Self assessment on HPC readiness for SMEs



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"Access to HPC resources by Greek SMEs" Info day

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- What is HPC?
- Why is HPC important?
- Why use HPC in Business?
- Adapting HPC for SMEs
- HPC services for SMEs

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 - _____>
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- Does this apply to my sector? Does this apply to my business?

Does this apply to my workflow?

- ⇒ What are my HPC needs?
- \Rightarrow Tools to cover my HPC needs.





What is HPC?

High-Performance Computing



What is HPC?

Technology that takes advantage of the power of **supercomputers** or **computer clusters** to solve computational problems that are advanced or massive, be it in terms of data volume or complexity.

Why is it useful?

HPC can lead to major advancements in fields like scientific research or technological product development, because it make it possible to analyse *huge volumes of data*, or perform complex simulations, that would otherwise be impossible to do with standard computers.



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Where is it used?

The adoption of HPC has been particularly robust in industries that need to *quickly analyze large data sets*, including genome sequencing, molecular dynamics, computational chemistry, etc. In the future, almost all industries will likely turn to HPC to tackle large volumes of data.

How does it work?

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HPC in the broader sense



HPC:

computing systems having extremely high computational capabilities. Today these systems are able to perform more than 10¹⁵ operations per second (petascale) and are expected in a few years to reach 10¹⁸ operations per second (exascale) HPDA = HPC + Big Data: Analyze extremely large datasets quickly and/or efficiently

AI: Systems capable of learning and making decisions **Cloud**: On-demand access to computing resources

such as servers, storage, databases, networking, software, analytics, and intelligence Quantum Computing

Self-assessment



- Are we moving towards compute-intensive workloads?
- Are we dealing with big data volumes?
- Are we relying on simulations?
- Are we using AI?
- Does our proprietary infrastructure seem overloaded?
- Have we seen improvement when using parallelism / GPUs / similar?





Why is HPC important?

Why is HPC important?



Reduced physical testing	By relying on HPC-powered simulations, physical tests can be eschewed. This can be very beneficial for industries where physical testing is costly and cumbersome, such as the automotive industry where crash tests can be replaced by simulations.
Fault tolerance	HPC clusters have more than one processing nodes, meaning that even if some of the nodes fail, the rest of the HPC system can continue its operation. Thus, even if overall processing is slowed down by the reduced computing power, there will be no problem of processing availability.
Higher Processing Speed	HPC clusters do not only exploit the availability of multiple nodes. They also contain highly performant processing and communication devices, such as the latest CPUs, graphics processing units (GPUs), and low-latency networking fabrics such as remote direct memory access (RDMA), coupled with all-flash local and block storage devices, HPC can perform massive calculations in minutes instead of weeks or months.
Lower Cost	The use of HPC shortens the time to complete production, given that it speeds up production processes. This translates to less wasted time and money. Furthermore, as remote HPC services become available, even small businesses and startups can afford to run HPC workloads, paying only for what they use and scaling up and down as needed (e.g. by relying on cloud-based HPC).
Improvement of existing processes	Faster processing time and quicker data analysis facilitates the automation and streamlining of workflows.
Innovation	Discoveries that are made possible for the first time through the use of HPC, make it a power that drives innovation across nearly every industry around the world.

Supercomputer vs. conventional computer







Supercomputer vs. conventional computer





Source: https://digital-strategy.ec.europa.eu/en/library/high-performance-computing-best-use-examples

Self-assessment



- Does my sector rely on scientific computations?
- Does my sector deal with simulations?
- Does my sector deal with ever-growing sets of data?
- Does my sector deal with data analytics?





Why use HPC in Business?

Why use HPC in business



Best Metric for Justifying HPC Investment



HPC significantly reduce R&D costs and development cycles, producing higher quality products and services, reducing the time of product development cycles.

- Example: HPC has enabled automakers to reduce the time for developing new vehicle platforms from an average of 60 to 24 months, saving EUR 40 billion while improving crashworthiness, environmental friendliness, and passenger comfort
- High return on investment in HPC: each Euro invested in HPC on average returned EUR 867 in increased revenue and EUR 69 in profits.

Sources: https://digital-strategy.ec.europa.eu/en/library/high-performance-computing-factsheet U.S. Council on Competitiveness report, "Solve. The Exascale Effect: The Benefits of Supercomputing Investment for U.S. Industry," Intersect360 Research, 2014

Example: Drug Discovery and Pharmaceuticals



CHALLENGES...

- Surfacing of new diseases
- Aging population means new patient profiles
- Medical data records growing exponentially
- Having to solve for enormous number of biological factors

Several years to decades to develop products

...AND HOW TO FACE THEM

- Make new discoveries faster than ever
- Work with larger data sets
- Collaborate more efficiently
- Scale up parallel simulations
- Exploit HPC-powered advances in genomics

Personalized treatments in shorter time

High-Performance Computing Enhances Treatment Precision in Breast Cancer



Who?	The Problem	The Challenge	
United Kingdom End User: CHOSA Oncology Ltd Domain Expert: Hellenic Mediterranean University Technology Expert: JADBio	 Many cancer patients fail to respond to their drug treatment, resulting in heavy human and economic loss Lack of efficacy is mainly attributed to host/tumour variations at the genetic and molecular level, which clinical practice still struggles to integrate New digital genomic technology delivers treatment regimens that assess and use the DNA, RNA, protein, and metabolites in the individual patient's tumour 	 Current technologies focusing on just one or a few genetic biomarkers or using complex ex vivo laboratory tumour models are predictive of treatment outcomes only in highly selected cases and difficult to implement effectively Building an easy-to-use and intelligent platform to identify effective drugs in each individual requires the analysis of huge data sets. 	

High-Performance Computing Enhances Treatment Precision in Breast Cancer

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The HPC Solution

The Business Benefit

- Extensive analyses of a huge volume of publicly available data (called NCI-60), which link different types of cancer to the anticancer activity of over 50,000 compounds
- Using the JADBio autoML platform and HPC resources, ML models for these selected compounds were built to estimate the models' performance in predicting treatment outcomes
- Analyses have required a prohibitive amount of time without the employment of HPC

- After further validation, the models will be used to set up a complete platform called 'Allied Intelligence for Drug Accuracy' (AÏDA) which predicts the efficacy of different cancer drugs for each individual patient
- No similar solutions exist at the moment
- With a focus on breast cancer, a business potential of up to €69m, based on an anticipated price of €3,000 per service.



Self-assessment



- Is time-to-market important for my business?
- Is my business operating in a competitive landscape?
- Are my competitors using HPC?
- Is the HPC ROI trend in my sector growing?





Adapting HPC for SMEs

HPC Needs by Stakeholder Type



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- May have in-house HPC capabilities
 - May have more liberal spending limits
 - May have easier access to technology experts
- May be more time constraintbound, in order to ensure competitiveness
- May have strict data or code confidentiality constraints.
- May have the capability of investing in research





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- May not have continuous flow of funding
- May have more freedom in
- accessing public HPC infrastructures
- May have HPC capabilities inhouse
- May have to create
- novel/custom procedures or workflows
- May be allowed limited access to proprietary solutions, due to copyright issues etc



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- May rely on limited funding
- May face more regulations or restrictions on where and how to spend funding

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- May be less deadline-bound
- May need robust HPC solutions, as decision-making may be slower

No "one size fits all"!

The challenges in the case of the SME

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COST

Prohibitive cost of in-house infrastructure

Limited budget for infrastructure hire

Limited budget for solution acquisition

FLEXIBILITY

Computational requirements and needs may fluctuate during development

Workflows may need to be adapted to available infrastructure

DATA

Data transfer time may be an issue

Data confidentiality may affect choice of infrastructure

Data storage needs may affect the cost

EXPERTISE

Adapting workflows to HPC may require experts outside of the SME's field

Experts should have a combination of backgrounds to better serve the SME's HPC need

INVESTMENT

Competitive markets

Must carefully choose where to invest time and budget

Exploratory research may be prohibitive



Access to infrastructure

HPC for hire

✤ Flexibility, more freedom of choice

 Extra cost that may be prohibitive

Cloud Solutions

Still incur cost, versatile under conditions

National Infrastructures

Lower cost

Eligibility may be restricted

EuroHPC JU Supercomputers

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Access to infrastructure





Self-assessment



- Do I need / where can I secure additional funding?
- What is my access profile (e.g. for JU supercomputers)?
- What type of data am I processing and what are the confidentiality levels?

HPC4SME Automated Assessment Tool



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HPC4SME Automated Assessment Tool

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HPC4SME Automated Assessment Tool

αναφορά

HPC4SME report

HPC4SME		

Πίνακας Περιεγομένων

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2 Τυνοπτική Αναφορά	
2.1 Επεξήγηση τελικού διαγράμματος ΗΡC4SME	
3 Εργαλείο Αξιολόγησης ΗΡC45ΜΕ	
3.1 Διαδικασία Αξιολόγγρης	
4 Asrapopà	
4.1 Ετοιμότητα	
4.1.1 Πιθανότητα Επί τευξης	
4.1.2 Οργανωτικοί παράγοντες	
4.1.3 Εσωτερική Ικανότητα.	
4.2 Υπολογιστικό Νέφος (Cloud)	
4.2.1 Eprenteureohtinta	
4.2.2 Tagingta	
43HPC	
4.3.1 Διαδικασία Αξιολόγησης	
4.3.2 Εργαλείο Αξιολόγησης	
5 Παράρτημα	
5.1 Μεθοδολογία	

HPC4SME 2 Συνοπτική Αναφορά

Από τις απαντήσεις σας στις ερωτήσεις, φαίνεται ότι ο οργανισμός σας έχει χαμηλές δυνατότητες για Cloud Computing και HPC. Μπορεί να υπάρχουν κάποια εμπόδια που τοποθετούν τον οργανισμό σας σε αυτήν την ομάδα - και σας συνιστούμε να διαβάσετε περαπέρω για να ανακαλύψετε ποια χαρακτηριστικά ήταν κρίσιμα και να ελέγξετε πώς θα μπορούσατε να βελτιώσετε τη θέση σας στο Διάγραμμα HPC4SME.

αναφορά



Το διάγραμμα δείχνει τη θέση του οργανισμού σας όσον αφορά τις δυνατότητες HPC και Cloud στους άξονες x και γ αντίστοιχα, και το χρώμα δείχνει την ετοιμότητά σας. Ανατρέξτε στο κεφάλαιο 2.1 για λεπτομερή εξήγηση σχετικά με το τι σημαίνουν οι θέσεις και πώς προσδιορίζεται η ετοιμότητα

Cloud:

Η συνολική αξιολόγηση των δυνατοτήτων του οργανισμού σας για χρήση υπηρεσιών cloud HPC δείχνει ότι οι εργασίες MPC σας δεν είναι ακόμη έτοιμες ή πιθανώς δεν είναι κατάλληλες για εκτέλεση σε τοποθεσία εκτός της δυσής σας. Δείτε τις προτάσεις στην ενότητα Cloud για να βελτιώσετε τις δυνατότητές σας στο cloud.

HPC:

Η συνολική αξιολόγηση του δυναμικού ΗΡC δείχνει ότι οι υπολογισμοί σας δεν είναι ακόμη έτοιμοι να εκτελεστούν στην υποδομή HPC. Ελέγξτε τις συστάσεις στην ενότητα HPC για να βελτιώσετε τις δυνατότητες



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Available resources and how to use them

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Enhancing innovation capacity in Business, Industry and Science by utilizing advanced High Performance Computing services



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https://eurocc-greece.gr/

Industrial Training Course



https://mssg.ipta.demokritos.gr/tng4hpc4ind/

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HPC Marketplace





HPC Marketplace

https://hub.eurocc-greece.gr/

HPC Tools Directory



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All Domains	
Life Sciences	10
Materials and Chemical Sciences	16
Earth System Scienc	ces 8
Engineering	30
Other	24
Generic	10

Machine Learning using Julia

EuroCC-Greece

This tutorial is about getting in touch with the Julia programming language that "makes it easy to express many object-oriented and functional programming patterns". It mainly focuses on (i) set up the Julia environment, (ii) run a set of simple examples on creating matrices, plotting charts, and executing simple forloops with CUDA, and (iii) go through introductory examples on machine learning (Regression and Decision Trees).

역 Engineering, Generic

🛛 Machine Learning / Al

Tutorial

1 https://github.com/EuroCC-Greece/ml-julia

Pytorch
Facebook's Al Research lab (FAIR)
An open source machine learning framework that accelerates the path from research prototyping to production deployment.
역 Earth System Sciences, Engineering, Life Sciences, Materials and Chemical Sciences, Other
A Machine Learning / Al

https://hpctools.chemeng.ntua.gr/

Call for expression of interest

- Are you an industry or government stakeholder looking for access to HPC resources?
- Apply to our program and secure assistance in your project projects by members of the High-Level Support Team of EuroCC@Greece.
- Fill out the form or e-mail
- <u>contact@eurocc-greece.gr</u>



Express Your Interest in HPC!





Get in touch and stay connected!

contact@eurocc-greece.gr





Contact Us!





Thanks!





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Q&A

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