going to exploit computational and/or HPC applications. The details of all the OGS activities, organized in different topics and research lines, are described in the scientific plan of the program “HPC Training and Research in Earth Sciences” (HPC-TRES), available on the HPC-TRES web-page (see following section).

### **3. Collaboration agreement between OGS and CINECA**

With the present agreement, OGS and Cineca want to regulate their collaboration for common interest activities concerning the development and elaboration of numerical simulations and the progress in algorithms and applications for geophysics, seismology and oceanography, already identified in the framework of the PRACE-Italy national research infrastructure, the extraordinary contribute of the MUR for the Italian participation to activities related to the international infrastructure.

It is our common interest that the present agreement, framed within the PRACE and EuroHPC roadmaps, will remain valid also if PRACE will be, for any reason, concluded or will change its status: this aspect is strategically important since it strictly connects the computational requests necessary to the development of the research lines described in the previous section with the infrastructural offer of PRACE-Italy, managed by Cineca, which is the national reference and European player for HPC and Big Data issues.

The human resources investment in modelling activities (for what concerns OGS: oceanography, ecology, biogeochemistry, seismology, geology) cannot indeed overlook a continuous update of the HPC infrastructure. This has to be matched with a high-level professional HPC support, able to: i) efficiently exploit the computational resources, ii) upgrade the numerical codes, and iii) keep the resources up with the technological advancement. Even with highly valued human resources, a delay in the management and upgrade of the HPC infrastructure would risk creating a gap difficult to regain in the capability to produce cutting-edge science, in particular in the frame of the EU projects goals and Horizon Europe initiative. The upgrade of the PRACE-Italy HPC infrastructure, national Tier-1 resource, is indeed planned within the activities of the NRRP project **TeRABIT**, started on 1<sup>st</sup> January 2023, led by INFN and where OGS acts as co-proponent.

Since 2012, in addition to the strengthening of the OGS scientific production activities and the development of new lines, the agreement has actually contributed to the global success of EURORA as one of the best energy efficient HPC facilities<sup>15</sup>. Such success was a result of the Cineca-OGS-Eurotech-PRACE cooperation, with Eurotech acting not only as an international player for HPC hardware supply, but also as important industrial enterprise of the Friuli-Venezia Giulia region. The continuation of the OGS-Cineca agreement allowed to keep the leadership in this field, also thanks to the installation in the second half of 2017 of the new prototype (codename DAVIDE), which was specifically meant to continue the work on energy efficiency started with EURORA.

OGS and Cineca, aware of the present change in computing paradigm which involves the growing heterogeneity of the HPC architectures, the increasing development of the scientific computing, and the consequent broadening of the gap between scientists and HPC professionals, have established, with the support of MUR, a training and research program to assist both undergraduate and graduate students (PhD/master students and PostDoc) to improve their knowledge in the field of the HPC tools for Earth Sciences applications. The program is called “HPC Training and Research in Earth Sciences” (**HPC-TRES**<sup>16</sup>), has already involved some national research groups, and plans to enlarge the cooperation, aiming also to support the national computational Earth Sciences community towards the Exascale.

This activity will allow Cineca to provide its services to research groups with scarce experience in the use of HPC resources, extending its users network and playing a fundamental role for the scientific and technological development of the national research community. This aspect is in line with the necessity to establish a collaborative environment able to maintain the HPC resources offer to the interested research groups in Italy even beyond the extraordinary contribute of MUR.

Given the previous conditions, OGS requests computational and storage resources and professional support for HPC activities related to the research lines described in Section 2. In particular, we refer to EuroHPC, PRACE and PRACE-Italy systems Leonardo, Marconi100, and Galileo100, and their corresponding upgrades, and to the interest in contributing to the exascale evolution.

Cineca commits to collaborate with OGS to provide:

1. professional support to the activities of OGS research lines described in the HPC-TRES scientific plan and other innovative applications (including: profiling, optimization,

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<sup>15</sup> <http://www.cineca.it/en/news/eurora-scores-first-green500-list>

<sup>16</sup> <https://www.ogs.it/en/high-performance-computing-laboratory-hpc-tres>

- porting of existing codes or innovative developing codes), also on cutting-edge hybrid/accelerated HPC architectures (towards Exascale);
2. adequate resources, both in terms of CPU-hours for computation: 3,6M core-hours per year on the Tier-1 system (Galileo100 and its planned upgrade) and 100k core-hours per year on Tier-0 system (Marconi100, then Leonardo), considering the activities to be carried out in the next two years, specifically related to the NRRP research projects (see Tab.1); and storage for data analysis/visualization (to be defined and agreed by both parties for each application in case that WORK and DRES environments may be not suitable), in order to carry out successfully preparatory tests of pre-production applications;
  3. long-term archiving (5TB on TAPE library until 31/12/2025);
  4. technical and professional support in the preparation of IS CRA / PRACE / EUDAT / EuroHPC proposals for production applications and of project proposals included in national or international calls (e.g. Horizon Europe, tenders for specific services), with updates and information about national and international funding initiatives involving HPC applications related to OGS activities (e.g. proof of concept for “ocean IoT”);
  5. technical support for the implementation and use of virtual systems on Cineca resources (e.g. virtual machine for applications/workflow monitoring, OGS thematic web pages), as well as light-virtualization such containers in order to ease the building of software stack and enhance flexibility of the computing environment;
  6. management of numerical simulation data, designed as an evolution of DRES toward a Database (e.g. exportation of the OGS DRES data to a DB) or other high-level archiving system with metadata linked to model outputs and high level easy to use interfaces similar to other cloud service like Dropbox, with the possibility to directly link data from outside (this is quite relevant since data are becoming more and more a publication asset that could be cited and can greatly improve the visibility and the impact of a research group/institute/organization);
  7. technical support for the development of high-level scientific visualization facilities, either at Cineca or at OGS (i.e supply expert advice for installation of ad hoc software like paraview or cinemascience for the Visual Lab of ECHO group), also in the frame of the “Summer of HPC” projects.

In the framework of HPC-TRES initiative, Cineca commits to support OGS for:

1. management of the training activities in the framework of the HPC-TRES program;
2. head hunting and human resources development in HPC applied to Earth Sciences;
3. organization of training activities online or at the OGS premises in Trieste (or in another feasible location in Trieste, also in collaboration with other scientific institutions of the Trieste Science System) for users at different levels, in particular courses on python including introductory lectures, specific lectures on debug, numpy, scipy, python objects (how to build a python library), courses on R, lectures on parallel computing and on the use of GPU architectures;
4. support to HPC-TRES fellows, specifically for parallelization of scientific codes;
5. dissemination and communication of HPC-TRES activities (e.g. through a web page managed with a virtual machine at Cineca).

| name NRRP project               | Application type (numerical simulation or data processing) | Reference name of the application                          | cluster currently used (G100, M100) | Use of GPU (Y/N/in progress) | configurazione attuale |  | Requirede computational resources (CPU-hours) | PI (email)                    |
|---------------------------------|--|--|-------------------------------------|------------------------------|------------------------|--|---|-------------------------------|
|                                 |  |  |                                     |                              | n. processors          | period simulated in 24 hours (for num. sim.) or time-to-solution for typical run |   |                               |
| CN Biodiversita' NBFC - Spoke 1 | numerical simulation                                       | OGSTM-BFM a 50+ PFT, run 1 biodiversita' con 500 variabili | G100                                | in progress                  | 480                    | 24 (10 years) TBC  | 1.000.000                                     | plazzari@ogs.it               |
| CN Biodiversita' NBFC - Spoke 1 | numerical simulation                                       | OGSTM-BFM a 50+ PFT, run 2 biodiversita' con 500 variabili | G100                                | in progress                  | 480                    | 24 (10 years) TBC  | 1.000.000                                     | plazzari@ogs.it               |
| CN Biodiversita' NBFC - Spoke 1 | numerical simulation                                       | OGSTM-BFM a 50+ PFT, run 3 biodiversita' con 500 variabili | G100                                | in progress                  | 480                    | 24 (10 years) TBC  | 1.000.000                                     | plazzari@ogs.it               |
| CN Biodiversita' NBFC - Spoke 1 | numerical simulation                                       | OGSTM-BFM a 50+ PFT, run 4 biodiversita' con 500 variabili | G100                                | in progress                  | 480                    | 24 (10 years) TBC  | 1.000.000                                     | plazzari@ogs.it               |
| CN Biodiversita' NBFC - Spoke 1 | numerical simulation                                       | OGSTM-BFM a 50+ PFT, run 5 biodiversita' con 500 variabili | G100                                | in progress                  | 480                    | 24 (10 years) TBC  | 1.000.000                                     | plazzari@ogs.it               |
| CN Biodiversita' NBFC - Spoke 2 | numerical simulation                                       | pollution SHYFEM   | G100                                | N                            | 14                     | 24 (1 month to 1 year)   | 300.000                                       | dcanu@ogs.it, claurent@ogs.it |
| CN Biodiversita' NBFC - Spoke 2 | numerical simulation                                       | marine spatial planning Nord Adriatico                     | G100                                | N                            | 28                     | 6 - 24 hours   | 300.000                                       | dcanu@ogs.it, claurent@ogs.it |

|                                  |                      |  |      |   |                  |                 |  |            |                                    |
|----------------------------------|----------------------|--|------|---|------------------|-----------------|--|------------|------------------------------------|
| CN Biodiversita' NBFC - Spoke 2  | numerical simulation | modellistica ensemble Species Distribution Models                                | TBD* | N |                  |                 |  | 100.000    | slibralato@ogs.it, dpanzeri@ogs.it |
| CN HPC ICSC - Spoke 4            | numerical simulation | RegESM Nord Adriatico ATM standalone hist+scenario                               | G100 | N | 240              | 24 (14 months)  |  | 350.000    | mreale@ogs.it                      |
| CN HPC ICSC - Spoke 4            | numerical simulation | RegESM Nord Adriatico ATM+OCN+RTM hist+scenario                                  | G100 | N | 260              | 24 (13 months)  |  | 410.000    | mreale@ogs.it                      |
| CN HPC ICSC - Spoke 4            | numerical simulation | RegESM Nord Adriatico ATM+OCN+RTM+BGC_offline hist+scenario                      | G100 | N | 360              | 24 (120 months) |  | 61.000     | mreale@ogs.it                      |
| CN HPC ICSC - Spoke 4            | numerical simulation | Mediterraneo Med-CORDEX OGSTM-BFM hist + 2scenari forzanti ICTP                  | G100 | N | 360              | 24 (120 months) |  | 187.000    | mreale@ogs.it                      |
| CN HPC ICSC - Spoke 4            | numerical simulation | Mediterraneo Med-CORDEX OGSTM-BFM hist + 2scenari forzanti ENEA                  | G100 | N | 360              | 24 (120 months) |  | 187.000    | mreale@ogs.it                      |
| CN HPC ICSC - Spoke 4            | numerical simulation | Mediterraneo Med-CORDEX OGSTM-BFM hist + 2scenari forzanti CMCC                  | G100 | N | 360              | 24 (120 months) |  | 187.000    | mreale@ogs.it                      |
| CN HPC ICSC - Spoke 4            | numerical simulation | Mediterraneo Med-CORDEX ATM+OCN+RTM+BGC (RegCM-ES) hist + scenario forzanti ICTP | G100 | N | 360              | 24 (6 months)   |  | 968.000    | mreale@ogs.it                      |
| CN HPC ICSC - Spoke 4 (link ICC) | numerical simulation | Mediterraneo online OCN+BGC (MITgcm + OGSTM-BFM) scenario forzanti ENEA          | G100 | N | 360              | 24 (3 mesi)     |  | 680.000    | mreale@ogs.it                      |
| CN HPC ICSC - Spoke 4 (link ICC) | numerical simulation | Mediterraneo online hi-res MITgcm+BFM online (ICCC follow up)                    | G100 | N | 800              | 24 (2 months)   |  | 12.000.000 | plazzari@ogs.it                    |
| CN HPC ICSC - Spoke 5            | numerical simulation | OpenQuake (parallelized through the <i>oqwrap</i> python wrapper)                | G100 | N | 48 cores per run | n.a. (3 hours)  |  | 300.000    | cscaini@ogs.it                     |

|                             |                         |                             |      |   |     |            |           |   |
|-----------------------------|-------------------------|-----------------------------|------|---|-----|------------|-----------|---|
| CN HPC<br>ICSC -<br>Spoke 5 | data processing         | track + rtklib              | TBD* | N |     |            | 100.000   | dzuliani@ogs.it,<br>amagrin@ogs.it,<br>ltunini@ogs.it |
| CN HPC<br>ICSC -<br>Spoke 5 | data processing         | gamit/globk                 | G100 | N |     | 36 months  | 100.000   | dzuliani@ogs.it,<br>amagrin@ogs.it,<br>ltunini@ogs.it |
| CN HPC<br>ICSC -<br>Spoke 5 | data processing         | Template Matching e LocFlow | M100 | Y |     | 1-2 months | 1.000.000 | avuan@ogs.it  |
| CN HPC<br>ICSC -<br>Spoke 5 | numerical<br>simulation | SPECFEM3D                   | G100 | N | 576 | n/a        | 1.000.000 | pklin@ogs.it  |

Tab 1. – Planned computational resources required to fulfill the research activities approved in the NRRP projects (\*new application).