

A person is standing in a server room, looking at a laptop. The room is filled with server racks and has a blue glow from the lights. The person is wearing a dark jacket and glasses.

HPC in Life Science

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A person wearing glasses and a dark jacket is standing in a server room, looking down at a laptop. The room is filled with rows of server racks, and the lighting is dim with blue accents from the server racks. The person is positioned in the center of the frame, looking at a laptop on a server rack.

Contents

1. HPCNow!
2. Why use an HPC?
3. How to use an HPC?
4. DEMO



Advanced supercomputing services for science and engineering

We plan, install & support

You run



| Company

- Young company (born in 2012)
- Staff: 35 HPC folks
- No financial dependencies
- Strong growth
- EU joint venture

**doitnow**

HPC Services

info@hpcnow.com - www.hpcnow.com

A light gray world map with two specific locations highlighted. In Europe, there are three small black dots above a larger green dot labeled 'Barcelona'. In New Zealand, there is a green dot labeled 'Auckland'.
Barcelona

Marie Curie, 8 - 08042 Barcelona (Spain)

Fernly Rise, 2019 Auckland (New Zealand)

Auckland

The company's core values are a deep understanding of the most advanced technologies in HPC along with extensive experience in customer and user support. The similarity of HPC technologies, both technically and commercially, with other growing IT sectors -Big Data, artificial intelligence, cloud computing- allow us to offer solutions in these areas as well.

Providing careful and detailed solutions and the successful customer response to our services has allowed HPCNow! to grow without external funding and to have the means to tackle any new challenge.



+200

years of accumulated
experience

+100

satisfied customers in
15 different countries on 5
continents

+100

HPC clusters installed

+50

distributed storage
solutions deployed

+3.000

users who have
received HPC training

We are passionate about new challenges and HPC technologies enthusiasts. Our goal is to take full advantage of supercomputing to provide solutions to our customers' scientific or engineering dares.



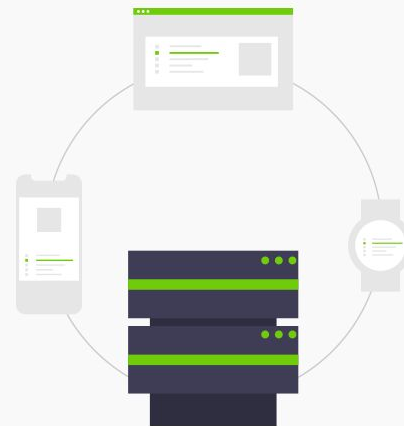
SW & HW & Cloud agnostics



User-oriented company



IT + scientific background



HPC services and solutions



Services and turnkey solutions adapted to your needs

HPCNow! provides its customers with the best solutions, getting the most out of their systems and maximizing the investment made.



Planning

HPCNow! performs detailed planning of all the required components for the optimal performance of an HPC system. On HPC systems already running, also consulting is offered in order to achieve the **best solution to enhance execution and user experience.**

● Consulting

● Solution Design

Installation

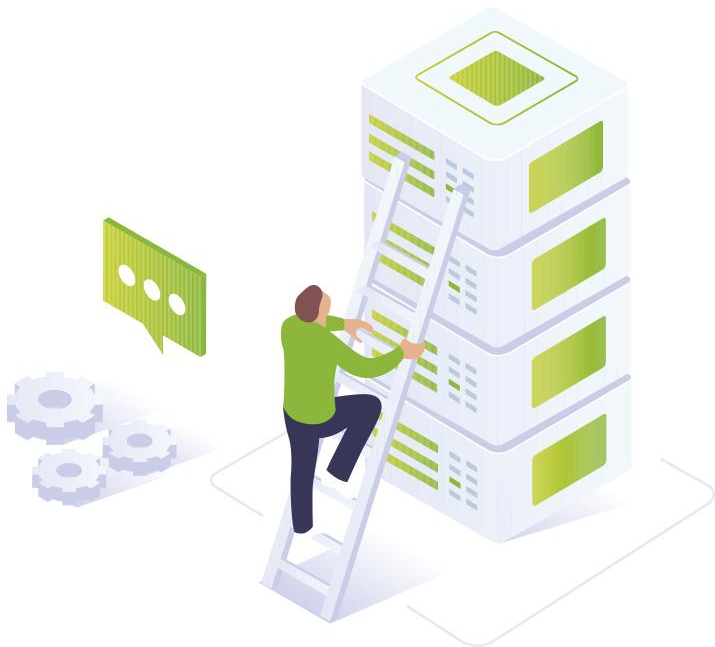
HPCNow! takes care of the full installation of an HPC system, **from the hardware to the final application**, including customized training that covers all necessary details for a successful administration and proper use of the resources.

- Infrastructure

- Software

- Training





Maintenance

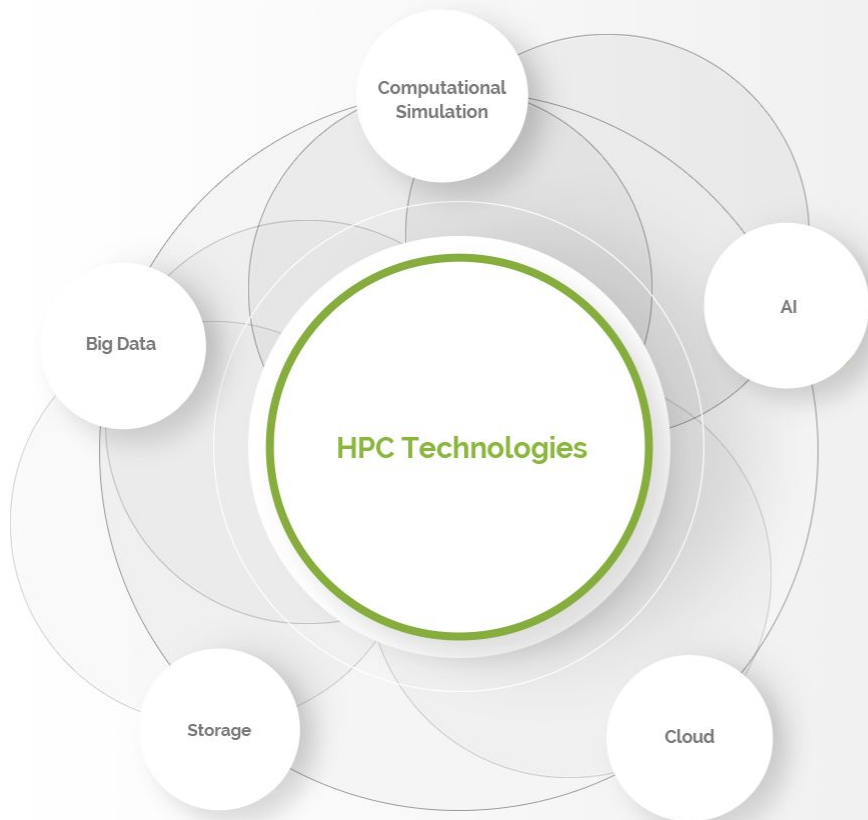
HPCNow! conducts the whole maintenance of an HPC system through its lifetime. It also offers the **best support to the users, advising and resolving any technical issues** that may arise, quickly and efficiently.

● Support

● Managed Services



| Solutions



| Sectors

HPC technologies are cross-cutting and cover an increasing number of areas. HPCNow! offers services and solutions applicable in all sectors and industries to accelerate and ensure your project success.

- Research
- Genomics
- Energy
- Pharma
- Automotive
- Banking
- Biotechnology
- Aeronautical
- Media

- Contribution to HPC community



EUROPEAN
TECHNOLOGY
PLATFORM
FOR HIGH
PERFORMANCE
COMPUTING



European
Extreme Data
& Computing
Initiative



MASTER en HPC *por*



EuroHPC
Joint Undertaking



We are hiring!

<https://hpcnow.com/jobs/>

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HPC: High Performance Computing

Multiple servers, (nodes)

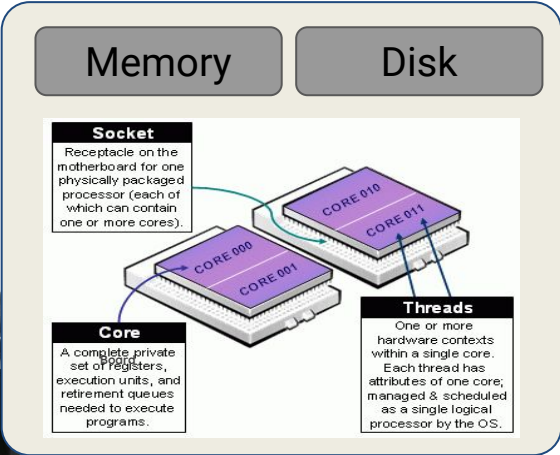
Working over an high speed network together as a cluster

Rack

Node



Data Center



Differences between Desktop Computer and HPC

- No Graphical User Interface (GUI)
- Programs are executed in batch mode
- Resources are shared between multiple users



HPCportals!!!!

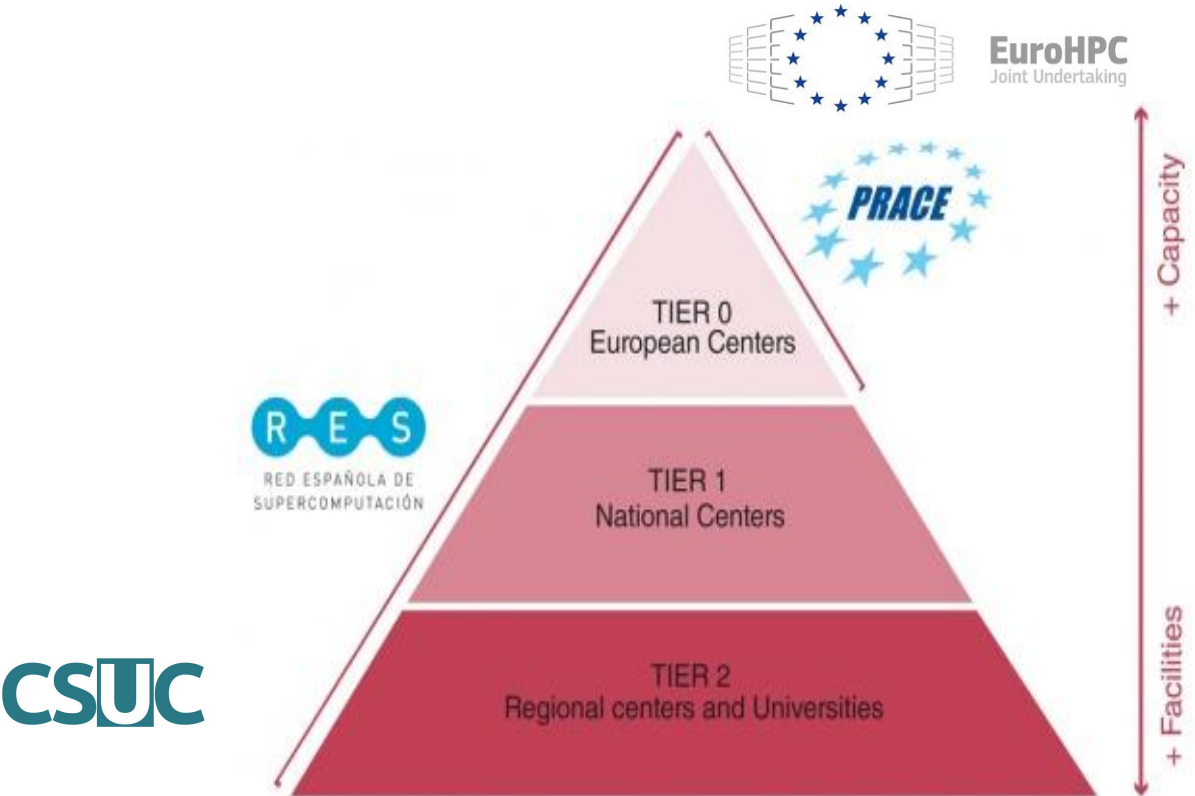
- Workstation
- Local Server

Local

- Cloud HPC
- HPC Provider Company
- HPC Public Center

Remote

HPC Public centers



Why use an HPC?

The key goal is to solve the problems faster.

- Speed → Split the work between several processors : the program will run N-ish times faster by using N processors.
- Volume → large data analyses
- Cost → faster results, reduced wet lab analyses
- Efficiency and convenience → shared resources used 24/7, no need to use all resources of your own PC

Why use an HPC?

The key goal is to solve

- Speed → Split the work across many processors.
- Volume → large data sets
- Cost → faster results
- Efficiency and convenience



...es faster by using N


...ources of your own PC

HPC Suitable Work

Suitable Work

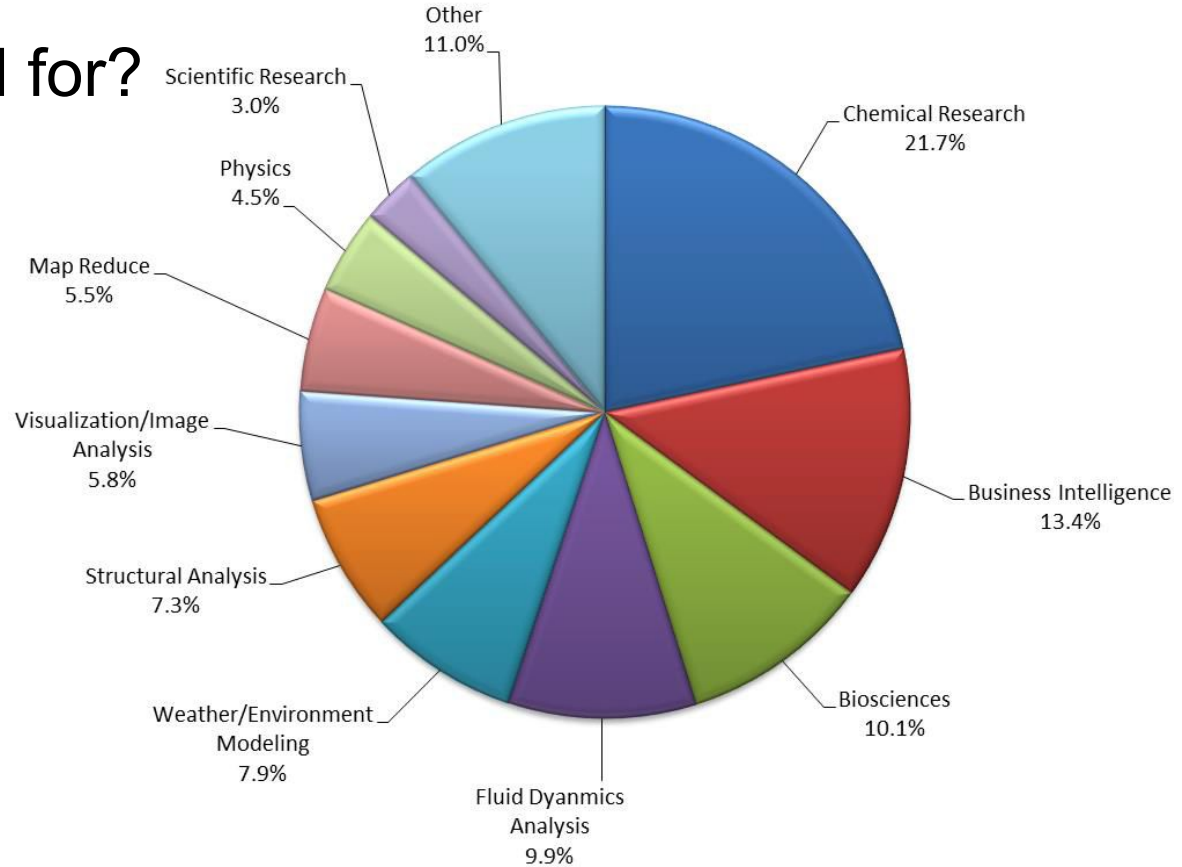
- When tasks take too long
- When one server is not enough
- When my problem consumes large amounts of memory

Less Suited Work

- Windows only software
- Interactive software i.e. GUI 
- Inefficient, un-optimised software

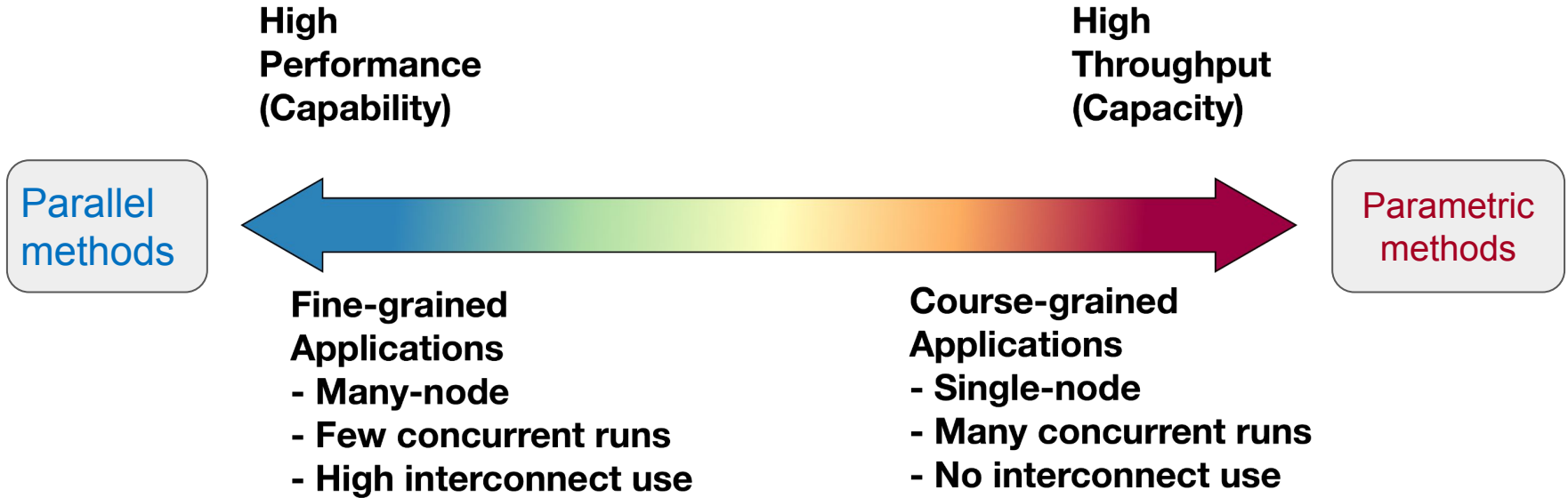


What HPC used for?



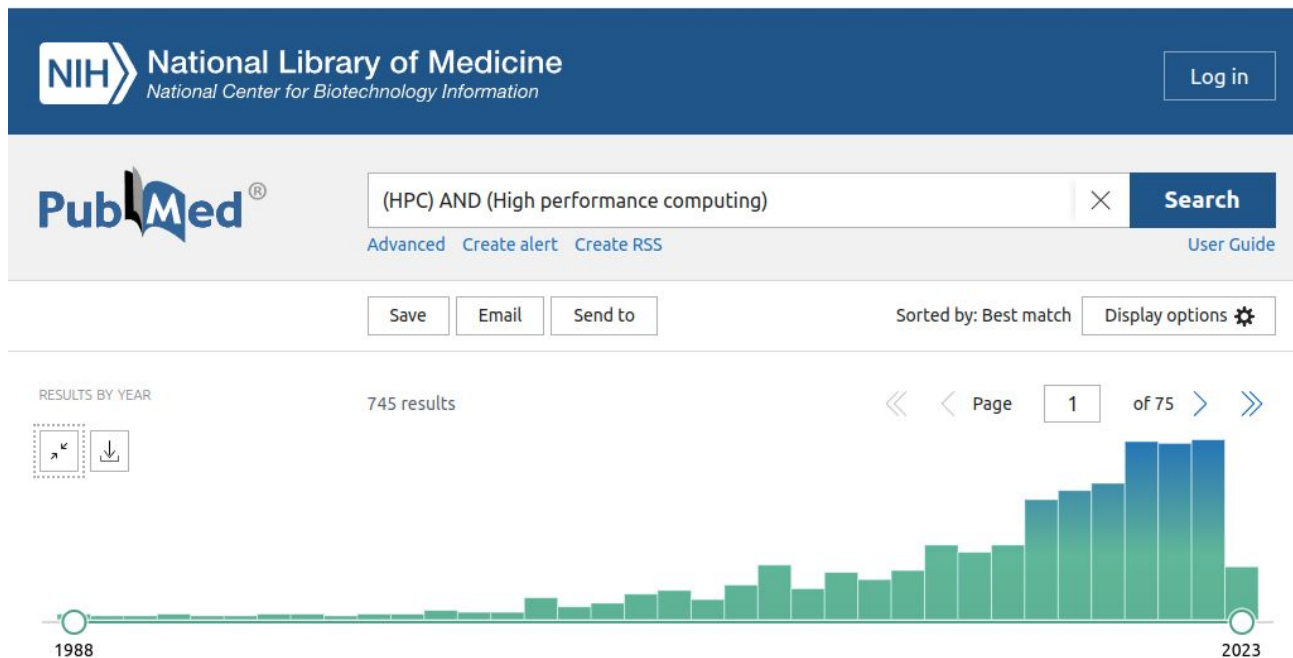
Storage: 1 PB = 10^{12} KB = 10^9 MB = 10^6 GB = 10^3 TB.

HPC or HTC?



HPC in Life Sciences recent papers :

Queried NCBI PubMed on April 11, 2023



HPC in Life Sciences recent papers

OXFORD JOURNALS Briefings in Bioinformatics

Brief Bioinform. 2017 Sep; 18(5): 870–885.
Published online 2016 Jul 7. doi: [10.1093/bib/bbw050](https://doi.org/10.1093/bib/bbw050)

Graphics processing units in bioinformatics, computational biology and systems biology

Editorial

Is high performance computing a requirement for novel drug discovery and how will this impact academic efforts?

Savins Puertas-Martin , Antonio J. Banegas-Lur , Juana L. Redondo , Pilar M. Ortigosa , Oihara 
Pages 981–985 | Received 16 Oct 2019, Accepted 17 Apr 2022
Download citation | <https://doi.org/10.1080/17445019.2022.2080171>

Immune Repertoire Analysis on High-Performance Computing Using VDJServer V1: A Method by the AIRR Community

Scott Christley, Ulrik Stervbo & Lindsay G. Cowell  on behalf of



Protocol | Open Access | First Online: 28 May 2022

4292 Accesses

Part of the [Methods in Molecular Biology](#) book series (MIMB)

Open Access | Published: 03 May 2018

Towards Portable Large-Scalable High-Performance Computing

Yuankai Huo , Justin Blaber, Stephen M. Damon, Brian D. Boyd, Shun Parvathani, Camilo Bermudez Noguera, Shikha Chaganti, Vishweshwar Greer, Ilwaj Landman 
[J Med Libr Assoc.](#) 2018 Oct; 106(4): 494–495.
Published online 2018 Oct 1. doi: [10.5195/jmla.2018.512](https://doi.org/10.5195/jmla.2018.512)

[Journal of High-performance computing service for bioinformatics:](#)

Jean-Paul Courneya

Bioinformaonist, Health Sciences and Human Services Library, UH

Alexa Mayo, AHIP

Associate Director for Services, Health Sciences and Human Services
21201

PMCID: PMC

Open Access Article

High Performance Computing PP-Distance Algorithms to Generate X-ray Spectra from 3D Models

by César González ^{1,*}, Simone Balocco ², Jaume Bosch ³, Juan Miguel de Haro ³, Maurizio Paolini ⁴, Antonio Filgueras ³, Carlos Álvarez ³ and Ramon Pons ^{1,*} 

- ¹ Institut de Química Avançada de Catalunya (IQAC-CSIC), 08034 Barcelona, Spain
 - ² Departament de Matemàtiques i Informàtica, Universitat de Barcelona, 08007 Barcelona, Spain
 - ³ Barcelona Supercomputing Center (BSC), 08034 Barcelona, Spain
 - ⁴ INTEL, 20090 Assago, Italy
- * Author to whom correspondence should be addressed.

<https://doi.org/10.3390/ijms231911408>

20 September 2022 / Accepted: 22 September 2022 / Published: 27 September 2022

Exscalate4CoV: Innovative High Performing Computing (HPC) Strategies to Tackle Pandemic Crisis

by Andrea R. Beccari ¹ and Giulio Vistoli ^{2,*} 

- ¹ EXSCALATE, Dompè Farmaceutici S.p.A., Via Tommaso De Amicis 95, I-80131 Napoli, Italy
 - ² Dipartimento di Scienze Farmaceutiche, Università degli Studi di Milano, Via Mangiagalli 25, I-20133 Milano, Italy
- * Author to whom correspondence should be addressed.

Hyperparameter Tuning with Learning for Imbalanced Alzheimer's Disease Data

by Fan Zhang ^{1,2,*}, Melissa Petersen ^{1,2}, Leigh Johnson ^{1,3}, James Hall ^{1,2} and Sid E. O'Bryant ^{1,2} 

- ¹ Institute for Translational Research, University of North Texas Health Science Center, Fort Worth, TX 76107, USA
 - ² Department of Family Medicine, University of North Texas Health Science Center, Fort Worth, TX 76107, USA
 - ³ Department of Pharmacology and Neuroscience, University of North Texas Health Science Center, Fort Worth, TX 76107, USA
- * Author to whom correspondence should be addressed.

[Appl. Sci.](https://doi.org/10.3390/app121336670) 2022, 12(13), 6670; <https://doi.org/10.3390/app121336670>

[Biocomputing](#) 2023, pp. 541–545 (2022)

HIGH-PERFORMANCE COMPUTING MEETS HIGH-PERFORMANCE MEDICINE

Anurag Verma, Jennifer Huffman, Ali Torkamani, and Ravi Madduri

https://doi.org/10.1142/9789811270611_0050 | Cited by: 0

Editorial | Published: 18 July 2018

Special Issue on High Performance Computing in Bio-medical Informatics

Luping Zhou, Islem Rezik, Chenggang Yan & Guorong Wu 

[Neuroinformatics](#) 16, 283 (2018) | [Cite this article](#)

2370 Accesses | 2 Citations | [Metrics](#)

Research | Open Access | Published: 16 December 2022

Profiling the BLAST bioinformatics application for load balancing on high-performance computing clusters

Trinity Cheng, Pei-Ju Chin, Kenny Cha, Nicholas Petrick & Mike Mikailov 

[BMC Bioinformatics](#) 23, Article number: 544 (2022) | [Cite this article](#)

987 Accesses | 4 Altmetric | [Metrics](#)



[Biol Methods Protoc.](#) 2022; 7(1): bpac032.
Published online 2022 Nov 15. doi: [10.1093/biomethods/bpac032](https://doi.org/10.1093/biomethods/bpac032)

PMCID: PMC9767868
PMID: 36561335

Teaching computational genomics and bioinformatics on a high performance computing cluster—a primer

Arjun Sethuramam 

High-Performance Computing in Cardiovascular Medicine of Multi-Dimensional Data Analysis—re, Shinichi Goto

Cardiovascular dynamics, Artificial intelligence, Neural network, Machine learning

High-Performance Computing in Bayesian Phylogenetics and Phylodynamics Using BEAGLE

Guy Baele , Daniel L. Ayres, Andrew Rambaut, Marc A. Suchard & Philippe Lemey

Open Access | 

Open Access | First Online: 06 July 2019

Accesses | 4 Citations | 8 Altmetric

[Methods in Molecular Biology](#) book series (MIMB, volume 1910)

Some topics covered and tools used

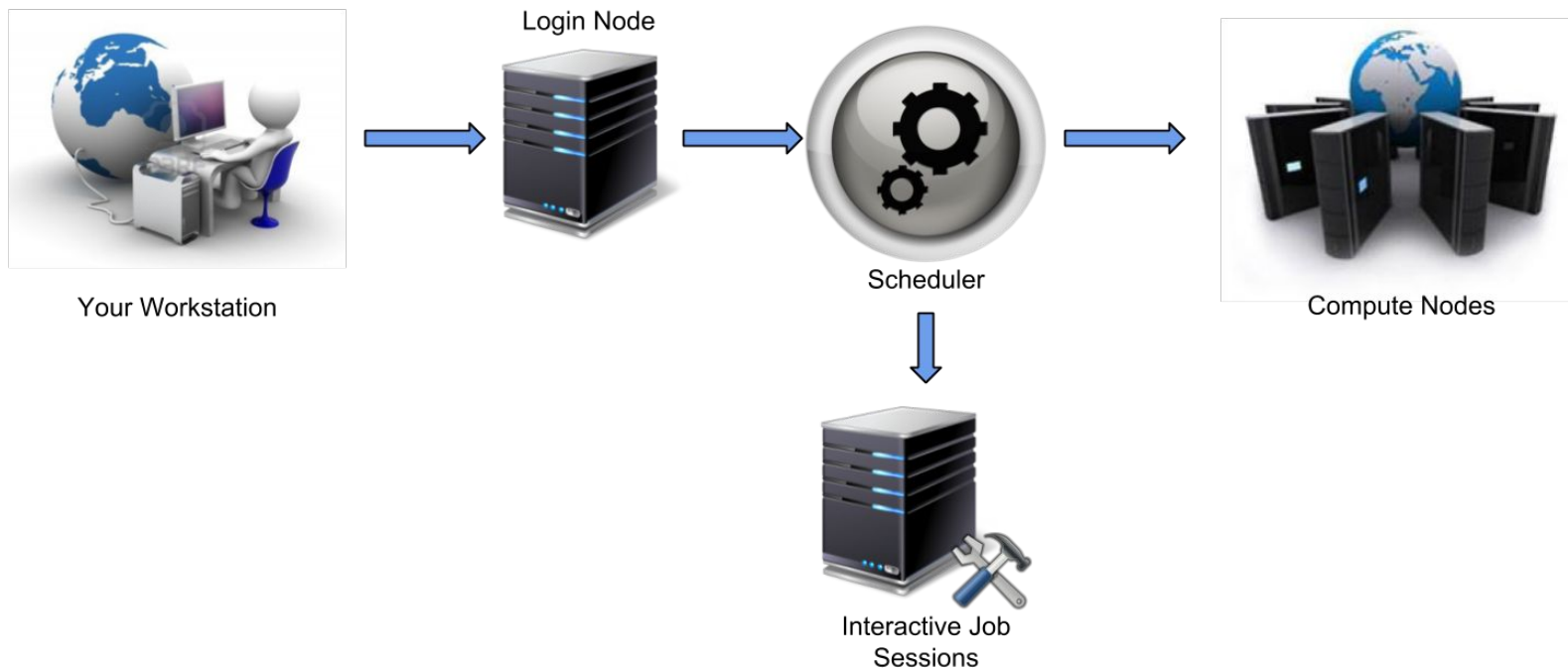
- protein folding
 - drugs design
 - genomics
 - WGS
 - RNAseq
 - proteome
 - metabolome
 - ecology
 - large datasets
 - precision medicine
 - ML / AI
 - simulations
- [AlphaFold](#)
 - [Nextflow](#) - workflow managers
 - CI/CD
 - containers
-
- Quantum computing is coming
 - cloud vs on-prem
 - [GPU](#)
 - Future directions in [HPC](#)
-
- [Heroes](#)

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User Workflow

On a HPC system you send your script to the queue to be run and use the computational resources



HPC Best practices

- **NEVER** run scripts outside of Workload scheduler
- Use the short or interactive queue to test your simulations
- Work on `/shared` or `/scratch` for light i/o jobs
- Work on `/tmp` for intensive i/o jobs
- Store temporary files on `/scratch`
- Move important files to `/projects`

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DEMO

<https://github.com/kErica/2023UB-formation/tree/master/2023-Workshop>