
EURO²
SUCCESS STORIES
2024
EURO4SEE

EuroCC 2/EuroCC4SEE Success Stories

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About the Projects: EuroCC 2/EuroCC4SEE

The mission of EuroCC 2 and EuroCC4SEE is to continue the establishment of a network of National Competence Centres (NCCs) in the most efficient way, while continuing to address the differences in the maturity of High-Performance Computing (HPC) deployment in Europe, for which improvement has already been noted since the first phase of the project.

Therefore, in addition to high-level management to monitor progress in the NCCs' development, the main task of the overall activity is to support national centres in setting up their individual operational frameworks, while accessing and making the most of the experience and expertise currently available at national and European level.

To support this, EuroCC 2 and EuroCC4SEE work together with CASTIEL 2, a Coordination and Support Action that is tailored to the needs of the NCCs, as well as the Centres of Excellence (CoEs).

The EuroCC activities – with 33 members and associated countries on board – are coordinated by the High-Performance Computing Center Stuttgart (HLRS). The project aims to elevate the participating countries to a common high level in the fields of HPC, High-Performance Data Analytics (HPDA) and Artificial Intelligence (AI).

The EuroCC 2/EuroCC4SEE projects have established National Competence Centres in the participating countries, which will be responsible for surveying and documenting the core HPC, HPDA, and AI activities and competencies in their respective countries. Ultimately, the goal is to make HPC available to different users from science, industry, public administration, and society.

Learn more about EuroCC 2/EuroCC4SEE here!

www.hpc-portal.eu

CASTIEL 2 – Coordination and Support Action

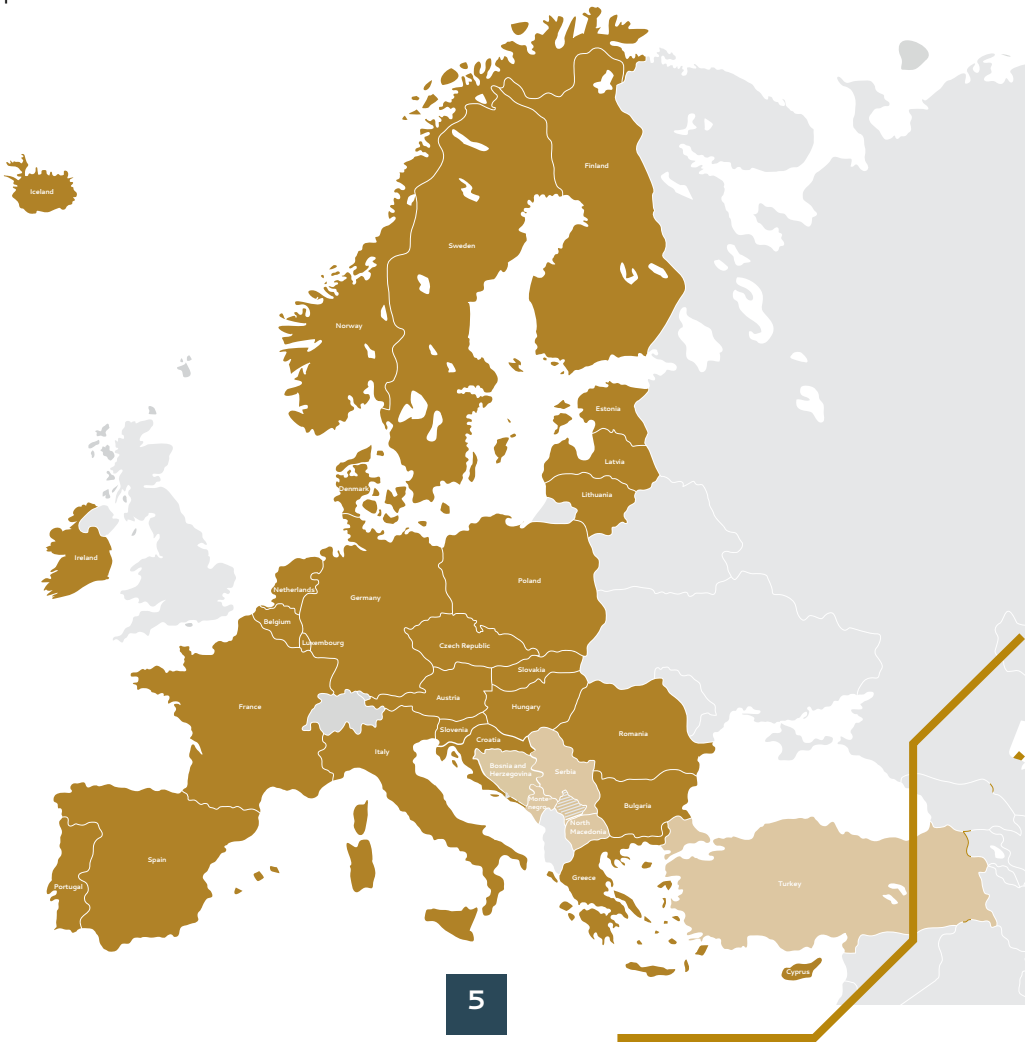
CASTIEL 2 coordinates and supports the NCC and CoE activities at the European level, and foster collaborations between NCCs and CoEs (and amongst each other) to achieve maximum impact to their user communities and the European HPC landscape.

What are the CoEs?

The Centres of Excellence cluster European Expertise with regard to specific topics. From Engineering to Biology and AI, everything is represented.

What is the relationship between CASTIEL 2 and EuroCC 2/EuroCC4SEE and the CoEs?

CASTIEL 2, the Coordination and Support Action (CSA) closely associated with EuroCC2/EuroCC4SEE, combines the National Competence Centres formed in EuroCC as well as the Centres of Excellence into a pan-European network. The aggregation of HPC, HPDA, and AI competencies demonstrates the global competitiveness of the EU partners.



NCCs Presenting the Success Stories

– NCC Belgium

The center operates in the area of high-performance computing (HPC) and high-performance data analytics (HPDA) and coordinates activities in all HPC-related fields and serves as a reference contact point on HPC/HPDA/AI at a national level. EuroCC Belgium consortium and partners: Cenaero, CECI, Innoviris Brussel and het Vlaams Computer Centrum (VSC) or Flemish Computer Center.

– NCC Bulgaria

It has been founded by the Institute of Information and Communication Technologies at the Bulgarian Academy of Sciences, Sofia University "St. Kliment Ohridski" and the University of National and World Economy. NCC-Bulgaria is focused on creating a roadmap for successful work in the field of HPC, big data analysis and AI, analyzing the existing competencies and facilitating the use of HPC/HPDA/AI in Bulgaria, and raising awareness and promoting HPC/HPDA/AI use in companies and the public sector.

– NCC Cyprus

The Computation-based Science and Technology Research Centre (CaSToRC) of The Cyprus Institute (CyI) acts as the National Competence Centre in HPC for Cyprus. It pioneers in the introduction, development and employment of intense computational methods and data to advance scientific and technological disciplines. CaSToRC aspires to cultivate the use of High-Performance Computing (HPC), Simulation, Machine Learning and Data Science in Cyprus and the Eastern Mediterranean and to serve the needs for computational and data intensive applications for academia, government and industry.

– NCC Czech Republic

The Czech National Competence Centre (NCC) for High-Performance Computing (HPC) and Data Analysis (HPDA) is represented by IT4Innovations National Supercomputing Center at VSB – Technical University of Ostrava. Its mission is to analyse, implement, and coordinate all the activities required to offer end users the services they need: from access to supercomputers and technology consulting to providing training for industry, public administration, and academia.

– NCC Estonia

NCC Estonia coordinates HPC expertise at the national level. Their mission is to analyse, implement and coordinate all necessary activities and offer services to end users to cover their needs, from access to resources and technological consultancy to providing training courses for academia, public administrations and industry.

– NCC Finland

The mission of NCC Finland is to build and enhance capacities in Finland for users in academia, research institutions, public administration and industry to harness the potential of EuroHPC high-performance computing and data analytics. NCC Finland is hosted by CSC – IT Center for Science Ltd. CSC is a non-profit state enterprise, which as part of the national research system, develops, integrates and provides high-quality information technology services and ensure that Finland remains at the forefront of IT development. CSC is the HPC hub of Finland.

– NCC France

The French NCC: CC-FR, dedicated to HPC, HPDA, AI technologies and Quantum Computing, brings together the community of technology providers and users. CC-FR federates the HPC, HPDA and AI ecosystem and supports SMEs on the use of intensive computing, high-performance data analysis and artificial intelligence.

– NCC Greece

The Greek NCC "EuroCC@Greece" is run by a consortium of 5 institutions namely GRNET – National Infrastructures for Research and Technology, National Center for Scientific Research "Demokritos", Foundation for Research and Technology – Hellas (FORTH), and Institute of Communication and Computer Systems of NTUA, Aristotle University of Thessaloniki. The consortium is coordinated by GRNET. The objective of the NCC is 3-fold: advance competitiveness in research; improve effectiveness of government services and promote innovation in industry.

– NCC Hungary

The HPC Competence Center (HPC CC) was established by the Hungarian Governmental Agency for IT Development (KIFÜ) in 2020. It promotes the High Performance Computing (HPC) and introduces the HPC infrastructure to potential academic and industrial users. Our experts assess the incoming project applications and manage the appropriate allocation of national HPC capacities. Additionally, the Competence Center maintains contact with users and international professional partners and represents the Hungarian HPC infrastructure and community in international professional forums.

– NCC Latvia

The High-Performance Computing Competence Centre in Latvia "SuperS" was developed in the framework of EuroCC project for supporting wider application of HPC in higher education, research, public administration, and industry. The Centre is coordinated by Riga Technical University HPC Centre and Institute of Numeric Modelling, University of Latvia.

NCCs Presenting the Success Stories

– NCC Luxembourg

Luxinnovation, the University of Luxembourg and LuxProvide are jointly managing the Luxembourg National Competence Centre in High-Performance Computing (HPC). Its mission is to promote the use of HPC linked to computing, data analytics and artificial intelligence and to support stakeholders such as industry – including SMEs and startups – academia and public administration to navigate the national and European HPC ecosystem. Luxembourg has a unique HPC infrastructure that is open to companies as well as to researchers. The Luxembourg National Competence Centre in HPC offers a wide portfolio of services to help you to set up and implement your HPC-enabled projects.

– NCC Montenegro

EuroCC Montenegro is part of the EuroCC project (Horizon 2020) and EuroCC2 (Digital Europe). National Competence Centre (NCC) in high-performance computing (HPC), established at University of Donja Gorica (UDG), coordinates all HPC-related activities nationwide and serves as a central contact point for industry, science, HPC experts, and the public.

– NCC Netherlands

NCC Netherlands is hosted by SURF, which is the ICT cooperative association that supports Dutch educational and research institutions to develop and/or acquire the best possible digital services and encourage knowledge sharing through continuous innovation. In particular, SURF hosts the national supercomputing and storage facilities of the Netherlands.

– NCC Poland

The National HPC Competence Centre is the Polish centre of expertise and a point of contact that enables users to benefit from national and European computing infrastructure. It offers advice to customers in all areas of HPC+ (HPC, HPDA, AI, Big Data, NLP, Data Analytics). Among the services, they provide access to computing resources, as well as technological support and training in high-performance computing, big data collection, storage, processing and analysis as well as artificial intelligence. Their offer is addressed to business entities (especially SMEs), universities, research institutes and public administration.

– NCC Slovenia

Slovenian National Competence Centre operates within Slovenian National Supercomputer Network – SLING who promotes the use of high-performance computers capabilities for research in science, industry, academia and the provision of public services. The most important task is raising the level of knowledge of users and general awareness of the benefits of using high-performance computers.

– NCC Spain

The Spanish National Competence Centre (NCC) aims to provide a broad portfolio of Supercomputing, Big Data and Artificial Intelligence services adapted to the respective needs of the industry (especially SMEs), the academic world and public administration in Spain.

– NCC Turkiye

Turkish National Science e-Infrastructure (TRUBA), operating under Turkish Academic Network and Information Center (TUBITAK ULAKBIM) is the coordinator of NCC Türkiye. Middle East Technical University (METU), Sabancı University (SU), and Istanbul Technical University (ITU) National Center for High-Performance Computing (UHeM) are the third parties of the NCC. While METU is a public university based in Ankara, SU is a privately-funded university in Istanbul. ITU UHeM, also based in Istanbul, provides supercomputing and data storage services to academic and industrial users. Their competencies include High-Performance Computing (HPC), High-Performance Data Analytics (HPDA), Artificial Intelligence (AI), CUDA, Materials Science, Computational Fluid Dynamics (CFD), and several other fields.

– Collaboration between NCCs Austria, Czech Republic, and Germany

NCC success stories – Collaboration of EuroCC Austria with EuroCC Czech Republic and EuroCC Germany

– Collaboration between NCCs Romania and Netherlands

NCC Romania is hosted by the National Institute for Research & Development in Informatics – ICI Bucharest, which is the most important institute in the field of research, development, and innovation in information and communication technology (ICT) from Romania.

NCC Netherlands is hosted by SURF, which is the ICT cooperative association that supports Dutch educational and research institutions to develop and/or acquire the best possible digital services and to encourage knowledge sharing through continuous innovation. In particular, SURF hosts the national supercomputing and storage facilities of the Netherlands.

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EURO4SEE

Section 1

IT and Software

Finnish start-ups have an exceptional competitive advantage – Candour Oy

NCC Finland

Industrial organisations involved:

Candour Ltd provides AI-powered biometric identification solutions that utilizes proprietary anti-spoofing and facial recognition technology. The company is based in Oulu, Finland.

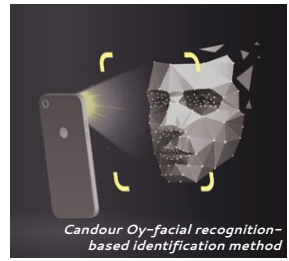
Technical /scientific challenge:

Candour Ltd's main product is Candour Identity, which is an online remote identity recognition service designed to complete the initial remote identity recognition process in under 1 minute and is easy to use for everyday scenarios. The product is based on AI-powered biometric identification and is patented.

Today almost every smartphone has a chip reader, which is used by the Candour app to verify the authenticity of passports. Candour authenticates using a standard smartphone. The user takes a picture of their passport, reads the passport chip with their mobile phone and then takes a selfie picture of themselves. Candour's technology compares the selfie image sample with the passport photo.

Above all, the identification must be sufficiently quick and easy. Few people today have the time to take numerous selfies or videos for an app. But when it comes to identifying a person, mistakes should not happen. Candour has managed to strike a good balance between easy yet secure identification.

Candour Oy – Concept


Candour Oy-facial recognition-based identification method

Solutions:

Its main product is a facial recognition-based identification method, which is being developed using machine learning requiring large-scale neural net training.

"We have already performed hundreds of iterations on the supercomputer. There have been improvements in model accuracy of tens of percent," says CANDOUR'S COO Harri Koskimäki. This means significantly better facial recognition and fewer errors. The more accurate the technology, the safer and also easier it is to use. "Time-to-market has been significantly reduced," says Koskimäki."The results are promising. We have been able to accelerate development and now have a very high level of model capability and maturity".

Business impact:

Initially, with Finnish innovation agency, Business Finland's support, the company was able to use the CSC supercomputers. Computing support is available for Finnish companies which are running product development projects, the results of which could be significantly improved with high-performance computing resources.

"Computing support complements existing product development funding and significantly improves the conditions for companies to develop internationally competitive products and services, especially those based on artificial intelligence," says Ecosystem Lead Outi Keski-Äijö from Business Finland.

The development of artificial intelligence and the activities of criminals are constantly evolving. "It's certain that we'll need the help of supercomputers in the future," says Koskimäki.

Benefits:

- Improved competitive advantage
- There have been improvements in model accuracy of tens of percent
- Steps towards internationalization
- Time-to-market has been significantly reduced

Keywords: Facial recognition, ID, Start-up, SME, Identification, App, Authentication

Industry Sector: Services & software providers

Technology: HPC, AI

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Machine Translation for Low-resource Finno-Ugric Languages

NCC Estonia

Scientific partners involved:

The University of Tartu is the leading university in the Baltics in the field of information technology and is one of the 250 best universities in the world in the ranking of Times Higher Education Universities in Computer Science. Examples of the University's Chair of Natural Language Processing's research directions include machine learning and data mining on text data, machine translation from one natural language into another, summarization of a long text document, automatic analysis of grammatical correctness, word meanings and sentence structure.

Technical /scientific challenge:

Neural networks have caused rapid growth in output quality for many natural language processing tasks, including neural machine translation (NMT). However, the output quality crucially depends on the availability of large amounts of parallel and monolingual data for the covered languages. Due to lack of training material, several lower-resource Finno-Ugric languages are not included in the existing massively multilingual models. In terms of the number of speakers, they range from 20 near-native speakers of Livonian to several hundred thousand speakers of Mordvinic languages.

TartuNLP team: research fellow Lisa Yankovskaya, Professor Mark Fišel and programmer Maali Tars (photo by Henry Narits).

Solutions:

An NMT system was developed between 20 low-resource Finno-Ugric languages and 7 high-resource languages. Monolingual corpora were collected mainly by crawling texts off the web and combining with pre-existing corpora. Three main categories of texts can be distinguished: news, Wikipedia, and biblical. All the NMT systems were trained on the LUMI supercomputer. All models were fine-tuned with the Fairseq framework implementation of M2M-100 for 350k updates with a batch size of 3840 tokens (the number was chosen to match earlier versions of models trained with the Huggingface implementation of M2M-100). The models were fine-tuned on 4 AMD Mi250X GPU-s.

Scientific impact:

23 Finnish-Ugric languages can now be translated using the machine translation engine of the University of Tartu. Most of these languages were added to a public translation engine for the first time. The translation engine allows researchers to translate materials that would otherwise be incomprehensible to them. It provides an opportunity to better study the history of languages and regions without knowing the respective language. Moreover, since most of Finno-Ugric languages are not widely spoken today, a translation engine is necessary to preserve these languages.

Benefits:

- Collection of parallel and monolingual corpora that can be used for training NMT systems for 20 low-resource Finno-Ugric languages
- Expansion of the 200-language translation benchmark FLORES-200 with manual translations into nine new languages (Komi, Udmurt, Hill and Meadow Mari, Erzya, Livonian, Mansi, Moksha and Livvi Karelian)
- The collected data can be used to create NMT systems for the included languages and investigate the impact of back-translation data on the NMT performance for low-resource languages

Keywords: Neural machine translation, Neural networks, Natural Language Processing, Finno-Ugric languages, TartuNLP

Industry Sector: Services & software providers, Natural Language Processing

Technology: Neural machine translation, HPC, HPDA, AI

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Powering Artistic Innovation: Tengrai 's Journey with HPC-Driven AI Art Creation

NCC Hungary

Industrial organisations involved:

A forward-thinking startup, Tengr.ai is dedicated to revolutionizing digital art creation. With a focus on user-friendliness and unbridled creativity, Tengr.ai's Image AI web application offers a seamless, language-inclusive, and fast experience for artists and creatives worldwide. Their mission is to democratize generative AI-assisted art creation, making it accessible and intuitive for users irrespective of their technical background.

Tengr.ai

Technical /scientific challenge:

The primary challenge is developing an AI-powered art generation tool that empowers artists by translating prompts into imagery. This involves training advanced models to execute artistic visions from text. Substantial computational power is crucial for enabling the parallel experimentation and refinement of diverse models and styles, ensuring a versatile, adaptive tool capable of catering to a wide spectrum of artistic needs through high-paced exploration and development.


Empress of Elegance: A Portrait of Gilded Grace


ARegal Rhapsody of Beauty and the Wildness

Contours of Creation, Tracings of Imagination

Solutions:

Tengr.ai leveraged the AI-partition of KIFÜ's robust 32 Nvidia A100 GPU HPC infrastructure across 4 HPE Apollo blades to rapidly iterate generative art models for photo-realistic rendering, illustrations, and more. Concurrent multi-model training increased throughput, enabling developing and A/B testing more models based on user feedback. Favored models were rapidly refined through additional training cycles, enhancing performance and responding to preferences.

Utilizing the expansive HPC capabilities, Tengr.ai accelerated its development cycle with a data-driven approach, rapidly closing the loop from development to deployment and fostering rapid advances in the AI art creation space.

Business impact:

The integration of HPC has significantly contributed to Tengrai ,s growth in the AI art generation sector. A notable 35-fold increase in website traffic over three months reflects a growing interest in the market. This increase in user engagement is attributed to the improved performance of the developed AI platform, and increase in model quality, facilitated by the HPC infrastructure. Tengr.ai's focus on uncensored creativity and multilingual support also contributes to its distinct position and helped differentiate its services in a competitive market.

Looking forward, the powerful HPC infrastructure is set to play a crucial role in startup's ongoing development. As the field of generative AI continues to evolve, the company is planning to broaden its range of models and tools, delving into new artistic styles and workflows, further enhancing the user experience to support continuous growth. The capability to experiment extensively will remain a key advantage for Tengr.ai. It enables the company to explore a wide array of creative possibilities, test new ideas swiftly, and respond agilely to emerging trends and user preferences in the digital art world. The ability to rapidly prototype and iterate different artistic styles, techniques, and model configurations enables Teng.rai to stay at the cutting edge of AI-driven art creation.

Benefits:

- Speed Optimization: Rapid model training and iteration
- Innovative Art Styles: Enabled experimentation with diverse generative AI models and techniques
- Scalability: future expansion and model complexity.
- Market Competitiveness: Leveled the playing field for a small startup in a rapidly evolving tech sector

Keywords: AI Art Generation, Generative AI, Machine Learning, Digital Creativity, User-Centric Design

Industry Sector: Services & software providers

Technology: AI and Machine Learning, focus on image generation models and great UX

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Analyzing the Efficiency of Ad Channels from Multiple Platforms

NCC Bulgaria

Industrial organisations involved:

Technical /scientific challenge:

In the evolving digital advertising landscape, brands and marketers invest across multiple platforms like Meta (formerly Facebook), Instagram, Google Ads, TikTok, LinkedIn, Snapchat, and more. Each platform provides a plethora of data related to ad performance, audience engagement, and conversion metrics. However, integrating and comparing data from these disparate sources with their specific APIs to derive a holistic view of advertising efficiency remains a significant challenge.

Marketers need a comprehensive solution to assess and compare the ROI of each ad channel to optimize their marketing budget. One of the key technical challenges of data analysis is to quickly and accurately integrate all available data, analyze the relationships, patterns, and trends, and provide actionable insights in a timely manner. HPC can be used to accelerate various data processing tasks, such as data cleaning and transformation, data preprocessing, and data analysis. This can be achieved through the use not only of HPC resources and techniques, but also other advanced technologies such as big data analytics (BDA) and artificial intelligence (AI).

AI could be very useful in solving another technical challenge - finding an appropriate attribution model. In the beginning, it could be based on data from Google Analytics, but a more comprehensive approach is to create and tune an attribution model based on feedback from the system itself.

Benefits:

- Unified View: A consolidated view of ad metrics from various platforms allows easier comparison and analysis
- Efficient Budget Allocation: Insights on ad performance across platforms help in optimizing ad spend, ensuring higher ROI
- Data-Driven Decisions: The analytics dashboard aids in making informed decisions based on real-time data
- Future-Proof Marketing: Predictive analytics provides foresight into potential future trends, enabling proactive marketing strategies
- Time Savings: automated data integration and visualization save significant time compared to manual data compilation and analysis
- Enhanced Personalization: understanding ad performance metrics across platforms can lead to better-targeted ads, enhancing user engagement

Solutions:

An effective multi-platform ad analytics dashboard provides a centralized view of the company's performance across various advertising channels. Here are the key components that the platform created for COCOSOLIS now incorporates:

- Integrated Analysis of Multi-Platform Marketing Data
- Data Integration Module: Module that interfaces with the APIs of Meta, Instagram, Google Ads, TikTok, LinkedIn, Snapchat, etc., to fetch ad performance data. This module handles varying data structures, frequency, and metrics.
- Data Cleaning and Normalization: Normalizing metrics like engagement, impressions, click-through rates, and conversions ensure comparability.
- Unified Analytics Engine: Implementation of an analytics engine that processes the integrated data to derive insights on ad performance, audience behavior, and platform conversion metrics. Use of statistical methods to compare and contrast the efficiency of each ad channel.
- Visualization and Reporting Dashboard: An interactive dashboard that provides marketers with real-time insights into the performance of their ads across platforms. It allows users to drill down into specifics, compare metrics side-by-side, and visualize ROI and other KPIs for each channel.
- Predictive Analytics: Machine learning models that predict the future performance of ads based on historical data. Guides marketers in allocating budget to channels that are forecasted to perform best.
- Feedback Mechanism: A feedback loop where marketers input results from offline conversion tracking or other external metrics to refine the analytics engine's accuracy.

Business impact:

- Optimized Ad Spend: By understanding the ROI of each platform, marketers can allocate their budgets more efficiently, maximizing the return on their advertising spend
- Informed Decision Making: A unified view of ad performance across platforms allows marketers to make data-driven decisions, be it for ad creative adjustments, targeting tweaks, or budget allocation
- Reduced Data Silos: Centralizing the analytics process breaks down data silos, ensuring that insights derived are comprehensive and holistic
- Future-Ready Marketing: Predictive analytics can guide marketers on future trends, preparing them to capitalize on upcoming opportunities

·Keywords: IoT, Big Data, Traffic events, Traffic alerts, Analytics,
·Technology: Various integrations, BigQuery, MySQL, or alternative data storage
·Industry sector: Retail, Services

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Quanscient prepares for quantum future with LUMI supercomputer

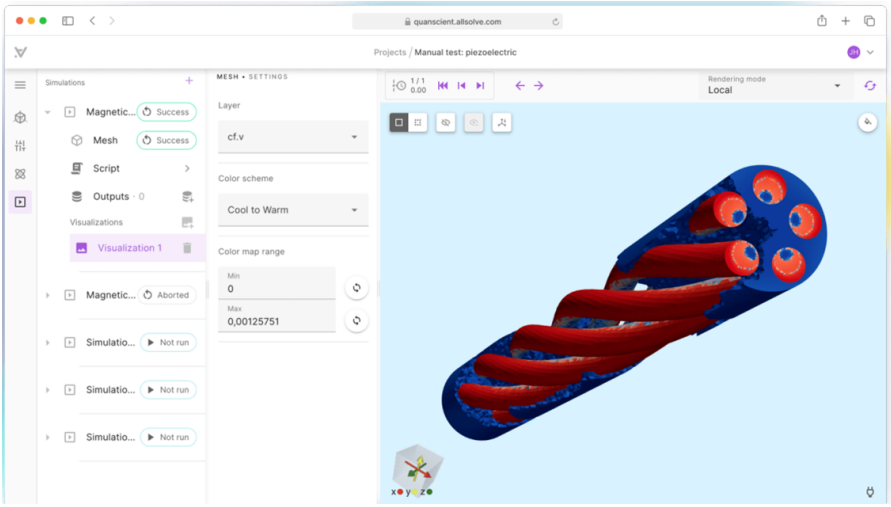
NCC Finland

Industrial organisations involved:

Founded in 2021, Quanscient's technology combines advanced cloud computing and quantum integration. It is expected to bring significant benefits to industrial applications based on, for example, computational fluid dynamics. Quanscient's vision is to make simulations matching reality by building a next-generation Simulation-as-a-Service platform utilizing cloud and quantum computing.

Technical /scientific challenge:

Quanscient uses real quantum computers in its development, but also supercomputing. Supercomputing is needed because quantum computers are still „noisy", i.e. very sensitive to errors. In other words, they can currently run only fairly small simulations. A supercomputer, on the other hand, can be used to emulate a quantum computer, allowing people to study how algorithms work on complex problems and as such the use of supercomputers is important for quantum algorithm development.



Solutions:

"You can test a quantum algorithm on a laptop, but you need a supercomputer such as the LUMI EuroHPC supercomputer if you want to scale the algorithm to realistic levels," says Dr. Ossi Niemimäki at Quanscient. "This will help identify problems and bottlenecks in simulations."

"In a couple of years, we may already be at the point where, in certain very precisely defined cases, quantum computers will be able to solve problems better than classical supercomputers," predicts Niemimäki. "As early as 2027, quantum software could be available on Quanscient's cloud service for the use of business."
In practice, companies can use the LUMI development environment to develop quantum algorithms and assess what the algorithms will make possible in the future when the number of qubits and the computing power of quantum computers increase. When the size of quantum computers increases, their ability to solve problems develops exponentially.

A quantum computer does not solve problems on its own, but needs a supercomputer to support it. Quantum computing can accelerate some parts of the computational model workflow, but much of it will continue to require the computing power of a supercomputer.

Business impact:

Quantum computing has the potential to revolutionise the way businesses process data in a more profound way than AI is currently doing. Quanscient is already preparing for future business needs and developing quantum software with the help of the LUMI supercomputer.

„Now is the time to develop quantum algorithms if you want to compete. When quantum computers are good enough to be really useful, we will have something ready to offer the automotive and aerospace industries," says Chief Scientist Valtteri Lahtinen. "In the future, the models could be used for modelling aircraft aerodynamics or for the product development of electric motors for cars, for example."

The LUMI supercomputer is used in particular to study how the software being developed can be scaled to the more powerful quantum computers of the future. Emulating a quantum computer requires a lot of computing power and the capacity available through EuroHPC enables Quanscient to run even the most challenging simulations.

Benefits:

- Emulating a quantum computer requires a lot of computing power
- Results on LUMI show how large simulations behave
- It also helped to identify problems and bottlenecks in simulations
- Quantum computing needs the computing power of a supercomputer for simulation and testing of quantum algorithms

·Keywords (Min 5): Quantum, Quantum computing, Emulation, Quantum algorithms, Algorithms, Future technology
·Technology: (HPC, HPDA, AI...): HPC, Simulations, Quantum, FEM, Cloud
Industry sector: Services & software providers

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EURO²

Machine Translation Post-Editing

NCC Estonia

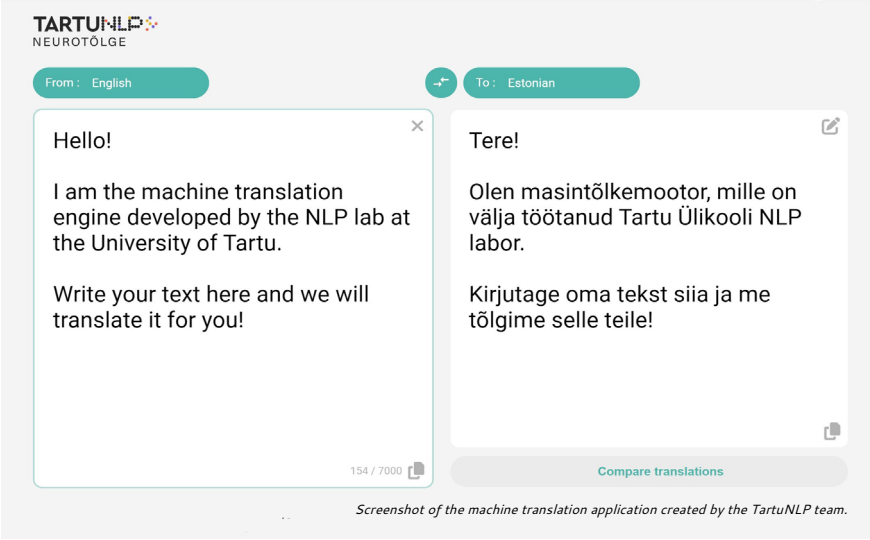
Industrial organisations involved:

Luisa Tõlkebüroo OÜ is the biggest translation agency in Estonia. The company offers over 50 services – including sworn translation, simultaneous and consecutive interpretation, layout work, machine translation and post-editing, subtitling and localisation.

LUISA
TRANSLATION AGENCY

Technical /scientific challenge:

The company needed a custom-made machine translation system to reduce the time of translations.



Screenshot of the machine translation application created by the TartuNLP team.

Solutions:

As the company had no previous experience neither in natural language processing nor in machine learning, they collaborated with the TartuNLP team. Training of the machine translation model was conducted by using University of Tartu HPC centre's Rocket cluster. Once the models were trained, the company considered different options for deployment. Their initial plan was to invest in their own infrastructure but soon they realized that it would not be justified for their use case and the TartuNLP group deployed the models alongside other services in the cloud.

Business impact:

Thanks to rapid advances in the technology and our extensive translation memory, the company is able to offer its customers machine translation service with post-editing in a range of language combinations and on a range of topics. The new service makes the company's service package more attractive, reduces costs and increases competitiveness in the market.

Benefits:

- Neural machine translation systems were built for 4 language pairs and several text domains
- The company enjoyed lower deployment costs and did not have to worry about maintaining their own hardware
- The innovative translation tool helps to save valuable time and human resources

Keywords: ·Natural Language Processing, Machine translation, Language technology, post-editing, TartuNLP

Industry Sector: HPC, HPDA, AI, Natural Language Processing

Technology: Services & software

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Revolutionizing Server Security: BitNinja Harnesses the Power of Komondor

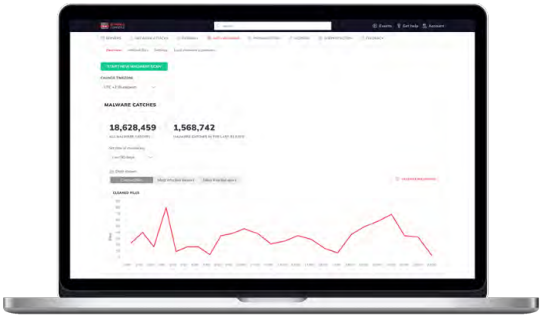
NCC Hungary

Industrial organisations involved:

BitNinja Technologies is an innovative leader in server security that specializes in proactive server protection. Utilizing a multi-layered, all-in-one security tool, the company secures web servers and customer websites against a wide range of cyber threats. Its comprehensive suite includes an AI-driven malware scanner, robust IP reputation list, advanced WAF (Web Application Firewall), and a global Defense Network, all in a centralized Dashboard for streamlined management.

Technical /scientific challenge:

In the rapidly evolving landscape of cybersecurity, traditional defences are often inadequate against AI-generated threats. The increasing sophistication of cyber threats, particularly those powered by AI, required a new paradigm in threat detection and analysis, one that conventional computing resources could not efficiently handle. Thus, the challenge was to enhance real-time threat detection and manage large-scale data processing for comprehensive cybersecurity solutions. This data included complex patterns and signatures of new and evolving malware.



BitNinja Malware Scanner Dashboard

Solutions:

To address these challenges, BitNinja significantly enhanced its AI algorithms by leveraging the advanced computing power of KomondorHPC, a high-performance computing system known for its exceptional processing speed and capacity for handling large-scale data. This upgrade allowed for deeper and more complex data analysis, leading to the development of more sophisticated and accurate threat detection models. Additionally, the supercomputer enabled real-time processing of vast datasets, ensuring that BitNinja's cybersecurity solutions remained agile and effective, even in the face of rapidly evolving threats.

Business impact:

Transformation of Cybersecurity Solutions

The integration of Komondor's computational power has significantly improved BitNinja's real-time threat detection efficiency, ensuring faster and more accurate responses to cyber threats.

Innovation in Threat Detection

Through the integration with Komondor's advanced processing power, BitNinja developed an AI model that significantly boosted their zero-day malware research. This new model streamlined the analysis of vast data sets, enabling quicker identification of unknown malware types with reduced human effort. This improved method was particularly effective in detecting emerging cyber threats, crucial for pre-emptive cybersecurity. By employing Komondor, BitNinja not only accelerated its threat detection capabilities but also enhanced the accuracy and efficiency in uncovering and responding to novel cyber threats.

Leadership in AI-Driven Cybersecurity

BitNinja's pioneering approach, powered by Komondor, has positioned the company at the forefront of the cybersecurity industry, providing their clients with the most advanced defenses against ever-evolving digital threats.

Benefits:

- Enhanced threat detection speed by 300%
- Improved identification of zero-day vulnerabilities
- Strengthened long-term cyber defenses

Keywords: Server Security, Artificial Intelligence, Real-time Threat Detection, Malware Scanner, Zero-day

Industry Sector: IT/HPC systems, services & software providers; Cybersecurity.

Technology: High-Performance Computing (HPC), Artificial Intelligence (AI).

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Supercomputer boosted R&D for speech recognition tech company Inscripta

NCC Finland

Industrial organisations involved:

Inscripta is a Helsinki-based company Finnish company founded in 2016, is a speech recognition company whose mission is to help healthcare professionals speed up their work. The Inscripta solution comprises of a dictation application, AI-powered speech recognition, and personnel and workflow management system.

Inscripta's technology is a product of years of work in training and experimenting with AI algorithms to find the best possible speech recognition models. Training AI models requires large amounts of data and computing power.

Technical /scientific challenge:

According to CEO Peter Smit and Senior Speech Recognition Engineer Emre Cakir, the number one advantage of HPC computing is speed, enabling efficient training of AI models.

In the CSC environment, computing capacity and GPUs have been well available. Access to supercomputing resources enables much faster deep neural network based speech recognition and spoken language understanding model teaching.

„Also, the user support is great. CSC's documentation is good, and if I can't find the answer to the problem, I can contact the service desk for support," Cakir says.

The familiarity of the computing environment was also a factor. Inscriptans got used to working in CSC's HPC environment already during their studies: Smit at Aalto University's speech recognition research group and Cakir at Tampere University.

Solutions:

Part of the daily routine work of healthcare professionals is keeping patient records. Inscripta has developed a dictation application, based on AI-powered speech recognition technology. Inscripta's solution significantly speeds up the work of healthcare professionals, enabling them to treat more patients.

"According to our survey, the app saves users an average of 45 minutes a day. Our solution has an impact on both users' work days and society at large as it's saving healthcare resources," says Peter Smit, CEO at Inscripta.

Inscripta's product development requires evaluating different machine learning algorithms to find the optimum models to improve speech recognition. Access to supercomputing enables much faster deep neural network based speech recognition and spoken language understanding model teaching.

Business impact:

With the help of CSC's Puhti supercomputer and Business Finland's compute grant, Inscripta has developed one of the most accurate medical oriented speech recognition solutions on the market.

The accuracy of Inscripta's speech recognition technology, is over 98%. The technology is very accurate accurate and is according to Inscripta, approaching the human level. The user reads and checks the text they dictate, but it is only rarely necessary to make corrections.

Inscripta is making plans for other European markets as well. The technology can be taught to understand any language, dialect, or jargon. It is also suitable for other industries.

Benefits:

- Ability to develop a technology that is highly accurate
- HPC is ideal for companies that run large amounts of data and require a lot of compute power
- R&D is easier in the HPC environment than in commercial cloud services
- User support

Keywords: Speech recognition, App, AI model, R&D, Dictation

Industry Sector: HPC Machine Learning, AI

Technology: Services & software providers

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EURO 4SEE

Section 2

Natural Sciences and Aeronautics

EURO²

Cosmic ray-based solutions for 3D imaging

NCC Estonia

Industrial organisations involved:

GScan was founded in 2018 to revolutionise inspection, security and medical scanning markets using Muon Flux Technology (MFT). GScan, as the pioneer of MFT having unique IP, tech & sales expertise in the field, is developing a new generation of Non-Destructive Testing (NDT) scanners and tomography systems for infrastructure management applications.

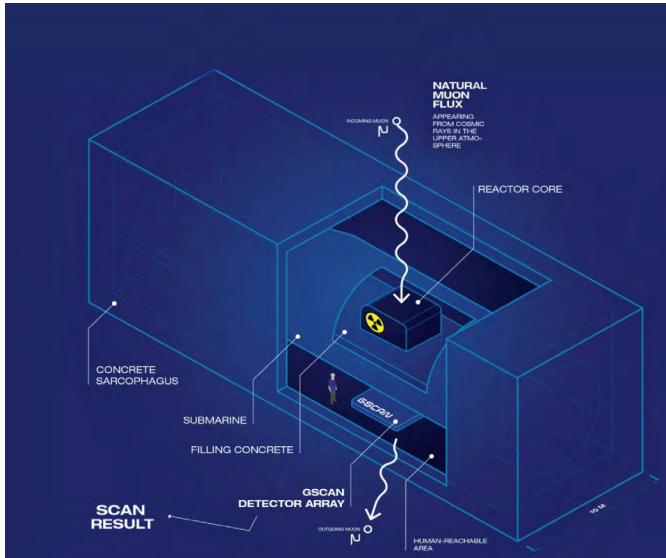
GSCAN

Technical /scientific challenge:

In 1968, Soviet Union built a nuclear submarine training base with two full-length submarines next to Estonian town of Paldiski. The site was handed over to the Estonian authorities, but no detailed specifications about the site were offered. The reactors and radioactive waste have been buried in concrete within the submarine bodies, which are further surrounded by a concrete sarcophagus. 3D scanning, mapping, and performing atomic detection of the now-defunct nuclear reactors were required to decommission these submarines safely.

Solutions:

Capitalising on the power of natural cosmic ray tomography, the technology tracks the trajectory changes or absorption of particles (muons, electrons, positrons) as they pass through the object of interest, thereby extracting crucial statistics about its material and shape. These insights are then translated into 2D and 3D visualisations of both internal and external geometries, along with data on chemical composition. The comprehensive output provides in-depth insights into the objects and materials under scrutiny – all meticulously tailored to fulfil customers' unique requirements. HPC plays an important role in translating the collected data into visualisations.



The principle of 3D-imaging of nuclear reactors for the safe decommissioning process.

Business impact:

GScan's muFLUX Infra detectors can be used for 3D imaging of abandoned nuclear reactors to ensure the safe decommissioning process. In order to minimise the risks of dismantling the site, a high-resolution 3D image and atomic composition analysis is needed. With time and space related digital data in terabytes, the detailed process of reconstruction enables to see inside of structures what was not possible before.

Benefits:

- Because HPC accelerates data processing, reconstructions are completed in less time
- With faster reconstruction, it is possible to apply wider range of algorithms during the post processing
- With a wider range of algorithms, the capability and efficiency of the technology grow and with better muon flux technology, the world can become safer thanks to more reliable data about critical infrastructure

Keywords: 3D imaging, Muon Flux Technology, tomography, nuclear reactors, cosmic rays

Industry Sector: HPC, HPDA, AI, Muon Flux Technology

Technology: Environment/climate/weather, Services & software, Maritime

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Advancing Maritime Design: HPC-Enhanced Hull Optimization in Wave Dynamics

NCC Slovenia

Industrial organisations involved:

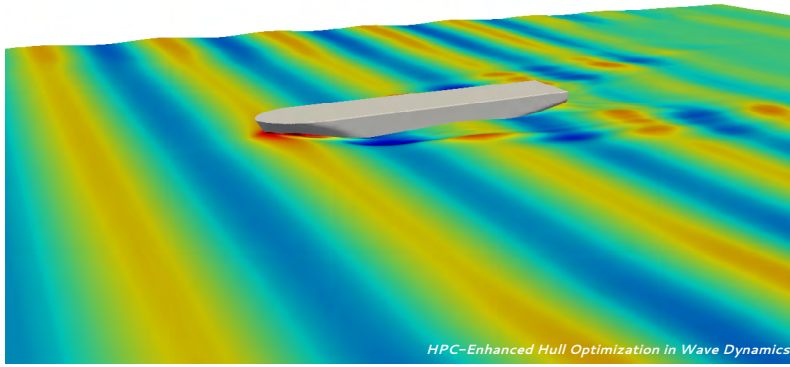
In silico specializes in numerical simulations of Computational Fluid Dynamics (CFD) for various engineering fields. The company's flagship service, Cloud Towing Tank (CTT), brings advanced CFD expertise to marine engineering. CTT offers comprehensive simulations, including ship resistance, self-propulsion, manoeuvring, seakeeping, and propeller-hull interaction, addressing a wide spectrum of maritime challenges.

Technical /scientific challenge:

Optimizing a container ship's hull for both calm water and added resistance in waves is a complex technical challenge. In calm water, the focus is on reducing resistance to enhance fuel efficiency and speed. This often involves streamlining the hull shape to minimize resistance. However, in wave conditions, additional factors like wave-induced motions, wave reflection and refraction come into play. This demands an iterative approach by employing CFD simulations and HPC resources to balance streamlined shapes for calm water efficiency hull geometry features that reduce added wave resistance.

Solutions:

To enhance the hull's performance, a two-stage optimization workflow was applied. Initially, the hull's global geometry parameters were optimized. Subsequently, a localized fine-tuning of the ship's bow was conducted. Furthermore, the employed approach preserved the required displacement of the vessel across all modifications. Testing encompassed three calm water speeds and one in regular wave conditions, analysing 27 variations per stage—totalling 216 CFD simulations. Performance was assessed through a consolidated propulsion power metric. The obtained data was then analysed through a surrogate model, which provided valuable insights into the influence of the selected variables on the vessel's performance, ensuring a robust and informed optimization process.



HPC-Enhanced Hull Optimization in Wave Dynamics

Business impact:

HPC significantly enhances our operational agility by enabling parallel simulations at a larger scale. The ability to run numerous computations simultaneously reduces the time required for complex analyses, allowing for rapid iteration. This rapid turnaround is crucial for staying ahead in a fast-paced market and meeting client expectations for swift project completions.

The elastic nature of HPC resources aligns perfectly with our project-driven workflow. By leveraging HPC services, we can scale our computing power to meet peak demands without the hefty investment in physical infrastructure. This flexibility ensures we can manage large-scale calculations during high-demand periods efficiently, maintaining smooth and uninterrupted project progression.

This scalability of HPC resources not only optimizes our operational costs but also empowers us to take on larger, more ambitious projects. It alleviates the stress of resource management, allowing us to focus on innovation and quality of service. Consequently, our business is more adaptable, responsive, and capable of seizing opportunities in a dynamic industry landscape.

Benefits:

- Drastically cuts simulation time
- Lowers operational costs
- Enhances design precision
- Boosts response to peak demands

Keywords: Computational Fluid Dynamics, Ship Design, Parametric Design, Added Wave Resistance, Marine Hydrodynamics, Naval Hydrodynamics

Industry Sector: services & software providers, Maritime

Technology: HPC

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EURO²

Faster processors communications to better understand fluid turbulence

NCC Belgium

Industrial organisations involved:

Pierre Balty graduated with a Master's degree from UCLouvain, in 2019 and is currently pursuing a PhD degree under the supervision of Prof. Philippe Chatelain at the Institute for Mechanics, Material, and Civil Engineering, UCLouvain. His research focuses on hybrid Eulerian–Lagrangian numerical methods, their deployment on distributed systems, and their applications to wind energy. To pursue his research, Pierre collaborates with an international research group from the Massachusetts Institute of Technology and the Argonne National Laboratory.

UCLouvain

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Argonne NATIONAL LABORATORY

Technical /scientific challenge:

One of the Vortex and Turbulence Research Group's interests lies in understanding and exploring fluid phenomena at an unprecedented level of accuracy. The latter often implies many different scales, requiring a substantial number of unknowns and, hence very large computational resources. This is where HPC comes into the picture.

In this project, we focused on developing an integrated software combining versatility, performance, scalability, and portability to solve the most time-consuming part of our simulation: the 3D unbounded Poisson problem required to impose the incompressibility of the fluid.

Solutions:

The Poisson problem is an elliptic problem, where each point in the domain influences all the other points. On HPC architecture, its resolution requires all-to-all communications, and the latter bound the resolution timings.

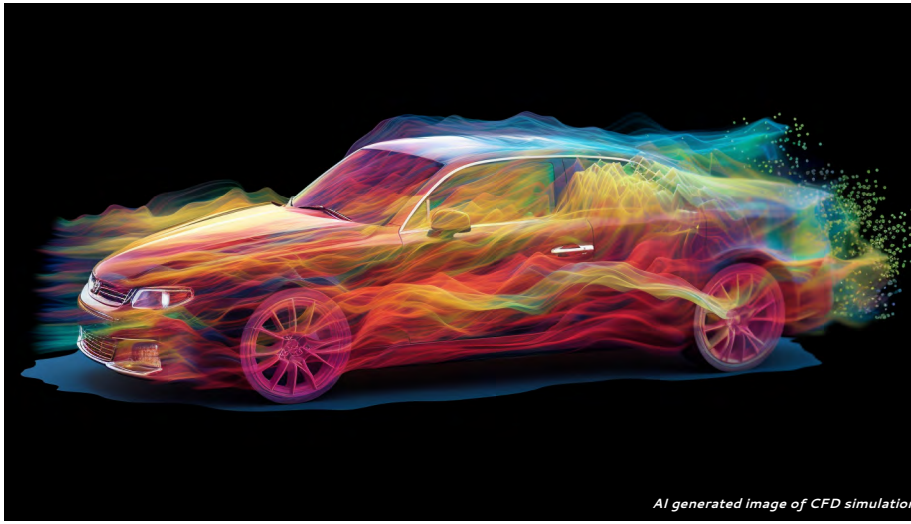
Among the existing approaches, we decided to use FFT-based methods, which are the fastest when dealing with uniform and regular cartesian grids. 3D FFTs are computed using a series of 1D FFTs, requiring aligned and continuous memory in the FFT direction. The transposition of the data implies processes communication and becomes the algorithm bottleneck. We proposed different implementations where the overall objective was to reduce the strong synchronization of the CPUs and improve the parallelization without impacting the flexibility and versatility of the solver.

Business impact:

The impact of our work goes well beyond computational fluid dynamics. Poisson equations are ubiquitous in computational physics as they concern problems ranging from particle physics to electromagnetism. Thanks to the enormous computational resources they provide, HPC is a keystone in such fields. Currently, the focus is on porting the existing frameworks on GPUs to benefit from the full computational power those supercomputers provide. For low arithmetic intensity problems such as the Poisson problem, the high bandwidth provided by the recent HPC architecture promises considerably reduced times-to-solution. Scalability is crucial for users when using HPC systems. For exascale architecture, where resources are tremendous, one of the key factors is the strong scalability, i.e., the ability of the software to decrease the time-to-solution proportionally to the increase of the number of processes. Let's say the user chooses an N/P ratio (N = unknown, P = proc). If the user uses 2P instead of P, it divides the time-to-solution by 2*eta (eta = strong scalability)—the highest the eta, the larger the time gain. In our case, the strong efficiency is remarkable for an all-to-all problem.

Benefits:

- Very large domain with a substantial number of unknowns > 250M unknowns
- Small time-to-solution for reasonable simulation
- Improved data post-processing



AI generated image of CFD simulation

Keywords: 3D Fourier Transform, Elliptic Problem, Free-space boundary, Poisson equation, Computational Fluid Dynamics

Industry Sector: Aeronautics, Automotive, Energy

Technology: HPC

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EURO²

Space Technology Company ICEYE praises LUMI user support

NCC Finland

Industrial organisations involved:

ICEYE is a Finnish space sector company that operates SAR (synthetic aperture radar) satellites. Instead of using conventional cameras, satellite images are taken with microwave radars which enable imaging 24 hours a day, and in difficult weather conditions, including through thick cloud cover. ICEYE leverages the high-performance computing capabilities provided by CSC – IT Center for Science Ltd. to train neural networks specifically designed for automated analysis of satellite imagery.

ICEYE

Technical /scientific challenge:

The areas to be monitored are sometimes extremely large:" In Japan, for example, one half of the land area may be at flood hazard at the same time. Or when we study the progress of deforestation, we can observe an area of up to hundreds of thousands of square kilometers", explains Tapio Friberg, Senior Machine Learning Engineer at ICEYE. Monitoring large areas based on satellite images is very intensive, which is why image interpretation must be automated to ensure efficiency and real-time monitoring.

Radar satellite image of the largest seaport in Europe – Port of Rotterdam, the Netherlands. The image was acquired with an ICEYE SAR satellite in the Spot imaging mode

Solutions:

To automate this procedure, machine learning-based neural networks are employed. In order for the neural networks to work as intended, they must be trained with large volumes of data, in this case with tens of thousands of satellite images. During the training, dozens or hundreds of tests are performed with the data before the model can be put to productive use. NCC Finland, as the company's partner, facilitates access to the substantial computing power and storage capacity needed for the effective training and testing of AI models.

"Data storage has been a particularly useful feature when working with CSC and NCC Finland", Friberg says. The data is kept safe until the prototype cycles, which may sometimes take up to a week, have been completed.

Business impact:

For ICEYE, ensuring the necessary support for deployment posed a fundamental challenge. Top performance and a very competitive price would not have sufficed if Tapio Friberg would have had to fight with the deployment process for weeks.

Ease of use and user support. These are the two points for which Tapio Friberg, ICEYE Machine Learning Engineer, gives special thanks. "And the very best experts supported us in the deployment process," says Friberg. When Friberg chooses new tools and operating methods, the factors affecting the choice are not only the price and technology but also how much working hours the deployment takes at ICEYE. When using a supercomputer, at first, you must always make some effort to match your own materials and software with the supercomputer.

"If I were to work on something on my own for a month without knowing whether it would bring results or not, I would probably spend my time on something else," Friberg said, when he described the selection process.
With the help of NCC Finland and CSC experts, ICEYE could select the right software and was able to match in house software libraries with LUMI.

Benefits:

- LUMI's cost efficiency enable ambitious testing
- CSC's user support helped match software libraries with LUMI
- Ease of use
- Data storage has been a particularly useful feature

Keywords: Real-time radar images, Radar images, Image interpretation, Data, Space technology
Industry Sector: Space manufacturing
Technology: HPC, AI, ML, SAR

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EURO²

More than 12,000 new periodic free-fall orbits for the three-body problem

NCC Bulgaria

Industrial organisations involved:

This work was developed in collaboration with colleagues from the Faculty of Mathematics and Informatics at the Sofia University, Institute of Physics Belgrade at the University of Belgrade, and the National Astronomical Observatory of Japan.

The Computer Informatics Department is part of the Faculty of Mathematics and Informatics (FMI) of Sofia University. It manages courses led by the faculty in programming, data structures, databases, artificial intelligence, and distributed systems. The department supports several masters' programs – Embedded Systems, Artificial Intelligence, Information Systems, IT Services, and Projects.

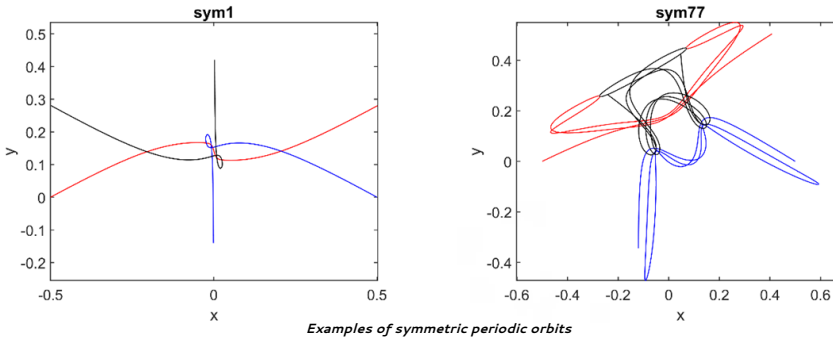
The Institute of Physics Belgrade (IPB) is a scientific institution whose program includes theoretical physics, physics of elementary particles, subatomic particle physics, and others.

The National Astronomical Observatory of Japan (NAOJ) is an astronomical research organization.

Technical /scientific challenge:

In 2019 Li and Liao announced the discovery of 313 initial conditions (i.c.s) for free-fall (or "brake") collisionless periodic orbits in the Newtonian three-body problem [1], 30 of these 313 i.c.s being for equal-mass case. They used TH-2 at the National Supercomputer Centre in Guangzhou, China to achieve these results. Although it was a breakthrough in searching for new periodic free-fall orbits at the time, this number of discovered and identified free-fall orbits does not compare favorably with thousands of other types of periodic 3-body orbits that have been found over the past decade. There were also some logical inconsistencies in the work of Li and Liao. Our goal was to find them and fix them and to conduct a new numerical search with better efficiency, limited to the equal-mass case.

[1] Xiaoming Li and Shijun Liao, "Collisionless periodic orbits in the free-fall three-body problem", New Astronomy 70, 22-26 (2019); arXiv:1805.07980v1 (online).



Examples of symmetric periodic orbits

Solutions:

The numerical algorithm that we use for finding periodic orbits is an optimized version of those used in [1]. This is the grid-search algorithm in combination with Newton's method, where the computing of the coefficients of the linear system at each step of Newton's method is done with the high-order Taylor series method used with high-precision floating point arithmetic. The obtained better efficiency can be explained with the use of a finer search grid, the use of a modification of Newton's method with a larger domain of convergence, and some technical improvements. Using the NESTUM cluster, the computation time was reduced more than a hundred times. Achieving the results is impossible without using the HPC cluster.

Scientific impact:

We searched for equal-mass periodic free-fall orbits, finding 24,582 initial conditions, corresponding to 12,409 distinct solutions. The distribution of initial conditions shows a remarkable structure (the „Maasai shield") similar to several other previously investigated properties of the free-fall problem. Some 236 orbits have geometric symmetries, compared with only a few known before. Several examples of so-called "stutter" orbits, predicted in 2012, have also been found. These are the news of interest to mathematicians. After the study of the stability of orbits, we shall know more about their astronomical and astrophysical interest.

A paper about the studies has been published: Hristov, I., Hristova, R., Dmitrašinović, V., Tanikawa, K. Three-body periodic collisionless equal-mass free-fall orbits revisited. Celest Mech Dyn Astron 136, 7 (2024). https://doi.org/10.1007/s10569-023-10177-w

Benefits:

- Reduction of computation time by using parallel compuuttions

Keywords: Three-body problem, free-fall periodic collisionless orbits, numerical search, supercomputer applications
Industry Sector:astronomy, physics, mathematics
Technology:HPC

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EURO 4SEE

Section 3

Environment, Energy, and Agriculture

EURO²

HiGh fidElity Modeling for small wINd Turbine (GEMINI)

NCC Greece

Industrial organisations involved:

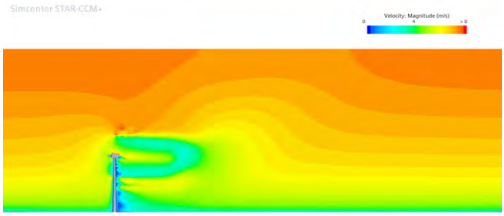
End User: Eunice Wind S.A., a subsidiary of the Eunice Energy Group, is the first wind turbine manufacturer in Greece. The small wind turbine EW16 Thetis, manufactured in Mandra, Attica is designed in accordance with IEC 61400-2, while Eunice Wind S.A. has a fully integrated production with ISO 9001: 2015 certified processes

Technical /scientific challenge:

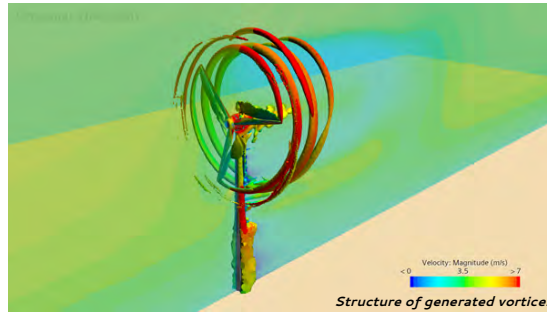
The improvement in the performance characteristics of wind turbines is a challenging task, and the need for optimum designs is significantly growing. Computational Fluid Dynamics (CFD) turns out to be a unique tool enabling the optimization of wind turbines during a detailed analysis of the rotors' blades shape and the tower design aiming to improve the overall efficiency of the structure. The consortium utilizes High Fidelity numerical models in order to assess and accurately simulate the aerodynamic performance of small wind turbines under various operational scenarios.

Solutions:

The project partners assembled a sophisticated suite of Computational Fluid Dynamics (CFD) simulation models, powered by High-Performance Computing (HPC) resources in order to rigorously assess and optimise wind turbine performance, with particular attention to the real-world operational conditions that the turbine would face on site. The simulations required, on average, over 485,000 CPU hours. In total, more than 125,000 CPU hours were allocated to this project. For the simulation process itself, dense computational meshes, comprising of more than 50 million cells, were used and a reduced time step approach was employed. Additionally, the implementation of the Detached Eddy Simulation method facilitated the modelling of complex physical phenomena. This comprehensive simulation procedure was subsequently validated using an experimental dataset, leading to a notable reduction in the uncertainty associated with the computed results.



Vertical sections at a stream-wise of velocity magnitude



Structure of generated vortices

Business impact:

For EUNICE WIND SA, the material and permitting cost of constructing a new wind turbine solely for testing purposes is approximately €300,000. Replacing those tests by HPC-based CFD simulations to analyze the wind turbine's operation in its actual location reduces costs to only 10-17% of the total expense, depending on the complexity of the HPC calculations. Simulation results lead to potentials for reduced costs through predictive maintenance and enable faster design cycles giving to EUNICE a competitive advantage.

By optimizing the turbine's operational settings, EUNICE WIND SA can now generate higher energy output from their wind turbines, an achievement with direct financial implications. Engineering P.C. gained experience in high-fidelity simulations by utilizing large-scale HPC resources allowing it to expand into new markets, like the wind energy sector.

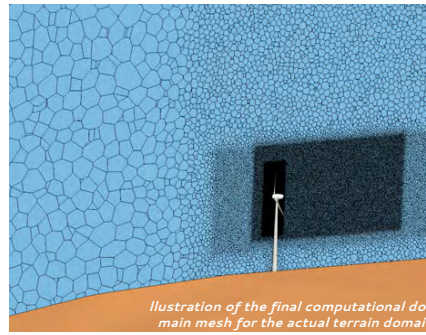


Illustration of the final computational domain mesh for the actual terrain domain

Benefits:

- Increased energy generation, higher reliability, and reduced maintenance costs
- Suppliers in the wind energy sector can capitalize on the improved performance and optimized designs by providing high-quality components and materials
- Service providers, including maintenance and consulting firms, can offer specialized services based on the project's findings, further enhancing their value proposition
- By leveraging the project's outputs, service providers can deliver more accurate and effective solutions to their clients; the project's outputs have created a cohesive ecosystem in the wind energy industry, where participants work together to drive continuous improvement and growth

Keywords:wind turbines, CFD, high-fidelity simulations, energy, aerodynamics, engineering

Industry Sector: Energy, Environment/climate/weather,

Technology: HPC

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Note: The work of the SME was performed within a business experiment funded by the FF4EuroHPC project(*). NCC Greece supported the development of the proposal."

*FF4EuroHPC has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 951745. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Germany, Italy, Slovenia, France, Spain.

Funded by the European Union

EURO²

Fuel and operational flexibility in micro Gas Turbine combustors for sustainable energy production

NCC Belgium

Organisations involved:

Alessio Pappa is a Postdoctoral researcher in the Thermal Engineering and Combustion Unit at the University of Mons, Belgium. He started his thesis as a teaching assistant in November 2017 under the supervision of Professor Laurent Bricteux and associate Professor Ward De Paepe. In October 2023, he defended his thesis entitled "Fuel and operational flexibility of micro Gas Turbines: assessment of combustor performances, emissions, and stability".

UMONS
Université de Mons

Technical /scientific challenge:

The pollution induced by combustion is considered one of the biggest challenges in our society. Therefore, the accurate control of turbulent flames is mandatory to answer the needs and challenges imposed by the advanced gas turbine cycles.

Besides the general geometric complexity of real combustors, a wide range of coupled problems are involved in turbulent flames. First, there are the fluid mechanical properties describing the mixing and all transfer mechanisms occurring in turbulent flames, such as heat transfer, molecular diffusion, convection, and turbulent transport. A precise knowledge of the chemistry is also required to predict ignition, stabilization, fuel consumption rate, or emissions. Among the other modeling difficulties, two- or three-phase combustion may also be encountered and real gas effects due to critical conditions limit the use of the perfect gas law and usual thermodynamical properties.

Solutions:

Computational Fluid Dynamics (CFD), which has been efficiently used in turbulent combustion modeling, appears as evidence to study and improve actual combustors. In this framework, Large Eddy Simulations (LES) offer a balanced solution to better assess the combustion behavior under the studied specific conditions (dilution and non-conventional fuels). In LES, the smallest length scales are modeled by performing spatial and temporal averaging, which ensures a limited computational cost while maintaining a reasonably good accuracy. Indeed, LES allows accurate assessing the unsteady effects coupled with the turbulent-chemistry interaction of reacting flows. However, this high-fidelity level of modeling becomes impossible without advanced and powerful numerical tools such as HPC. A typical simulation of the reacting flow in a burner of 300kWth requires usually 25 days using 1000 cores on a Tier-1 supercomputer.

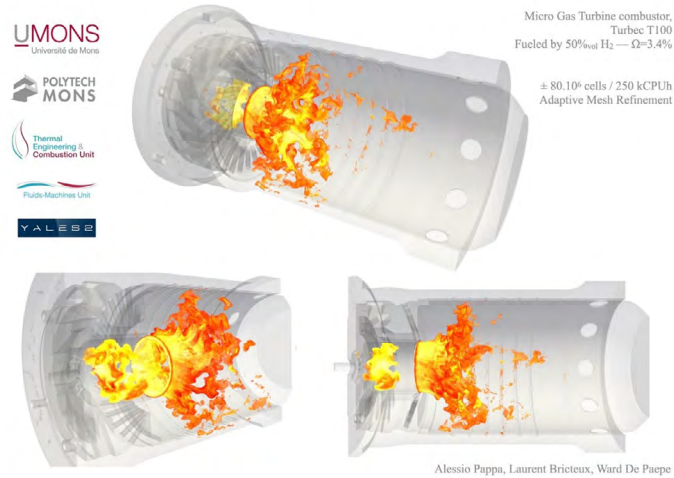
Business impact:

The objective of the research was thus to assess and analyze, using LES, the impact of various fuel and fuel blends, and/or unconventional diluted conditions such as water and exhaust gas recirculation (EGR), on the combustion stability, performance, and emissions, especially for micro Gas Turbine (mGT) combustors. This research was built on three main axes: numerical development, operational flexibility, and fuel flexibility.

Fuel flexibility means that the mGT combustor must be able to work with different fuels such as hydrogen from renewable energies using Power-to-Fuel, while operational flexibility means that the combustor must work under diluted conditions (water and/or CO2) coming from different advanced cycle modification such as humidification or EGR. Therefore the mGT combustion chamber has to face unconventional diluted conditions and/or different fuels but has still to ensure complete, stable, and efficient combustion. In addition, accurate data assessing the impact of such diluted conditions and/or different containing fuels on the combustion performance, stability, and emissions for actual mGT combustor geometries and operating conditions are mandatory to address this need for flexibility.

Benefits:

Decentralized systems in combination with small-scale Combine Heat and Power production, like micro Gas Turbines (mGTs), and performing Power-to-Fuel to store the excess electricity coming from renewable energy, are two important studied paths for the future energy production sector. Both trends require combustion flexibility in terms of fuel utilization and operation. Considering these statements, mGTs offer advantages related to their easy and high adaptability and flexibility and can fulfil the requirements of the future power generation market. The adaptability of the mGT system allows to perform cycle humidification, which enables a separated heat and power production control, increasing the efficiency and operational flexibility. It also allows reducing the operating cost of carbon capture, utilization, and storage (CCUS).



Turbulent flames in a combustor

Keywords: CFD, Large Eddy Simulation, Micro Gas Turbine, Hydrogen, Fuel

Industry Sector: Energy

Technology: HPC

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At the Forefront of Supercomputing: Whiffle and Lux-Provide Transform Weather Prediction Capabilities

NCC Luxembourg

Industrial organisations involved:

Whiffle B.V. was founded in 2015, starting as a spin out of the Dutch Delft University of Technology. With its roots in science, the company continues to use cutting edge R&D to further develop Large Eddy Simulation (LES) models and its unique implementation on high performance computing systems. This resulted in the world's first LES based operational weather model that produces highly accurate and ultra high-resolution weather forecasts. Application areas of Whiffle's model include wind and solar power projects and air quality.

Technical /scientific challenge:

The technical/scientific challenge lies in harnessing the power of HPC as a backend solution to expedite computations and enable scalability, ultimately enhancing the accuracy and efficiency of models, also time to solution. This necessitates overcoming complexities inherent in integrating HPC infrastructure, optimizing algorithms for parallel processing, and ensuring seamless scalability to meet evolving computational demands.

Weather forecasts and simulations on a hyper local scale

Solutions:

Whiffle uses LuxProvide's HPC infrastructure to enhance the computational capabilities of its Large Eddy Simulation (LES) technology, enabling high-speed processing of vital weather data (such as wind patterns, turbulence, and wakes) for wind energy projects. MeluXina, the innovative supercomputer, plays a central role with its versatile software ecosystem, designed for scalable HPC, data analytics, and AI. It supports containerized workflows, ensuring efficiency in complex computational tasks.

Whiffle plays at the forefront of scientific computing. Their innovative GPU-based model is highly flexible and can adapt to the latest developments in cloud and HPC technology. Working with LuxProvide allowed them achieving further enhancements to fully leverage the available high-end HPC infrastructure. They can now meet the expanding needs of multi-gigawatt wind farms, providing precise weather insights for large domains, in a fraction of the time. Leveraging the extensive number of interconnected GPUs that are available on demand, they have markedly improved the speed and scale of our modelling processes. This advancement lays the groundwork for future continental-scale LES applications.

Business impact:

LuxProvide, along with its infrastructure MeluXina, in collaboration with the expertise of LuxProvide, facilitates the identification of bottlenecks through profiling, thereby enhancing accuracy and efficiency. Leveraging the power of HPC, they can envision a future where weather prediction reaches unprecedented levels of precision and reliability.

Benefits:

- Facilitating the acceleration of time-to-results
- Providing rapid deliverables to end customers
- Enhancing efficiency and customer satisfaction

Keywords: Weather prediction, energy systems, LES, CFD, atmospheric forecasting

Industry Sector: Energy, Environment/climate/weather

Technology: HPC, AI

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EURO²

HPC for the Acceleration of Materials Discovery and Design

NCC Belgium

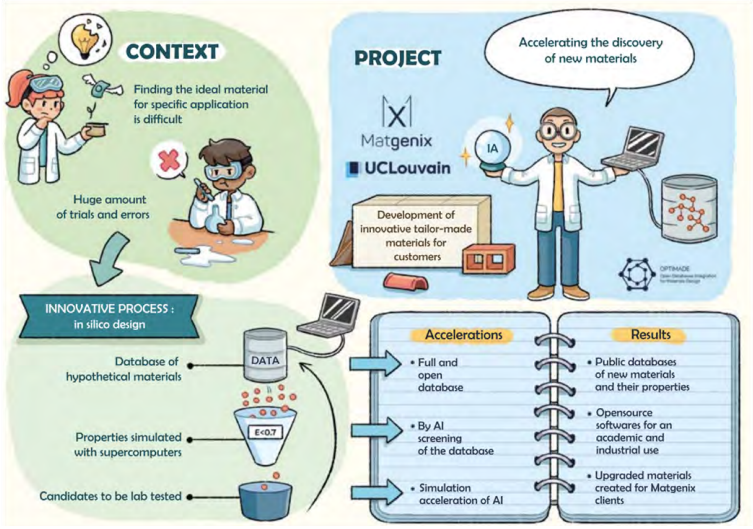
Industrial organisations involved:

Matgenix is a Belgian start-up. The company offers tailored solutions to boost research and development activities in chemistry and materials science.

The project has been developed in collaboration with the Catholic University of Louvain through the BEWARE Fellowship of Dr. Matthew Evans.

Matgenix

UCLouvain



How AI and machine learning help design new materials

Technical /scientific challenge:

Active in the energy sector, Matgenix is working – for example - on batteries and photovoltaic devices. Matgenix needs to virtually test thousands of materials rapidly without needing to synthesize them, then select the most promising ones to be tested for expensive validation. The space is too large to even virtually screen all possibilities, and for some applications, calculations of properties are extremely computationally intensive.

Solutions:

Matgenix develops and extends open source software that enables high-throughput calculations to be performed on tens of thousands of materials that exist in open databases to find the optimal solutions for a given application, as well as the ability to robustly suggest new hypothetical materials with targeted properties. Machine learning is also used to accelerate these steps; either by training a surrogate model that can suggest which of the thousands of potential materials to study in detail, or by training models on a particular set of materials that can predict the targeted properties with sufficient accuracy much more efficiently than traditional first principles calculations. This combination of high-throughput automated jobs and machine learning approaches allows for unprecedented scope and scale of materials design and discovery.

Business impact:

Being able to virtually test materials candidates provides a significant competitive advantage over traditional trial-and-error approaches, allowing companies and researchers to explore many more ideas with greater fidelity for the same or even lower cost. The inclusion of machine learning-based approaches can also allow for significantly larger system sizes to be studied in detail, providing a much better match to the real physical system. Matgenix also leans heavily on the robust automation of calculations. Combined with sizeable HPC resources, this means that the time taken to reach a reliable and systematic answer is considerably shorter than it would be otherwise.

Benefits:

- The use of HPC & simulations allows to predict the properties of materials and compounds even before having synthesized them
- Using large scale HPC resources greatly accelerates the time-to-solution, enabling much broader systematic searches
- The sizeable datasets created can then be repurposed for machine learning studies, which accelerates future developments by generating surrogate models that circumvent the need for further calculations

Keywords: R&D, Chemistry, Materials, Processes, AI

Industry sector: Material Science, Energy

Technology: HPC

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EURO²

Optimization of the anaerobic digestion process for biogas generation

NCC Spain

Industrial organisations involved:

NORVENTO is a company focused on the promotion and development of energy production facilities based on renewable energies (wind, sun and biomass), as well as in the manufacture of wind turbines. ENERGYLAB is a Spanish (non-profit) private technology centre specialized in energy efficiency and sustainability, including research topics related to biogas.

Technical /scientific challenge:

Anaerobic digestion is the process by which microorganisms degrade organic matter in the absence of oxygen, producing a methane-rich biogas stream that can be used for energy generation. Industrially this process occurs in large full tanks called anaerobic digesters. The main motivation was to prove that an optimal energy balance between energy consumption and production can be achieved in small-scale anaerobic digesters.

Solutions:

A new open source-based solution that allows the simulation of flow (fluid dynamics) and biological aspects of an anaerobic digester was developed. Due to the scales involved in the process (300 m3 for anaerobic digester and particles around 0.01 cm3), the numerical solution of this coupled problem is very complex. Highly refined meshes are needed, which results in large computation times. Consequently, the solution requires HPC capabilities to provide results in an affordable time which model the engineering processes.


Biogas Plant

Business impact:

Design and optimization developed tools allow Norvento to reduce volume and cost of industrial anaerobic digesters, increasing the amount and quality of the produced biogas while reducing the energy consumption (needed for mixing and heating). As a result, Norvento renewable energy power plants are able to increase their electrical and thermal production.

For Norvento, a cost reduction in investment and maintenance as a direct outcome of reduced size digesters, will improve and support a profitable and sustainable business, and favour new business lines, such as the implementation of on-site digesters for cattle raising installations.

EnergyLab obtained a valuable knowledge of fluid-dynamics, HPC and simulation models. Potentially, new services focused on energy efficiency, based on the HPC simulation tools developed, can be set up and included in the EnergyLab service portfolio.

Benefits:

- ·5% increase of thermal and electrical production of Norvento's biogas plants
- ·More efficient digesters will contribute to the reduction of greenhouse gas emissions
- ·New strategic services in the EnergyLab service portfolio and growth expected by 30% in total sales; the growth in turnover of the EnergyLab non-profit centre will result in increased staff

Keywords: CFD, simulation, OpenFOAM, optimization, computational modeling

Industry sector: Energy

Technology: HPC

Note: This success story was performed in a business experiment of the Fortissimo 2 (*) project involving the NCC member CESGA; the success story was included in this EUROCC booklet as it provides inspirational material for the take-up of HPC by SMEs.

*The Fortissimo 2 project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 680481.

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EURO²

Supercomputing and molecular dynamics paving the way to a circular economy

NCC Belgium

Organisations involved:

Mats Denayer is a PhD student at the General Chemistry Research Group (ALGC) of Vrije Universiteit Brussel. He started his PhD under the supervision of prof. Frank De Proft (affiliated with UGent (Center for Molecular Modeling) at that time but who is now affiliated with VUB).

VUB VRIJE UNIVERSITEIT BRUSSEL

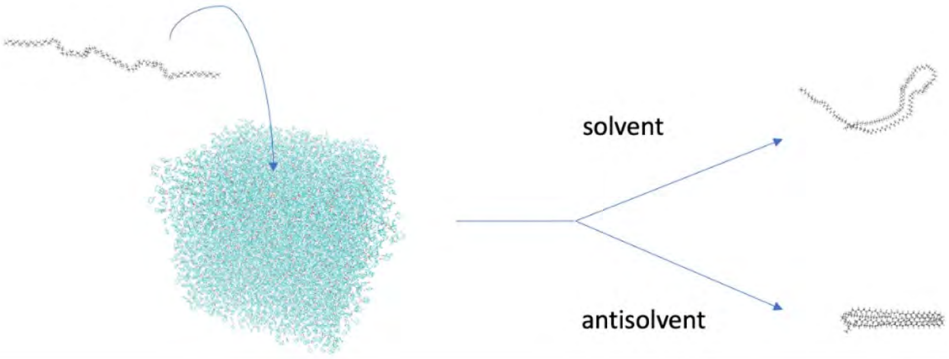
ALGC GENERAL CHEMISTRY RESEARCH GROUP

UNIVERSITEIT GENT

CENTER FOR MOLECULAR MODELING

Technical /scientific challenge:

A polymer is a substance or material consisting of very large molecules composed of many repeating subunits [1]. Polymers can be found in shopping bags or water bottles for example. In his PhD, Mats Denayer developed a new computer-based protocol to predict whether polymers will dissolve in certain liquids (solvents). Proven valid, the program can be used for industrial purposes such as polymer recycling. Mats' research fits within the context of transitioning from our current linear „use and dispose" economy to a circular economy through the development of (polymer) recycling processes. Mats uses classical molecular dynamic simulations to study how polymers behave when put in a liquid. The simulations help him understand the different steps in the dissolution process on an atomic level.



Picture displaying the different conformational behaviour of a single polymer chain in a good versus bad solvent

Solutions:

For his simulations, Mats uses the Tier-1 supercomputing infrastructure of the Vlaams Supercomputer Centrum (VSC) for two key reasons. Mats Denayer (ALGC-VUB): "Firstly, when it comes to simulating systems with a vast number of atoms, such as one to two million in our case, time becomes a critical factor. We explicitly model every polymer and solvent atom, making these simulations incredibly large. Running these simulations on standard computers or Tier 2 systems would take too long. Tier-1 supercomputers offer the computational power we need to tackle such complex simulations efficiently. Secondly, we aim to explore a large number of polymer/solvent combinations, ultimately translating into a high-throughput screening process.

Business impact:

The computational method developed by ALGC-VUB is a viable tool to predict the behaviour of a polymer in a liquid, and it is also a viable tool to understand observed polymer-solvent interactions.

The developed protocol was also built so that it can be used very easily by the industry. It works like a black box: industrial users can just give the input (a polymer) and ask which solvent to dissolve or precipitate. Or the input could also be: 'I have polymer A and solvent B, and the output will tell what will happen to the polymer. The industrial user doesn't have to know and does not get to see the calculations needed to give the result. And there is more: the protocol is not restricted to polymer recycling but to any application examining the affinity between certain molecules. Mats Denayer (ALGC-VUB) is now working on adapting the protocol to be used in other fields like polymer-assisted drugdelivery.

Benefits:

- Viable tool for theoretical polymer solubility prediction
- Viable tool for rationalization of observed polymer-solvent interactions
- Developed protocol applicable as 'black box', no user knowledge required
- Window opened towards other applications such as polymer assisted drug delivery, biochemical analysis

Keywords: Chemistry, polymer recycling, molecular modeling, plastic pollution, environment, in silico experiments

Industry sector: Chemicals, Environment, Material sciences, Plastic Recycling

Technology: HPC

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EURO²

HPDA service for estimating the brown bear population in Bulgaria

NCC Bulgaria

Industrial organisations involved:

The Department of Scalable Computing and Applications (SCA) with HPC Centre is part of IICT-BAS. It manages the HPC centre with the supercomputer Avitohol. The department develops and deploys Cloud middleware and software components, methods, algorithms, and applications suitable for Cloud and HPC computing systems.

Being the first and the richest natural history museum in the Balkans, the National Museum of Natural History (NMNH) at the Bulgarian Academy of Sciences studies, preserves and disseminates information about living and non-living nature both in Bulgaria and throughout the world. NMNH is the only national institution directly engaged with the preservation of scientific collections of live and non-live nature from Bulgaria and the world.

The Executive Environment Agency (EEA) under the Ministry of Environment and Water in Bulgaria is responsible for managing environmental control and protection. It oversees the National System for Environmental Monitoring, providing information on environmental factors countrywide, and serves as a National Reference Centre for the European Environment Agency.

Institute IICT
INSTITUTE OF INFORMATION AND COMMUNICATION TECHNOLOGIES

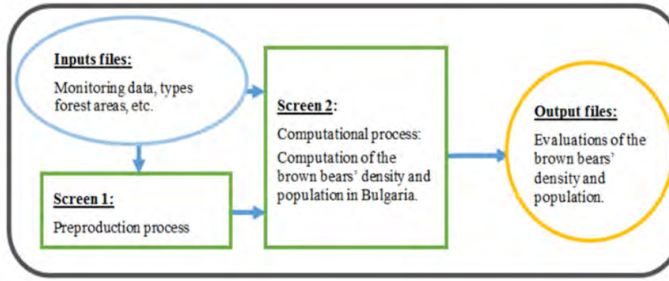
NATIONAL MUSEUM OF NATURAL HISTORY
Bulgarian Academy of Sciences

Executive Environment Agency

Technical /scientific challenge:

The problems were related to the reliability of the provided data from the national monitoring, the approaches to determine the unique traces, and the application of the statistical algorithms. We encountered challenges when we integrated the sample areas (quadrats – 10 x 10 km) using ETRS89 and bear habitats in different forest types, through the CORINE Land Cover-2018 product.

Other technical issues arose when we plugged into the HPDA service the GPS coordinates for the found bear's foot-prints during the National monitoring.



Scheme of the HPDA Service for estimating the brown bear population in Bulgaria

Solutions:

The HPDA service was developed for the needs of EEA. By integrating statistical methods for bear population estimation it gives additional knowledge in the field of wildlife conservation. This service enhances the accuracy of estimates for the bear population by processing large datasets and by incorporating advanced statistical techniques that consider various factors affecting population dynamics as forest type, climate, threats, food availability, and settlements near the habitats.

It enables faster analysis for making informed decisions taking into account multiple variables, such as habitat changes, climate fluctuations, and human impact in order to develop effective strategies for the conservation of the species. The service allows data integration from various sources: (i) data received from the National monitoring – number of bear footprints, number of discovered winter dens and other bear traces, type of food in different forests, etc. (ii) data from GPS tracking, and camera trap data as well as simulate different estimates by using no-real data closely to those from National Monitoring to create different management and conservations scenarios on the bear population.

Benefits:

- Conservation and management of the species
- Human-Bear conflict management
- Biodiversity Preservation
- Economic value through tourism and ecotourism

Keywords: route method, maximum likelihood method, bear's footprint
Industry Sector: statistical and data analysis, biological diversity, IT
Technology: HPDA

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EURO²

Environment water quality: Opening of public bathing sites in natural environment

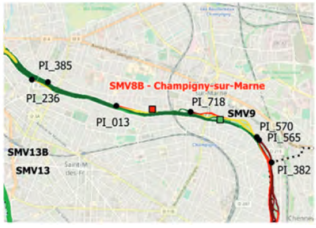
NCC France

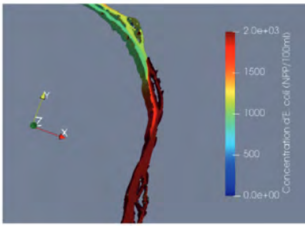
Industrial organisations involved:

The NCC CC-FR is managed by TERATEC the European Pole of Competence in high performance digital simulation, in partnership with CERFACS the European Center for Advanced Research and Training in Scientific Computing, with Inria Academy, a continuing education program dedicated to open source software, with CRIANN, the regional computer centre and digital applications of Normandy , and ROMEO the Regional Computing Center of the University of Reims Champagne-Ardenne.

Technical /scientific challenge:

How to succeed in opening swimming sites in the river la Marne after the Paris 2024 Olympic Games? The Public authorities need to obtain a fine modeling of dispersion bacteriological strains since their point emission. In order to support the management plans settled by public authorities in these highly urbanized areas, Prolog engineering has developed a model coupling hydrodynamics and water quality on the Criann supercomputer.





Fine modeling of the dispersion of bacteriological strains from their point of emission

Solutions:

PROLOG INGÉNIERIE group, specialized in the field of water and environment was supported by CC-FR to deploy a code coupling hydrodynamics and water quality on the CRIANN Supercomputer to obtain a fine representation of the dispersion of pollution at a bathing area in 3 steps:

1. 2D modeling by the Telemac-Mascaret system representing the conditions hydrodynamics of a 40 km long section of the Marne
2. Prioritization of pollution sources due to permanent or accidental wastewater discharges and rainwater discharges
3. Focus on a potential bathing site. 3D modeling for a fine representation of local dispersion of pollution- Proof of concept that was achieved:
   - 3D hydrodynamic simulation of a section of the river Marne with consideration of pollution sources
   - Deployment 3D hydrodynamic simulation on HPC architecture
   - Getting started with the HPC environment

Business impact:

Thanks to CC-FR and CRIANN with a high-level expertise in intensive computing, PROLOG INGÉNIERIE group has been able to significantly increase their expertise to deploy 3D hydrodynamic simulation on HPC architecture. Individual and personalized support has also enabled the company quickly become autonomous in the use of supercomputer and to enable large client to be carried out with a significant productivity gain.

Benefits:

- Speed of calculation time
- Fine representation of pollution dispersion at bathing area level
- More than 120,000 CPU hours was needed

Keywords: HPC, Simulation, dispersion of pollution, Environment water quality

Industry Sector: Environment/climate/weather and Finance/Insurance and Public services/Civil protection

Technology: HPC, Simulation

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EURO²

Improvement of the remote expert system based on software OTEA

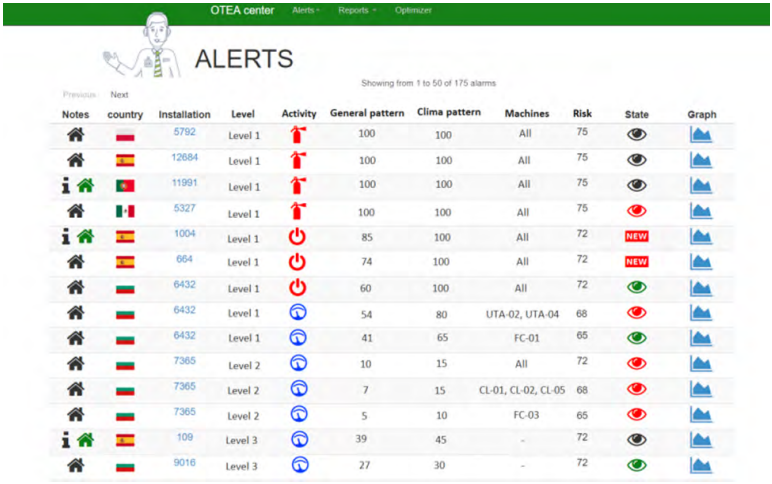
NCC Spain

Industrial organisations involved:

EcoMT is an ICT company that develops and integrates remote control and monitoring of facilities.

Technical /scientific challenge:

New facilities with a growing number of Heating, Ventilation and Air-conditioning (HVAC) machines produce huge amounts of data. Usually, a deterministic system with brute force conditions was applied to detect comfort anomalies in more than 3,000 installations worldwide, with 600,000 variables monitored resulting in 3 trillion records for 5 years. The challenge of this experiment was to replace the brute force solution with a superior ML model. Like the brute force model, the ML model is numerically intensive and needs the use of HPC.



Notes	country	Installation	Level	Activity	General pattern	Clima pattern	Machines	Risk	State	Graph
		5792	Level 1		100	100	All	75		
		12684	Level 1		100	100	All	75		
		11991	Level 1		100	100	All	75		
		5327	Level 1		100	100	All	75		
		1004	Level 1		85	100	All	72	NEW	
		664	Level 1		74	100	All	72	NEW	
		6432	Level 1		60	100	All	72		
		6432	Level 1		54	80	UTA-02, UTA-04	68		
		6432	Level 1		41	65	FC-01	65		
		7365	Level 2		10	15	All	72		
		7365	Level 2		7	15	CL-01, CL-02, CL-05	68		
		7365	Level 2		5	10	FC-03	65		
		109	Level 3		39	45	-	72		
		9016	Level 3		27	30	-	72		

Visualization of the final product

Solutions:

The OTEA remote expert system (OTEAres) was developed as an expert remote management system with an aim for energy optimization through the premature detection of incidents based on historical records. The savings of clients connected to the OTEAres platform operated by EcoMT, would be immediate using ML algorithms and HPC which is essential for real-time operations. OTEAres enables decision support in real time offering a 24/7 service through its control centre, which is the department in charge of controlling the proper functioning of the installations, remotely resolving incidents in the shortest time possible.

Business impact:

The update of the deterministic previous version into a new ML model capable of predicting and organizing a wider range of incidents. It is estimated an energy saving of 7% per installation, a reduction of 30% in preventive maintenance visits and a reduction of 20% in corrective maintenance.

Benefits:

- Energy saving of 7% per installation,
- Reduction of 30% in preventive maintenance visits
- Reduction of 20% in corrective maintenance

Keywords: ML, model, preventive maintenance, remote monitoring, optimization

Industry Sector: Energy

Technology: HPDA

Note: This success story was performed in a business experiment of the Fortissimo 2 (*) project involving the NCC member CESGA; the success story was included in this EUROCC booklet as it provides inspirational material for the take-up of HPC by SMEs.

*The Fortissimo 2 project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 680481.

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EURO²

Implementation of High-Performance Computing Pipeline for Agricultural Research Institute

NCC Cyprus

Industrial organisations involved:

The Agricultural Research Institute (ARI) is a Department under the Cyprus Ministry of Agriculture, Rural Development and Environment. Its vision is to be a model center of knowledge and innovation, and lead Cyprus to a better future by strengthening rural development, improving the quality of life, and ensuring the sustainable use of natural resources. Research at ARI aims to create and transfer knowledge for the development of the primary sector and to solve problems at the farmer's level, with research results transferred to stakeholders through modern educational programs.

Technical /scientific challenge:

ARI aimed to adapt a computational pipeline to HPC to enhance agricultural research. The initial focus was on the feasibility of installing the RStudio Server on the CYCLONE High Performance Computing (HPC) infrastructure. The goal was to harness RStudio's statistical computing alongside CYCLONE's computational resources for managing extensive agricultural datasets. Next step was adapting the computational pipeline for HPC, which involved detailed planning and execution to ensure the seamless integration and utilization of HPC resources. The objective was to establish a scalable, efficient, and robust pipeline to manage diverse datasets crucial for modern agriculture.

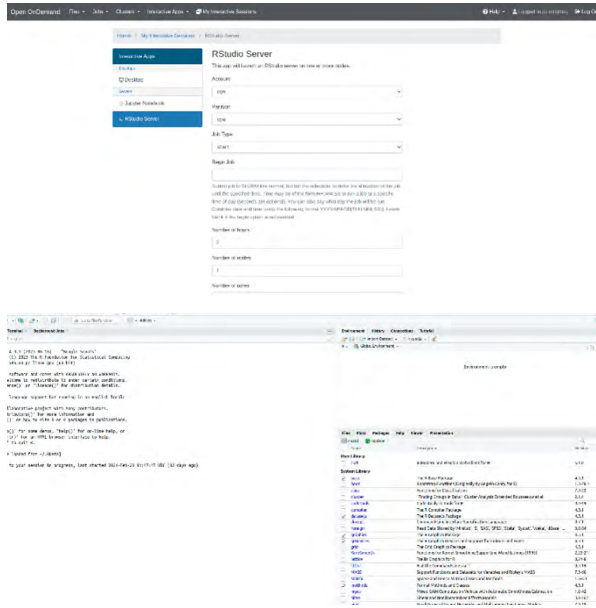
Solutions:

The solution involved seamlessly integrating RStudio Server with CYCLONE's HPC infrastructure. This process began with a feasibility study, confirming that RStudio could efficiently operate within CYCLONE's environment, inspired by successful implementations at Princeton and Iowa State Universities. Subsequently, a detailed plan for adapting the computational pipeline to HPC was developed and executed. This adaptation focused on scalability, efficiency, and robustness to handle large and diverse datasets.

Business impact:

The implementation of HPC at ARI has revolutionized its research capabilities. Previously, the handling and analysis of extensive agricultural datasets were constrained by computational limitations, slowing down the pace of discovery and innovation. With the adoption of HPC, ARI can now process large volumes of data much faster, enhancing the efficiency of research activities. As a result, ARI's research is increasingly data-driven, allowing for more precise and impactful scientific outcomes.

The use of HPC in agricultural research is expected to continue driving significant scientific advancements. It empowers researchers to tackle previously unfeasible problems, contributing to more sustainable and productive agricultural practices. This advancement not only strengthens rural development but also plays a vital role in addressing global challenges such as food security and climate change.



Graphical interface for the submission of Jobs to the Cyclone HPC through the RStudio server

Benefits:

- Accelerated data analysis, reducing research timelines
- Enhanced efficiency, lowering operational costs
- Enabled precision agriculture, optimizing resource use
- Significantly reduced data processing waste

Keywords: High-Performance Computing, Agricultural Research, Data Analysis, Precision Agriculture, Sustainable Development

Technology: HPC, Statistical Computing

Industry sector: Agriculture, Environment/climate/weather

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EURO²

Using HPC-Cloud tools for optimal positioning of mini wind turbines

NCC Spain

Industrial organisations involved:

KLiUX Energies is a Spanish manufacturer of vertical-axis wind turbines for urban and residential environments.

The University of Zaragoza is a Spanish public research institute that hosts its own computing centre, and provided application expertise. nablaDot is a Spanish company providing CFD consultancy services.

Gompute is a leading Swedish simulation and HPC solution provider. It provided the HPC expertise in this experiment.

nablaDot: is made of a group of engineers with a wide experience in fluid simulation and its application to the industry.To do this, we use Computational Fluid Dynamics (CFD) techniques to solve fluid flow, heat transfer and chemical reaction problems.

Technical /scientific challenge:

This challenge was about developing an application that combines GIS (Geographic Information System), NWP (Numerical Weather Prediction), CFD (Computational Fluid Dynamics) and analytical software in a cloud environment.

The company needed a cloud environment, to provide detailed information about wind flow in urban environments for small wind turbine manufacturers, suppliers and also potential customers.

Solutions:

The performed work allowed the development of a computational tool based on HPC-Cloud that provides an accurate estimation of wind potential in an urban area, including identification of acceleration, channelling, blocking, recirculation and turbulence zones.

Note: This success story was performed in a business experiment of the Fortissimo 2 (*) project involving the NCC member CESGA; the success story was included in this EUROCC booklet as it provides inspirational material for the take-up of HPC by SMEs.

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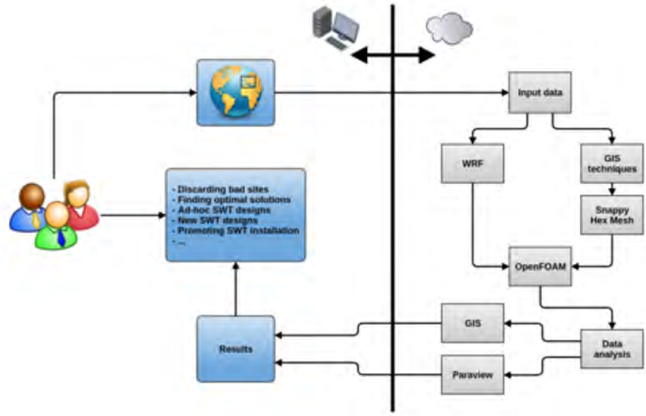

Workflow diagram representing the interaction between Cloud computing software solution and users/decision makers for wind-turbine position optimization

Business impact:

The application developed in this experiment can provide the potential of wind energy in urban areas at a competitive cost compared to current methods. Currently, the time required for a measurement campaign is in the range of 4 months to one year, with the cost being between 4000 and 12000€, which is high considering the scale of small wind turbine projects, as in some cases, the price is similar to that of the turbine.

The estimated cost of using the application is around 1500-2000 €, requiring approximately 15 days of computational calculations.

Benefits:

- Time savings: from 4 to 12 months to 15 days maximum
- Cost saving: in terms of money, from 4000-12000 € cost to 1500-2000 €

Keywords: turbulence, wind turbines, numerical weather prediction, computational fluid dynamics, analytics software, HPC

Industry sector: Energy, Manufacturing & engineering

Technology: HPC, AI

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EURO²

Analysis of defects in reactor pressure vessel of nuclear power plants

NCC Belgium

Industrial organisations involved:

Cenaero

TRACTEBEL ENGIE

Technical /scientific challenge:

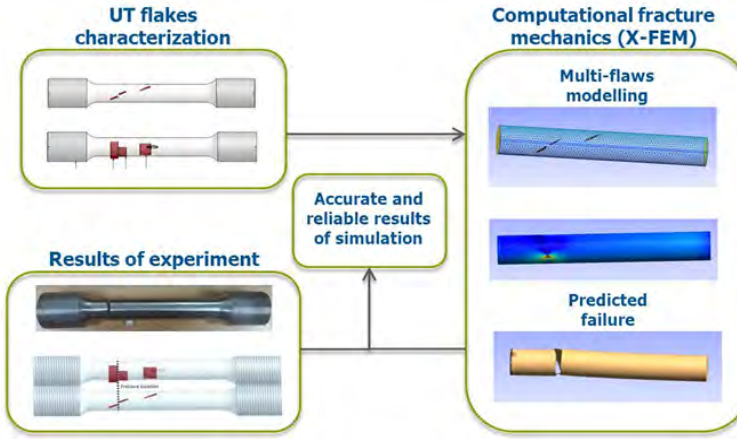
During a major maintenance of Doel 3 (3rd reactor of a nuclear plant located at Doel) in 2012, a periodic inspection of several parts of the reactor vessel was performed. This inspection, with a new equipment, led to the detection of the presence of flaw indications (hydrogen flakes) in the reactor vessel of Doel 3, and later of Tihange 2 (2nd reactor of a nuclear plant located at Tihange). To evaluate the structural integrity of the vessels, these inclusions have been considered as „cracks" by the evaluation team which is the worst case possible.

Among a lot of analyses, numerical simulation has been chosen by Tractebel to assess the risk level. Due to the number of the cracks and proximity between them, such computation required HPC resources due to the amount of memory required for one computation as well as the number of computations to be performed.

Solutions:

Based on the inspection, Tractebel defined the cracks equivalent to the observed inclusions and first asked to Cenaero to make Linear Elastic Fracture Mechanics computations to assess the risk of crack propagation with such conservative hypothesis (equivalent cracks).

"Morfeo Crack" software, developed at Cenaero, was used to perform the computations based on its ability to easily define multiple cracks in a numerical model and evaluate the risk of crack propagation under various loading conditions. The first ones started with a limited number of simultaneous cracks. This first computations demonstrated the ability of the model to evaluate the crack propagation risk with a lot of multiple cracks and loading conditions. Then, thanks to first positive results, the number of simultaneous cracks has been increased to improve the representativity and accuracy of the results. The amount of required memory depended on various factor including the number of the cracks and the distance between the cracks. Moreover, at this time (2012), it was not possible to run the computation on multiple nodes. This induced that the amount of memory on the biggest available nodes limited the mesh sizes. The configurations with a lot of cracks required a lot of caution and expertise to perform the computation within the available hardware resources (amount of memory on one node) while satisfying high quality standards in the results. Moreover, Cenaero developed methodologies to face the number of configurations and the post-processing operations to be carried out.



Business impact/Benefits:

The collaboration on crack analysis between Tractebel and Cenaero is considered as a success and led to the relaunch of the nuclear reactors. This collaboration still goes on with significant extensions. Recent works dealt with lifespan assessment by numerical simulations considering residual stresses due to welding process.
For all these computations, the amount of resources needed, because of the memory needs and the number of computations, is such that an HPC infrastructures is necessary.

From a scientific point of view, the specific needs of Tractebel helped Cenaero to improve the used methodologies and tools. Among these improvements, some work was carried out to extend computation to elastic-plastic fracture mechanics hypothesis. Moreover, the hardware limitation has been over-come by developing an adapted methodology, ensuring that a computation on more than one node is possible which the same accuracy.

From a business perspective, Tractebel has acquired Morfeo Crack's software licenses to conduct its own analyses on various part of nuclear power plants. Since then, Tractebel acquired a unique expertise in this field that it can make available to its partners.

·Keywords: Nuclear power plant, crack propagation assessment, high memory needs, configuration management
·Industry sector: Energy
·Technology: HPC

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EURO 4SEE

Section 4

Pharmacy and Medicine

Application of HPC Tools for the Optimization of 3D-printed Orthopaedic Devices

NCC Latvia

Industrial organisations involved:

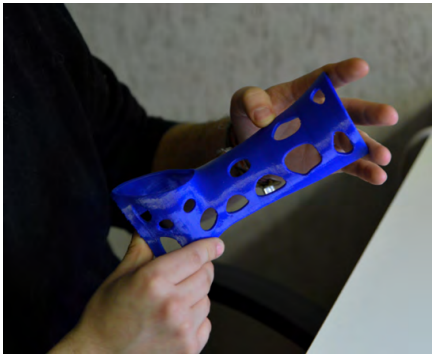
CastPrint SIA is the leading custom-made 3D printed assistive device manufacturer in Europe. As such CastPrint has a team of medical engineers, 3D designers and medical specialists - technical orthopaedists and medical doctors.

The University of Latvia is a leading national higher education institution in Latvia. The Institute of Numeric Modelling offers expertise in mathematical modelling and optimisation. The Institute for Mechanics of Materials provides technical capacity for material testing.

Riga Technical University HPC centre provides HPC resources and expertise in HPC software setup.

Technical /scientific challenge:

CastPrint has been providing custom 3D printed medical devices since 2016, addressing the demand for improved patient-centric solutions. The creation of these devices is challenging due to the complexity of 3D scans and the manual operations involved. This process is time and resource-intensive, often leading to software crashes and data loss. High Performance Computing (HPC) has provided an opportunity to overcome these challenges, enhancing the efficiency and capacity of production.

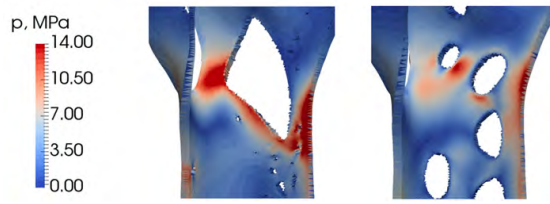


Topologically optimized 3D printed cast

Note: The work of the SME was performed within a business experiment funded by the FF4EuroHPC project(*). NCC Latvia supported both the development of the proposal and the execution of the business experiment.

*FF4EuroHPC has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 951745. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Germany, Italy, Slovenia, France, Spain.

Funded by the European Union



Stress distribution comparison between original and optimized design

Solutions:

The challenge of manufacturing custom 3D-printed medical devices was addressed by incorporating parametric model optimization and HPC tools. The process involved selecting test cases, developing a software system for numerical studies, optimizing model parameters, validating model results, and implementing the model in the manufacturing workflow. The implementation of the project led to reduced design time, material usage, and printing times.

Business impact:

Business- product time to end user decreased by 25%. This is achieved through shorter design and print times for the ordered 3D printed medical devices that reduces production costs by up to 15% and increases production capacity by 25%. Reducing the time between scanning and printing opens up opportunities in new markets.

Society- Shorter printing times and less materials used result in lower costs and thus CastPrints become more accessible for patients.

Environment- Despite the fact that CastPrints are made out of Poly-lactic acid plastic that is made from sugar-cane and is biodegradable, a 25% reduction in plastic use means less plastic waste. Similarly, a 25% decrease in printing times result in electricity consumption used in printing the device itself. By reaching the goals set out in this experiment, the experiment partners will contribute in the reduction of plastic waste and electricity usage while improving the durability and wearability of the product.

Benefits:

- 20% reduction in personnel hours for cast design due to automation
- 25% less material used and 25% decrease in production time after topological optimization
- 15% decrease in production costs and 25% increase in production capacity for CastPrint

Keywords: 3D-Printed Assistive Devices, Custom Manufacturing Optimization, Numerical Modelling, Material testing, Topology Optimization, Orthopedics, Medical Device Production, Cost Reduction, Healthcare Technology

Industry Sector: Healthcare

Technology: 3D printing, 3D scanning, HPC

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EURO²

PediDose: A pediatric simulated dosimetry platform for clinical use

NCC Greece

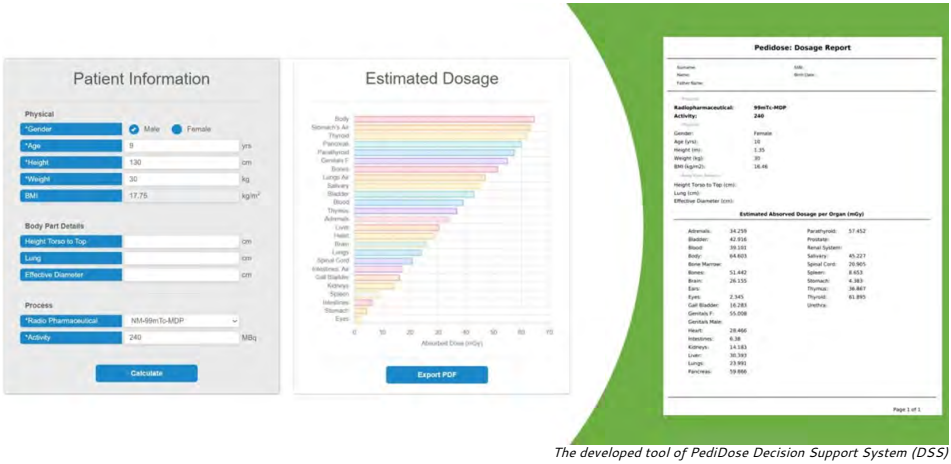
Industrial organisations involved:

BIOEMTECH is a Greek SME in the field of biomedical engineering, bridging the gap between ex vivo studies and in vivo molecular imaging. The company develops benchtop molecular imaging systems and provides imaging services for the preclinical evaluation of nanoparticles and other novel radiopharmaceuticals. BIOEMTECH consists of a multidisciplinary team with a strong background in biomedical engineering, medical physics, bioinformatics, radiochemistry, biology and nanomedicine.

BIOEMTECH

Technical /scientific challenge:

Personalized internal dosimetry is of great interest in children undergoing medical imaging examinations with ionizing irradiation. PediDose aims to exploit advanced Monte Carlo simulations, anthropomorphic computational phantoms, and Artificial Intelligence techniques to develop a realistic, simulated dosimetry database. The goal is to develop a novel software that will offer clinicians the possibility to assess internal pediatric dosimetry and optimize Nuclear Medical Imaging clinical protocols in terms of personalized prediction models.



The developed tool of PediDose Decision Support System (DSS)

Solutions:

MC simulations in combination with anthropomorphic digital phantoms provide accurate dosimetry estimations for clinical acquisitions (gold standard for dosimetry). Such simulations, with low statistical uncertainty, are highly intensive in terms of computational needs. A realistic simulated dosimetry database was produced using a digital pediatric population of 30 phantoms. ML algorithms were trained on the simulated data to develop a prediction dosimetry model, based on the specific anatomical characteristics of each patient. The developed tools have been integrated in a novel software product, which could be further exploited in clinical practice. PediDose brings together 2 innovative SMEs (BIOEMTECH & IKnowHow) experts in medical physics & bioinformatics and 1 HPC expert (GRNET) to efficiently implement the project.

A beta version of PediDose GUI has been integrated to the evorad® clinical suite by IKH. The next steps include the development of a standalone beta version of PediDose by BIOEMTECH with additional visualisation features. The goal is to extensively evaluate the novel SW in clinical environment. In parallel, both SMEs co-work on the definition of the IPs and the development of a common Marketing Strategy plan.

Business impact:

Industrial access on HPC is necessary for advanced computational solutions, however there is the need for training personnel of HPC activities. Through PediDose BIOEMTECH explored other opportunities to utilize HPC for more company's activities. In addition, PediDose success story showed that supporting SMEs in both funding and allocating HPC resources, in a business-oriented program (FF4EuroHPC), may result in final novel products.

PediDose is expected to significantly strengthen IKH and BIOEMTECH in the EU industry of medical software and provide the SMEs with great advantages in this highly competitive area, addressing both the European and US Market. PediDose has been technically integrated into the evorad® suite, a competitive healthcare software for medical imaging (PACS) from IKH. PediDose will permit BIOEMTECH to enter the medical software market (personalised dosimetry) through business partnership with IKH extending its portfolio.

Benefits:

- Currently, PediDose is the only solution which is based on AI predictive models and the gold standard of MC simulations, which provide a competitive advantage to the existed dosimetry estimations
- PediDose has been technically integrated into the evorad® suite, a competitive healthcare software for medical imaging (PACS) from IKH
- This add-on is expected to generate additional net income for IKH of about €1.25 Mio within the next five years
- PediDose will be offered on a license basis to other vendors of medical software
- Medical market entry for BIOEMTECH facilitated through partnership with IKH

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Keywords: personalized dosimetry, pediatrics, monte carlo simulation, anthropomorphic computational phantoms, nuclear medicine imaging

Industry Sector: Biotechnology/Bioinformatics, Health care / Pharmaceuticals / Medical devices, Life sciences

Technology: HPC, AI

Note: The work of the SME was performed within a business experiment funded by the FF4EuroHPC project(*). NCC Greece supported both the development of the proposal and the execution of the business experiment.

*FF4EuroHPC has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 951745. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Germany, Italy, Slovenia, France, Spain.

EURO²

Transforming Burn Care with Mathematical Modelling and Supercomputing

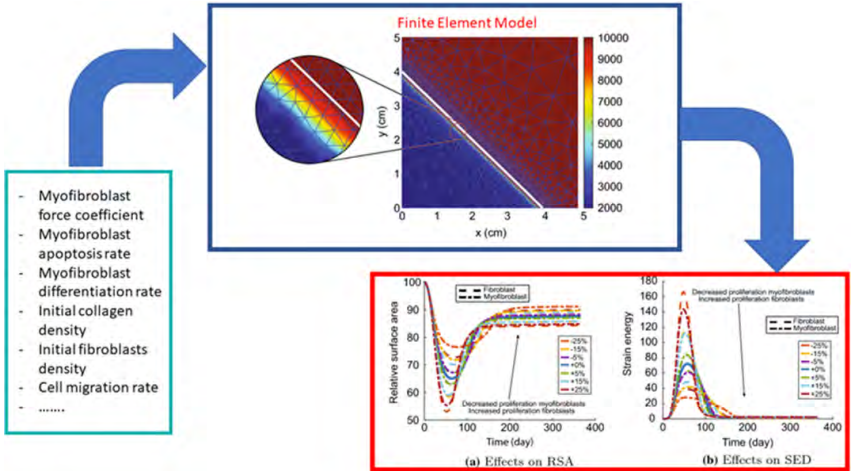
NCC Belgium

Industrial organisations involved:

The Computational Mathematics Group (CMAT) is a research group at the University of Hasselt conducting research inspired by real-life applications. The Data Science Institute (DSI) is affiliated with the same university and brings together over 150 researchers working in the broad field of data science. The Nederlandse Brandwonden Stichting (the Dutch Burns Foundation) was founded in 1971 by a group of concerned physicians and healthcare providers wanting to make a difference for burn patients. Their mission is to prevent burns and minimise the suffering caused by burns to a minimum.

Technical /scientific challenge:

Every year about 120,000 individuals in Belgium endure severe burn injuries, whereas about 10,000 individuals need hospitalisation; the aftermath extends far beyond visible scars. The recovery process also introduces skin contractions. These contractions, in turn, can result in mobility problems for the patient, which can even lead to disability. These limitations in movement have a profound impact on patients' daily activities and lives. Therefore, doctors aim for treatments that minimise skin contraction when treating burn injuries. Mathematical modelling emerges as a powerful tool, offering a virtual canvas to simulate the complex dynamics of human skin contraction.



Solutions:

Mathematical modelling gives insight but can also be used to estimate the chances of successful treatment through (clever) multiple realisations of the simulation framework. Since this step is expensive from a computational point of view, neural networks are used to speed up the simulations so that the mathematical framework can be used in clinical practice. For this purpose, training the network and generating data is necessary.

The Tier-2 Vlaams Supercomputer Center (VSC) infrastructure was used to generate the data needed to train the neural network. The computing infrastructure enabled generating data in parallel using multiple computing nodes. It enabled a fast generation of data and fast training of the neural network. Eventually, a reliable and fast neural network that can reproduce lengthy finite element simulations was obtained. Thanks to using a neural network, simulation times are much shorter.

Business impact:

Mathematical modelling can replace animal testing by developing a „virtual patient", thus eliminating the need for such experiments on animals.

In the future, the simulations can also be used to see the impact of certain therapies on the progression and evolution of skin. Another possibility for future research is to create the potential for doctors to take a picture of a wound and insert that wound geometry into the computation framework, then calculate the probabilities that this wound will be problematic in terms of conjunction and extreme scaring. This may lead the way to more patient-specific healthcare.

Benefits:

- Shorter simulation times by use of neural networks
- Fewer animal experiments are needed
- Patient-specific health care
- Estimation of the impact of treatment

Keywords: Mathematical modelling, neural networks, burn injuries, mathematical biology, partial differential equations

Industry Sector: Numerical Mathematics, Life Sciences, Health Care

Technology: Finite Element Methods, HPC, AI

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EURO²

Drug Discovery on an Unprecedented Scale – Machine Learning Boosted Molecular Docking

NCC Finland

Industrial organisations involved:

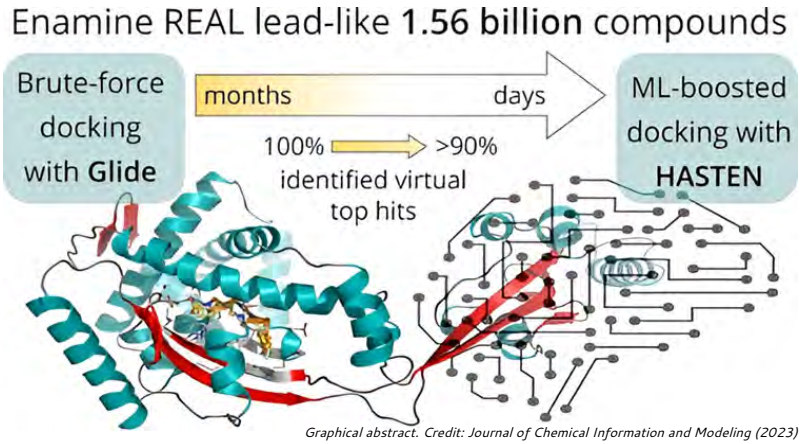
Orion is a globally operating Finnish pharmaceutical company with more than 3,500 employees around the world. Orion products are sold in over one hundred countries.

The University of Eastern Finland is a multidisciplinary university in Finland. The university comprises four faculties with Campuses located in Joensuu and Kuopio.

Technical /scientific challenge:

Drug design involves examining astronomical amounts of molecules, which requires massive computing power that only a supercomputer can provide. „The calculation required by a single molecule may be simple, but when it has to be done 1,000 billion times, it's just not possible without a supercomputer," explains Professor Antti Poso from the University of Eastern Finland.

Because the number of calculations is so huge, the computation time is very long, even for a supercomputer. „Purchasing computing resources from cloud service providers would be very expensive. For example, a medium-sized company would not be able to spend such vast amounts on securing the dataset for a single calculation method", adds Professor Antti Poso.



Graphical abstract. Credit: Journal of Chemical Information and Modeling (2023)

Solutions:

One of the world's largest virtual drug screening trials was carried out in 2023 in cooperation between the University of Eastern Finland, Orion Oy and CSC – IT Center for Science Ltd. With machine learning, virtual screening could be performed more than 11 times faster than with the traditional method, saving about 90–95% of resources. Prior to deploying artificial intelligence for expediting the screening process, the researchers initiated by establishing a foundation. An extensive virtual screening campaign was performed, evaluating 1.56 billion drug-like molecules against two pharmacologically relevant targets. This process spanned nearly six months and leveraged the computational power of the CSC supercomputers Mahti and Puhti, alongside molecular docking techniques. Molecular docking involves computationally fitting small molecules into specific binding regions of the target and generating docking scores to quantify their suitability. Consequently, docking scores were initially calculated for all 1.56 billion molecules.

The results were compared to a machine learning-boosted screen using HASTEN, a tool developed by Dr Tuomo Kalliokoski from Orion Pharma, "HASTEN uses machine learning to learn the properties of molecules and how those properties affect how well the compounds score. The machine learning model can predict docking scores for other compounds in the library much faster than the brute-force docking approach," Kalliokoski explains.

Business impact:

- Businesses will have access to the computing capacity provided by a supercomputer
- Free computational resources are available in EuroHPC for research and development carried out in cooperation with higher education institutions. This phase in the cooperation process is designed to promote innovation and scientific research before the results are applied to business activities. This enables even smaller companies in Finland to seek competitive advantage with good ideas without major investments.
- The knowledge and competence gained will benefit both businesses and the academic community:
- Intellectual property rights will remain fully with the company, but the method developed together will be available to the academic community as well. Enhanced processes will more broadly benefit the entire Finnish academic community.
- Businesses will have access to expertise that they do not have:
- NCC Finland (CSC) provides expertise and support for the implementation, which is particularly valuable for the success of projects. Cooperation brings technical expertise to the project that would be difficult to acquire elsewhere.

Benefits:

- A total of 1.56 billion compounds were processed in the screening. With the help of machine learning, the virtual screening could be carried out in more than 90 percent less time
- With the help of machine learning, it was possible to get forecasts in less than ten days instead of half a year
- An accurate comparison was made between machine learning-enhanced docking and traditional docking in a very wide range of data
- The project is an example of collaboration between academia and industry and demonstrates the importance of access to world class HPC resources; An ambitious goal could be achieved by combining ideas, resources and technology of different parties
- The resulting research datasets have been made available to the public: a ready-made screening library to speed up docking for other targets and the results of docking the entire 1.56 billion compounds for two targets

Keywords: Drug discovery, Pharma, Molecular modelling, Docking, Machine Learning
Industry Sector: Biotechnology/Bioinformatics/Pharmaceuticals
Technology: HPC, Docking, HPDA, AI

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EURO²

Treatment Precision in Breast Cancer

NCC Greece

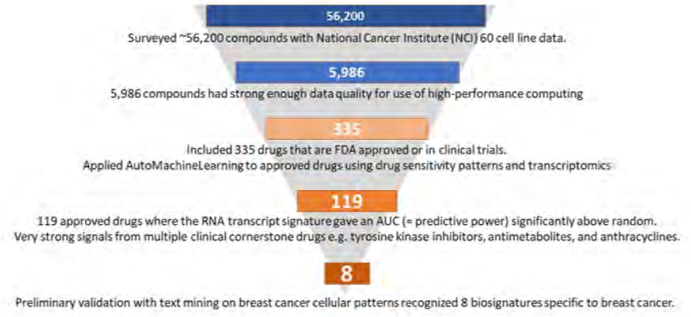
Industrial organisations involved:

JADBio is a robust AutoML platform focused on BioMed and Multi-omics. They make it easy and affordable for data scientists and life-science professionals to use data science to discover knowledge, while reducing time and effort by combining an end-to-end machine learning platform for data analysts with a wealth of capabilities ranging from smart feature selection to the reuse of predictive models. By providing off-the-shelf models for common healthcare use cases and automating many of the manual processes involved in traditional data science tasks, JADBio allows data analysts to focus on what really matters, the problem and its solution. JADBio is headquartered in the Technology and Science Park in Crete, Greece and in LA, California, US.

JADBio®

Technical /scientific challenge:

In cancer treatment, it is a clinical challenge to select the right drug which will work for a specific patient, as the efficacy of cancer drugs is highly dependent on individual characteristics on a molecular level. The solution developed by the experiment helps to narrow down the most promising drugs, using an HPC-backed machine learning approach to analyse a huge initial dataset. The aim is to implement an easy-to-use and intelligent platform which can identify the drugs most likely to achieve high effectiveness in each individual patient based on the specific patient's molecular profiles.



Vertical sections at a stream-wise of velocity magnitude

Solutions:

The experiment carried out extensive analyses of a huge volume of publicly available data. The NCI-60 data set links 60 human cancer cell lines representing different types of cancer to the anticancer activity of over 50,000 compounds. Using specific quality criteria, which were defined at the start of the experiment, 5,986 compounds out of those over 50,000 were selected for further analysis, including 335 drugs that are FDA-approved or in trials.

Using the JADBio autoML platform and HPC resources, ML models for the selected compounds were built to estimate the models' performance in predicting treatment outcomes. As a means of early validation of the ML models, biological text mining was carried out independently. It revealed eight specific models which are particularly interesting for breast cancer, which was among the promising 119 models also identified by ML. They include models for key anticancer drug classes used in breast cancer, corroborating the value of the HPC-backed ML approach and building the basis for further clinical validation.

Business impact:

With a breast cancer incidence of over 780,000 cases in 2018 in the EU and USA alone, there is a huge market potential to be exploited with such a commercial response prediction test – even using very conservative assumptions. The market launch is expected in mid-2024 in Germany and Nordic countries, where 23,000 cases of breast cancer are newly diagnosed per year, offering a business potential of up to €69m, based on an anticipated price of €3,000 per service.

Benefits:

- The business model is highly scalable and the system can be applied to any tumor type and any drug that has demonstrated toxicity
- Besides direct economic and clinical benefits, all partners will enjoy increased visibility in the biomedical market and scientific community, generate new intellectual property, and foster company growth
- The HPC-based solution can play a role as a use case for promoting other diagnostic/prognostic/predictive applications in the field of personalized medicine, fostering wider application

Note: The work of the SME was performed within a business experiment funded by the FF4EuroHPC project(*). NCC Greece supported both the development of the proposal and the execution of the business experiment.

*FF4EuroHPC has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 951745. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Germany, Italy, Slovenia, France, Spain.

Funded by the European Union

Keywords: breast cancer, oncology, drug effectiveness, personalized medicine, machine learning

Industry Sector: Bioinformatics, Health care / Pharmaceuticals / Medical devices

Technology: HPC, AI

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EURO²

Bringing Bio Foundation Models to the Fingertips of Scientists

NCC Luxembourg

Industrial organisations involved:

Helical builds the first open-source platform for researchers, biologists & developers to explore bio foundation models, and build cutting-edge applications to accelerate drug development. As a Luxembourg-based startup, they drive innovation in the biotech industry. Specializing in harnessing the power of Generative AI for Genomics and Transcriptomics, Helical empowers biotech firms through intelligent genomics data collection, scientific feedback incorporation, and scalable model fine-tuning. Helical democratizes the use of bio foundation models, enabling organizations to build scalable processes to fine-tune and use the models for specific biological applications and research objectives.

Technical /scientific challenge:

Bio Foundation Models have been trained on thousands of genomes or RNA which enables them to extract important features from biological data. These models will enable a new range of applications, but they are different from traditional AI methods, requiring a dedicated IT infrastructure and optimized frameworks to run. From training, fine-tuning to the usage of the models in different workflows, all of these processes are not readily available for scientists to use within their applications. With the HPC these models can be democratised and put to work.

```python
from helical.models.uce.uce import UCE


model_config  = { ...
}

files_config = { ...
}

data_config = { ...
}

helical_model = UCE(model_config,data_config,files_config)
data = helical_model.process_data(test,species=data_config["species"])
embeddings = helical_model.get_embeddings(data)

```

Python code snippet demonstrates how to utilize Helical's foundation models

Solutions:

Using the HPC enabled Helical to use the necessary computational power to develop and use the bio foundation models for different applications such as biomarker discovery. Working with large AI models has been made easier through the resources of the HPC. Additionally, the high data throughputs allowed Helical to run various optimizations for large datasets to improve the applications that are developed as part of their platform. To test and deploy their models, Helical uses the HPC and its resources to investigate how bio foundation models can be hosted and made easily available for scientists to query them. Making these models available to bioinformaticians will be crucial to enable a new range of bio applications.

Business impact:

Through LuxProvide, Helical was able to start developing its platform on a much larger scale by being able to use a wide range of bio foundation models directly with the distributed network of GPU nodes. Reducing the development time is important for Helical which in turn will accelerate the number of new applications that can be enabled. In a first phase, Helical focused on biomarker discovery with RNA sequencing data. Using the Jupyterlabs interface on the HPC enabled for quick development cycles and the batch jobs will enable Helical to do optimizations on a larger scale in the future. Additionally, Helical is deploying AI methods to further enhance outcomes for the biological applications it is developing. For these methods, larger clusters of nodes will result in more precise and better solutions, giving the algorithms more computational power which they are able to leverage to scale well.

This strategic partnership with LuxProvide signifies a significant step forward in advancing genomics research and innovation. By combining Helical's cutting-edge capabilities with LuxProvide's state-of-the-art infrastructure, they aim to revolutionize genomics, unlocking new frontiers in healthcare and biotechnology. Together, Helical and LuxProvide are poised to drive transformative progress in understanding and leveraging the intricate complexities of the biological world.

Benefits:

- Quicker turnaround times through faster inference
- Development of a high-performance oriented platform for bio
- Large Scale Optimization which was not possible before enabling better results

Keywords: Genomics, Bio Foundation Models, Platform
Industry sector: Biotechnology, Bioinformatics, Healthcare, Crop Sciences
Technology: HPC, Generative AI, Evolutionary Algorithms

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EURO 4SEE

Section 5

Manufacturing and Engineering

EURO²

How to speed up Fire-Safety simulations using supercomputer resources

NCC Poland

Industrial organisations involved:

Building Research Institute (Client) is a public funded research institute that conducts research in the field of construction and related fields, aimed at their implementation and application in practice. The department we cooperated with deals with fire safety issues. It carries out both scientific research and commercial projects (e.g., expert assessments of fire safety of existing buildings and also those in the design phase). Prior to project, the Client performed simulations with its own infrastructure, which often was insufficient (e.g. during surges of commercial orders).

Technical /scientific challenge:

The analysis of fire events in a presence of wind is not an easy task since it requires taking into account the simultaneous impact of the wind and the fire development changing with time. To obtain a statistically valid result, it is necessary to carry out dozens of simulations taking into account various directions of wind and its speed. This, in turn, requires extensive HPC resources and scalable computational models. As part of the project, optimal set of simulation parameters was determined – number of simulated scenarios, the size of the numerical grid and the method of simulating thermal radiation.

Solutions:

Client had prior knowledge on CFD methods and software as well as a ready-to-use case that exceeds his hardware capabilities. During tests, we demonstrated that simulation using 480 CPU cores leads to an optimal speedup (simulation time vs number of cores shown in the figure below; simulation time on the Client's infrastructure provided for comparison).

Moreover, using HPC allows for running multiple simulations at once, which is important since same geometry must by simulated multiple times for different wind conditions, i.e., wind speed or directions. Although it was not a merit part of the PoC, it is worth to mention that the use case has been set up by the Client beforehand in a manner so the change of wind speed or direction could be accessed with just "one-liner" script. Taking into account the case of 1° wind direction resolution (i.e., 360 different wind directions taken into account) and at least few wind speeds to make the assessment valuable, the problem rises of having thousands of variants that must be simulated independently. And as the assessment considers multistorey car park, where the location of simplified car bodies can be defined in set of uncountable variants, the number of cases that needs to be simulated is very large.

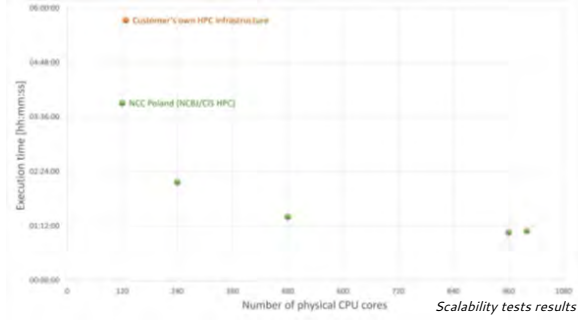
Business impact:

Unlocking possibility to use HPC in short periods of time, when Client's own infrastructure is insufficient:

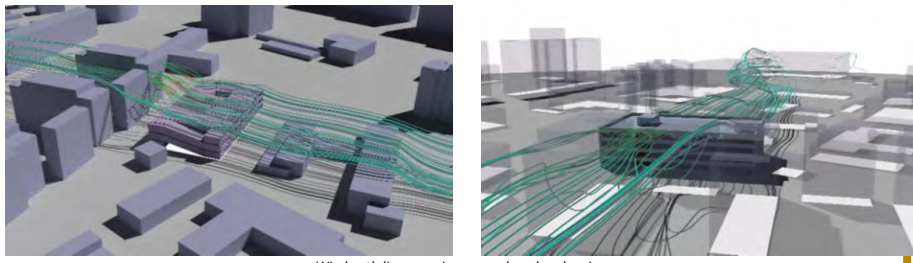
- Prior to the project, the Client used in-house HPC (supercomputer) of previous generations to carry out the simulations. Thanks to the project, the Client gained awareness that the problems they research can be scalable across a larger number of computer nodes to significantly reduce the computational cost and time, thus allowing higher simulation yield than methods previously available to the Client. The process of carrying remote simulations in a cloud environment was far easier than the Client had earlier expected.
- Scaling of HPC resources for the tasks required by the Client required technical skills related to automatization and management of parallel simulations on a larger number of nodes. After the project, the Client could use HPC resources on his own.
- Cost awareness: Although the demonstration was free, we provided detailed billing info to the Client after the project was completed. This way we freed up one source of Client's uncertainty limiting future use of HPC, as he knows exactly how much will he have to pay for computing power when using HPC for simulations in future.
- Usage of professionally managed and well-structured HPC resources leads to reduction of required time to results

Benefits:

- Significant simulation speedup (up to 6 times) when compared to in-house infrastructure owned by the Client
- Possible simulation quality improvement thanks to usage of more detailed physics model (due to additional computing power available) in simulation – leading to lower uncertainty on results



Scalability tests results



Wind path lines passing car park under planning

Keywords: CFD, fire simulation, HPC, fire safety, simulation speedup, engineering, construction optimization analysisIndustry

Sector: Construction, Public services/Civil protection,

Technology: HPC (CAE)

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EURO²

Leveraging expertise

NCC Belgium

Industrial organisations involved:

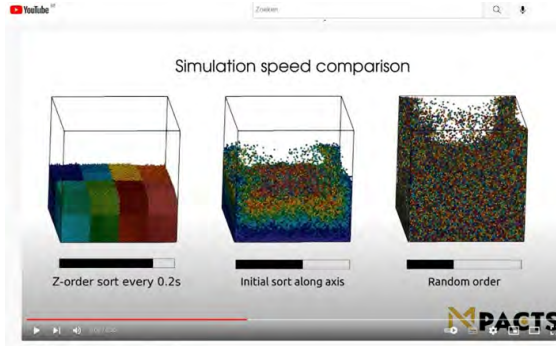
The simulation software Mpacts can simulate the behaviour of a large number of particles through machines enabling the improvement of the machine by testing designs in a software environment before actually having to build a physical machine. This way is much more time-efficient and cost-reducing. Mpacts uses the Discrete Element Method (DEM) to understand, predict and solve industrial problems. To simulate a lot of particles, a lot of computational resources are needed. To perform simulations for clients the organization uses the VSC (Vlaams Computer Centrum) infrastructure.

MPACTS

Technical /scientific challenge:

While granular dynamics is conceptually very similar to molecular dynamics – particles are moving because of interaction forces and external forces, it is also much more complex.

As the particles move in (simulated) space, interacting particles don't stay close together in memory. This complicates memory access which in turn has a direct impact on performance. The hierarchical structure of memory on modern CPUs (L1, L2, L3 cache levels, RAM) is based on the assumption that computationally expensive loops will access data through arrays in a more or less contiguous way. Memory access patterns that deviate from this will suffer from cache misses, which means that data needed by the CPU has to be fetched from more distant regions of the memory. This can cause a significant slowdown of the code. By the nature of particle flows, the neighbourhood of a particle changes continuously and inevitably, the processing of the contacts between particles will, after some time, access the particle data in a random manner, causing many cache misses and slowing down the application.



Effect of positional sorting on simulation performance

Solutions:

One of the services is helping users to improve their software so it can run more efficiently on the VSC infrastructure. In the case of Mpacts, VSC recommended sorting the particles so that particles close in (simulated) space are also close together in computer memory. This programming technique made the software more efficient and, thus, faster.

Business impact/Benefits:

Simon Vanmaercke (Co-Founder of MPacts): "By sorting the particles in memory, we obtain maximum efficiency from the existing hardware, which translates into faster computation times by factor two. The increase by factor 2 means we are able to deliver a simulation in one month instead of two. When we use GPU, the difference is even more pronounced: performance then increases by a factor of five! This improvement has a high impact on our responsiveness in solving engineering problems."

The effect on the computational time is illustrated in this YouTube movie for single-core performance. When using GPU's also the available hardware capabilities are used to the maximum.

Keywords: Particle Based Simulation, Discrete Element Modeling, Granular Dynamics
Industry sector: services & software providers, manufacturing & engineering
Technology: (HPC)

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EURO²

Neural networks in the steel industry

NCC Czech Republic

Industrial organisations involved:

The company ITA technology & software was founded in 1991 and is a supplier of software solutions and technologies in the field of metal rolling, forming, heat treatment and metallurgy. ITA is engaged in modern hot and cold rolling technologies, as well as computer simulation and prediction of mechanical properties after heat treatment. It supplies know-how and software solutions to leading and major producers of rolling equipment, technologies, and control systems. Many of their software solutions have been successfully installed in rolling mills around the world.

ITA technology & software

Technical /scientific challenge:

The main objective was to analyse the possibilities of applying machine learning (ML) methods to predict the best parameters to use in the cooling process following the steel rolling. The correct setting of these parameters is necessary to properly control the cooling in order to maintain the required quality of the final product. The aim of the analysis was to find out if the prediction given by ML models can surpass currently established methods based on combinations of previously used values.

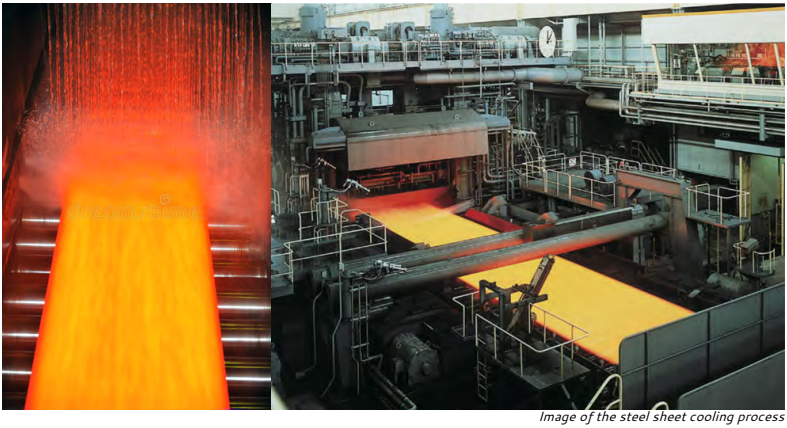

Image of the steel sheet cooling process

Solutions:

The ML model is based on multi-layered feedforward neural networks. The material and physical properties of the metal sheet, together with the water coolant temperature, were set as the input variables. The output of the neural network is the predicted value of the cooling parameter. The training sets consist of historical data from previously processed sheets. The data include values of the parameters that were used in the cooling setup and their optimal values that were calculated after the cooling. We designed several models that included distinct sets of input parameters and performed an analysis of how each variable affected the output. Also, the possible effect of outages on the prediction was studied. The comparison of the ML model with the established one was based on the difference between optimal values and the predicted ones (values given by the established model correspond to those already used in the cooling setup).

Business impact:

A large amount of water is used to cool the steel strips, the volume of which is determined by the calculation of the automation software module. This module is based on solving a temperature model to estimate the temperature of the following belt. For this temperature model to work properly, it needs to be adapted, using two or three adaptation parameters, depending on the actual measured cooling temperature. Currently, this adaptation is performed based on the experience of the chiller operator.

The aim is to replace the need for correction by the user with automatic correction based on artificial intelligence methods. This substitution will allow for a more accurate calculation of the estimated belt temperature after cooling, thus making the entire cooling process more efficient.

Benefits:

- AI deployment enables more accurate temperature calculations
- time and cost savings due to more precise adjustment of the cooling process
- a reduced environmental impact due to optimisation of the cooling process

Keywords: Cooling of steel sheets, High-performance computing (HPC), Neural networks

Industrial sector: steel manufacturing

Technology: HPC, Artificial Intelligence

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EURO²

HPC-Cloud-based simulation of flange tightening

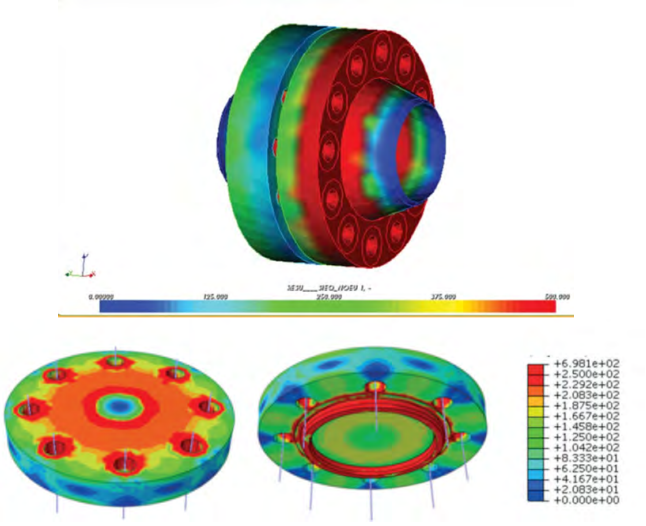
NCC Spain

Industrial organisations involved:

Texas Controls is a Spanish SME that offers tightening and sealing solutions to large industrial facilities in the industrial, power generation and oil & gas sectors. The mechanical division of Texas Controls is the only engineering company in Spain specializing in tightening and sealing. Its long experience over many years of achieving critical safe mechanical joints, and its ongoing research projects allow Texas Controls to address critical tasks, offering its customers the highest confidence in the implementation and operation of leak-free and safe flanged joints.

Technical /scientific challenge:

The challenge of this case study was to simulate and optimize the tightening of flanges. This required the development of a computer model for simulating the tightening process and a front-end application to control the simulations in order to improve the design of the tightening process. Given the complexity of the problem, HPC resources were needed to model the tightening process accurately.



HPC-based simulation of joints

Solutions:

A computer model was developed which represented all the functional parts of a flange including the gasket and the tightening bolts. This model was driven by a user interface, which enabled different tightening scenarios to be evaluated. The model was implemented using both open-source and proprietary simulation codes. Several sizes of case studies were run.

Business impact:

Based on previous experience in the field (when no simulations were carried out), a nonoptimized tightening of a 24-stud bolt flange took 108 man-hours while Texas Controls can reduce this type of process to 72 man-hours using simulation. In all this comprises a 33% time saving per flange. Whilst this represents considerable savings in labour costs, the most important outcome is the reduction in downtime of industrial installations such as refineries. Using advanced simulation, a flange can be tightened in 18 hours as opposed to 27 without advanced simulation.

During the shut-down of a hydrocracker, the maintenance and tightening of such heat exchangers are included in the critical path of the shutdown and maintenance projects, so any delay in these operations has a major impact on the final completion date of the commissioning of the hydrocracker unit.

The cost of down time for a medium-sized hydrocracker is about €21k per hour ($500k per day). This means a saving to the end-user of ~€180k because the critical path is shortened to the same extent that the tightening process is optimized.

Benefits:

- Up to 33% time saving per flange: a flange can be tightened in 18 hours as opposed to 27 without advanced simulation
- Potential saving to the end-user of ~€180k

Keywords (Min 5): simulation, cloud, HPC, optimization, computer model

Industry sector: Mechanical engineering

Technology (HPC, HPDA, AI...): HPC

Note: This success story was performed in a business experiment of the Fortissimo (*) project involving the NCC member CESGA; the success story was included in this EUROCC booklet as it provides inspirational material for the take-up of HPC by SMEs.

*The Fortissimo project has received funding from the European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement No 609029.

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EURO²

CCUPAR: Optimum Design of CO2 Capture and Utilization Processes in Parallel Infrastructures

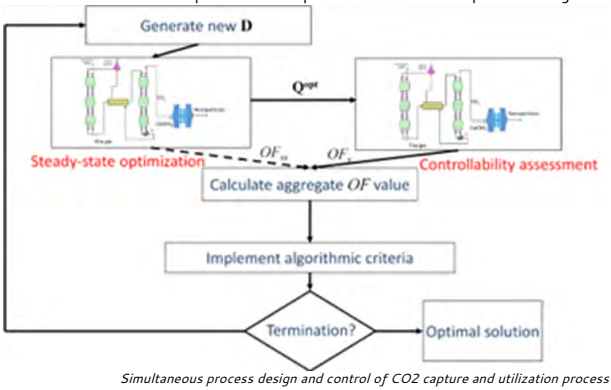
NCC Greece

Industrial organisations involved:

Y Squared (YSD) is an SME that specializes in the area of designing process systems for the chemical industry. In recent years YSD has identified enormous future potential in the area of CO2 capture and utilization systems, as there are strict commitments by the EU for decarbonization with specific targets within the next decade. YSD has great experience in the design of reactive separation systems, which are exactly the type of systems used in CO2 capture and utilization. By combining in-house knowledge regarding the chemical process industry, YSD will be in a unique position to exploit the very extensive capabilities of HPC-capable algorithms. The Centre for Research and Technology Hellas was founded in March 2000. It is a legal entity governed by private law with non-profit status, supervised by the General Secretariat for Research and Innovation (GSRI) of the Greek Ministry of Development. CERTH' main mission isthe promotion of innovative research for the benefit of society. Dedicated to this purpose, CERTH lies at the forefront of basic, applied and technological research to provide solutions to society's modern challenges.

Technical /scientific challenge:

The design of CO2 capture and utilization (CCU) systems requires the consideration of a large number of design options and operating scenarios to attain optimum and realistic design solutions of low cost. The problem is computationally very challenging, due to the need to consider multiple different materials, different process structures and operating conditions. As a result, existing algorithms for integrated process design and controllability assessment and computing practices that are based on personal computers result in suboptimal designs.



Simultaneous process design and control of CO2 capture and utilization process

Solutions:

CCUPAR developed a parallel algorithm for integrated process design and controllability assessment of advanced CCU systems. The algorithm accounts simultaneously for different materials and process structures and a broad range of operating scenarios. We have demonstrated the ability of the algorithm to identify designs that reduce the capture and utilization costs compared to conventional designs, with limited computational effort. The algorithm was implemented in the design of CCU solutions for the cement and quicklime industries. Partners CERTH and Y Squared collaborated to provide consultation to the considered and other industrial sectors (e.g., power, refining etc.) on design studies that will motivate investments in CCU infrastructure. Partner YOTTA demonstrated the ability to host this type of application in their HPC system.

Y Squared and CERTH have already integrated the capabilities of the algorithm and the process models into their consultation and research services. In parallel. the partners plan to continue upgrading the algorithm in order to include additional processes and capabilities.

Business impact:

Due to the speed up achieved through employing HPC, the company engineers managed to increase their efficiency and produce improved designs in short amount of time. The significant decrease in computation time allows Y Squared to take on more clients simultaneously and provide them with its customized and specialized services. The increased workload is expected to result in the creation of several job vacancies, as well as internship opportunities for young trainees to get exposure to chemical process design and modelling, advanced computing techniques, and HPC.

Benefits:

- Y Squared and CERTH have already integrated the capabilities of the algorithm and the process models into their consultation and research services
- The significant decrease in computation time allows Y Squared to take on more clients simultaneously and provide them with its customized and specialized services
- The improved software provides Y Squared with a competitive advantage in the market and the opportunity to expand its market reach in Greece and other European countries

View of CO2 capture plant at CERTH's PSDI Lab

Remote control of CO2 capture plant

Keywords: CO2 capture, CCU systems, Optimization, Parallelized Algorithms, Controllability Assessment, Climate Change

Industry Sector: Construction, Manufacturing & engineering, Raw materials, metals, minerals and forest-based

Technology: HPC

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Note: The work of the SME was performed within a business experiment funded by the FF4EuroHPC project(*). NCC Greece supported the development of the proposal.

*FF4EuroHPC has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 951745. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Germany, Italy, Slovenia, France, Spain.

Funded by the European Union

EURO²

Understanding physics at the micro-scale in filter media with HPC

NCC Belgium

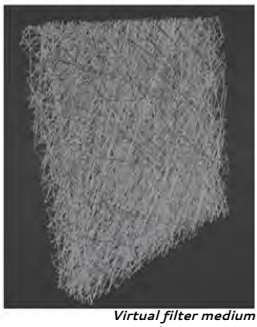
Industrial organisations involved:

Atlas Copco specialises in the design, development and manufacture of, amongst others, industrial compressors and expanders, vacuum solutions and air and gas treatment equipment.

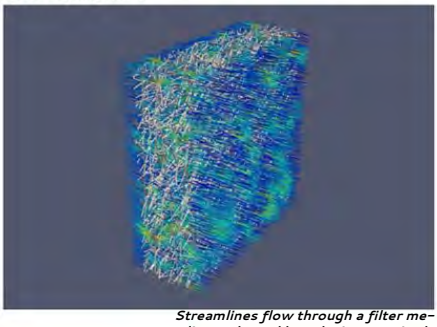
Customers tend to be companies in various industries, from food and beverage, oil and gas, semiconductor, transportation, and construction to medical applications. Atlas Copco extensively uses computing, computer models and digital twins to predict the behaviour of various products in different conditions. The same models are also used to allow engineers to better understand products on a fundamental level.

Technical /scientific challenge:

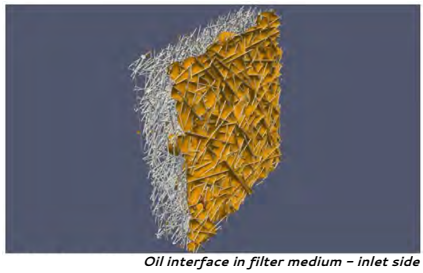
The flow geometry and physics at the microscale in filter media are complex and require state-of-the-art computational fluid dynamics techniques to resolve. The required computational resources are extensive and need world-class high-performance computing.



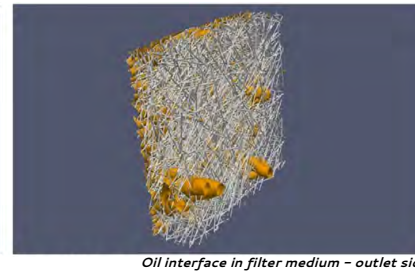
Virtual filter medium micro-structure



Streamlines flow through a filter medium coloured by velocity magnitude



Oil interface in filter medium – inlet side



Oil interface in filter medium – outlet side

Solutions:

VSC proposed to run these calculations on the VSC Tier-1 cluster Hortense. Simulations were first performed to build the necessary experience in efficiently running large-scale calculations and exploring the computational limits. Using Hortense gave Atlas Copco access to new simulation techniques to investigate the microscale behaviour of oil aerosol filter media.

Business impact/Benefits:

Tom Saenen (Atlas Copco, Technology developer Computational Fluid Dynamics): "We think that the VSC is an excellent organisation for the Flemish industry to get easy access to a powerful computing infrastructure at a modest price. It truly democratises large-scale simulations otherwise out of reach for many companies. Finally, organisations can expect quick and skilful support from the VSC team in setting up the simulations and software tools."

Keywords: air quality, oil aerosol, filter, CFD, compressors, vacuum pumps, hpc

Industry sector: General industrial machinery, automotive, construction, power generation, chemical and petrochemical industry.

·Technology: HPC, CFD, OpenFoam, ParaView

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EURO²

Major time savings with high-performance computing in fire engineering

NCC Finland

Industrial organisations involved:

Ramboll Finland is a multi-sector engineering and consultancy company whose services include building fire safety designs. The focus of fire engineering is ensuring that the premises of public and corporate clients are safe for occupants and property, as well as for the emergency services personnel in the event of a fire.

CSC's Customer Solution Manager Juhani Huttunen proposed launching the cooperation as a Try & Buy test project, which includes also expert support for their deployment. The company Ramboll sought to ensure that the FDS software, widely used in the fire safety sector, was compatible with LUMI's computing environment.

'With the help of Jarmo Pirhonen, the software was LUMI compatible in no time, and the actual work could start way sooner than we thought. Jarmo's help was paramount in this', Hämäläinen praises.

Technical /scientific challenge:

Time is often a critical factor for designers in construction projects. This certainly applies to fire safety engineering where clients' schedules are tight, fire safety regulations create a mandatory framework for fire safety design that must be followed, and permit processes take time. Delivery times for fire rated materials can, unfortunately, also be long.

Marko Hämäläinen, a fire safety expert at Ramboll Finland, is used to these challenges. The intended use of the building meant that complying with the fire safety regulations was not going to be so straightforward. In these cases, designers can use performance-based design methods, simulations, to prove the safety of the building.

Ramboll HQ - Photo Adam Mørk

Solutions:

As the project this time was so time-critical, a former supercomputing user Marko Hämäläinen from Ramboll had the brilliant idea to introduce advanced computing methods to expedite these simulations.

"Our work was speeded up, and we saved both time and money. We could run an individual simulation around four times faster than before. As the simulations were run in parallel the entire set of simulations was completed almost 20 times faster. The simulation models were optimized based on computing needs rather than the computer's terms. In the end, our customer got the results of the fire dynamics analysis quickly, which quite obviously meant that they could also be submitted to the authorities for approval earlier than usual. And I was able to tackle the next projects sooner." says Marko Hämäläinen from Ramboll.

Business impact:

In LUMI, the number of cores used can be scaled freely as required by the simulation model instead of modifying the simulation model on the computer's terms. This is impossible to do in cloud.

'From the designer's point of view, the flexibility to use only the number of cores required by the simulation model at any one time is fantastic." 'We at Ramboll clearly see that the various high-performance computing applications combined with the possibilities offered by AI will definitely have a role to play in our design projects also in the future,' says Hämäläinen.

Benefits:

- The entire set of simulations was completed almost 20 times faster
- The price was competitive, no need to apply for public funding
- Time savings
- The simulation models were optimized based on computing needs rather than the computer's terms

Keywords: Fire safety, Fire safety engineering, Fire safety designs, Building, Designs

Industry Sector: Construction, Engineering

Technology: HPC,FDS Fire Simulation, CFD

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EURO²

Simulation of airflow in concentric chimneys

NCC Spain

Industrial organisations involved:

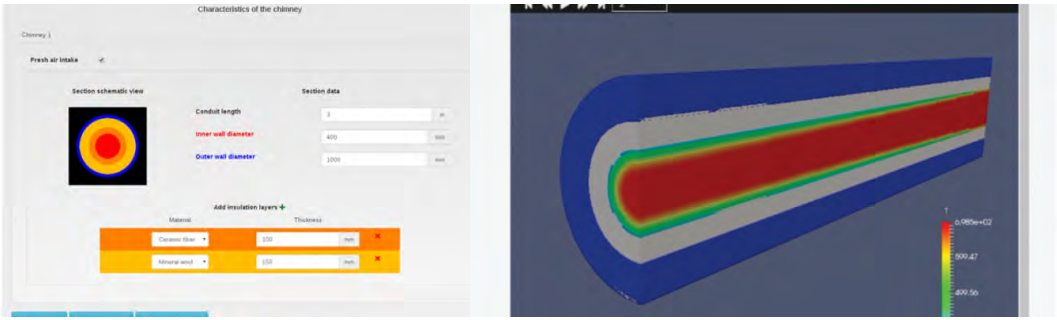
DINAK is a Spanish SME expert in designing, manufacturing and installing domestic and industrial chimneys and ventilation systems. DINAK needs a simple and powerful tool to analyse and test the design of exhaust chimneys. The developed tool should help them to improve the design of concentric chimneys and gain understanding of the physical phenomena involved in exhaust processes. To reduce design times to reasonable levels, High Performance Computing (HPC) has become an essential component in the development of such a design tool.

DINAK

La fuerza de la marca líder

Technical /scientific challenge:

If a chimney is not properly designed, not enough oxygen will reach the stove and combustion will be inefficient. There are many variables involved in the optimization of the design of a chimney and physical testing is not feasible on the grounds of cost and time. Consequently, it is necessary to use advanced numerical tools. The problem is complex because there are many variables, and the simulation must be sufficiently accurate and detailed. High performance computing (HPC) is needed for a fast time-to-solution, supported by a user-friendly interface to make the simulations easily accessible.



HPC-based simulation

Solutions:

The performed work produced a reliable HPC-based simulation, based around the open-source Open Foam package and successfully validated against commercial software and experimental data. There was also the development of a user interface that provides the ability to explore the design space in a systematic way which can improve the quality of the resulting designs.

Business impact:

Before this experiment DINAK did not have access to HPC-based simulation and had no experience in its use. It needed approximately a month of work for the design and testing of a new chimney. Every new product required the work of 3 specialized engineers and 2 craftsmen to assess the different options, to design prototypes and manufacture them and to test complete chimneys to verify the initial design concept. With this solution, DINAK can shorten the whole design process down to one week.

HPC simulation thanks to the NCC Spain support enabled DINAK to accelerate and optimize the design of concentric chimneys. Faster design will allow DINAK to enter new markets and to increase its competitiveness. Experience shows that the first company with a new design of chimney increases its market by 5% to 10%. Currently, DINAK develops around 3 to 4 new products per year and this advantage would increase its turnover by approximately €100K. The optimized design through the use of HPC, enables DINAK products to pass CE Mark tests with a zero-failure rate with a consequent cost reduction.

Benefits:

- Shorten of the whole design process for a chimney reduced down to one week
- Successful pass of CE Mark tests with a zero-failure rate with a consequent cost reduction.
- Increase of the number of new produced designs

Keywords: CFD, simulation, HPC, design optimization, OpenFOAM

Industry Sector: Manufacturing & engineering

Technology: HPC

Note: This success story was performed in a business experiment of the Fortissimo (*) project involving the NCC member CESGA; the success story was included in this EUROCC booklet as it provides inspirational material for the take-up of HPC by SMEs.

*The Fortissimo project has received funding from the European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement No 609029.

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EURO²

Unveiling the Nanoscale: Supercomputing-Driven Insights for Advanced Manufacturing

NCC Luxembourg

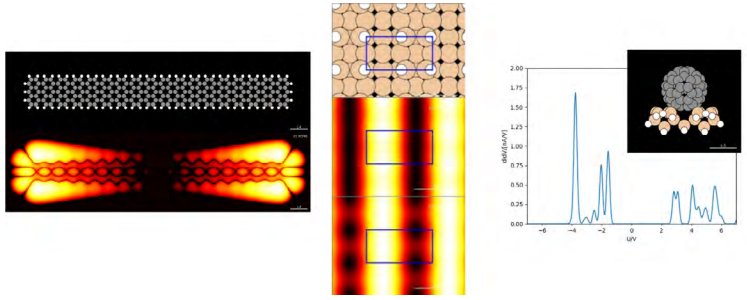
Industrial organisations involved:

Espeem, a private research institute located in Luxembourg, was established in May 2018 by Dr. Mads Engelund. Espeem's mission is to bridge the gap between industrial research needs and supercomputing solutions, translating complex research use cases into actionable proof-of-concept simulations on supercomputers. The goal is to empower the company's product research teams to conduct their simulations independently, enhancing efficiency and innovation.

Technical /scientific challenge:

In the realm of advanced manufacturing, the quest to forge new frontiers in material science and develop groundbreaking products necessitates a profound understanding of materials at the atomic level. This intricate knowledge is pivotal across various manufacturing domains, each with its unique challenges and requirements:

- Computing: The realm of computing, especially quantum computing qubits, demands surfaces engineered with precision at the atomic scale. Furthermore, as classical transistors shrink in size, the necessity for atomic precision becomes increasingly critical.
- Energy: The energy sector's advancements, from solar cells to batteries and hydrogen storage solutions, are significantly driven by the need for an atomic-level understanding.
- Chemicals: The production of chemicals was the first industry where atomic-level understanding was important, but this need has only increased with the advent of on-surface synthesis.
- Amid these endeavors to navigate new material processes and forge innovative products, manufacturers face the formidable challenge of safeguarding their intellectual property. Since insights are often hard won, easily replicated, and represent the future income of a company, the data is highly sensitive – surpassing even financial data.



STM prediction use case, left-to right: Carbon nanoribbon image, Si(001):H image under different conditions, spectroscopy of buckyball on a surface

Solutions:

Enough Power and Experts to Scale; Supercomputers like Meluxina offer the computational power required for delving into the nanoscale and HPC expertise. The latter is required to craft precise models that replicate complex material interactions at the atomic level. These models require substantial computational resources to simulate accurately. By working closely with dedicated supercomputer staff, Espeem's simulation experts can optimize these models to take full advantage of the hardware's capabilities, ensuring that every calculation is executed with maximum efficiency and accuracy.

An Environment for Safe Collaboration: cornerstone of utilizing supercomputing in advanced manufacturing is establishing a secure collaborative environment. The delicate nature of nanoscale innovation, especially concerning proprietary materials and processes, calls for an infrastructure capable of protecting intellectual property while fostering idea exchange. Supercomputing centers like Meluxina adhere to stringent security protocols, offering data protection in line with GDPR and ISO 27001 standards.

Business impact:

The main technological advancements of the developed solution are in materials and surface science. From ancient metallurgy to modern computer chips, the exploration of new materials and manufacturing methods expands the horizons of possibility. The immense potential impact is paired with the challenge of realizing this impact, since material innovations may require the entire supply chain to re-tool before the benefit reaches consumers. Still, a breakthrough, such as a battery with double the energy density, could swiftly revolutionize electrification and transform society.

Benefits:

- Simulating and analyzing materials at the atomic level allows for the design of products needing fewer raw materials
- Reduced energy consumption during production due to optimized material design
- Longer products' lifespans
- Smaller environmental footprint
- Enables development of new, environmentally friendly materials

Keywords: Supercomputer, material science, Surface-mount technology (SMT)
Industry Sector: material science, data security, smart-manufacturing
Technology: Simulations and smart-manufacturing technology.

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Customizing Scene in Virtual Environments using Neural Networks

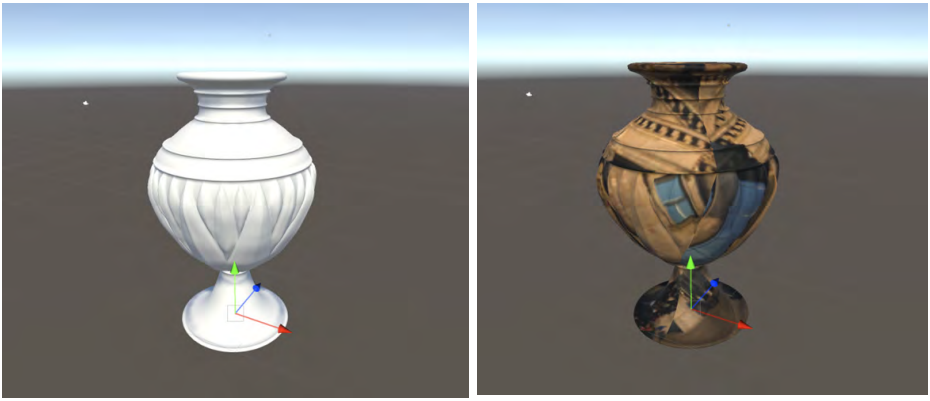
NCC Türkiye

Industrial organisations involved:

VLMedia created in 2014, is a rapidly growing, mobile focused team reaching millions of smartphone users with social network projects, which are available on AppStore, Google Play and Web platforms. VLMedia has more than 200 million registered users in over 50 countries and supports 19 languages.

Technical /scientific challenge:

The main technical challenge consisted in implementing intricate style transfer techniques from 2D to 2D and 2D to 3D using neural networks. AI played a pivotal role in creating a robust hybrid method for style transfer. This innovative approach combined the Neural Neighbor Style Transfer (NNST) method with traditional style transfer, integrating AI's deep learning capabilities. Leveraging AI's neural network architectures, specifically the VGG19 model, allowed feature extraction and content-style balancing, essential for faithful and detailed style transformations across dimensions. The hybrid method, fusing style and content loss computations, preserved target styles while significantly enhancing realism and comprehensiveness in the style transfer process.



Original and Stylized 3D Object

Solutions:

The challenge was addressed by developing a hybrid style transfer method, merging NNST with conventional techniques. Leveraging VGG19 (Visual Geometry Group consisting of 19 convolutional layers – https://viso.ai/deep-learning/vgg-very-deep-convolutional-networks/) model for feature extraction and content-style balancing, this method optimized style and content loss computations. Iterative adjustments fine-tuned processing times and weight ratios, achieving a balance between preserving target styles and retaining original content details.

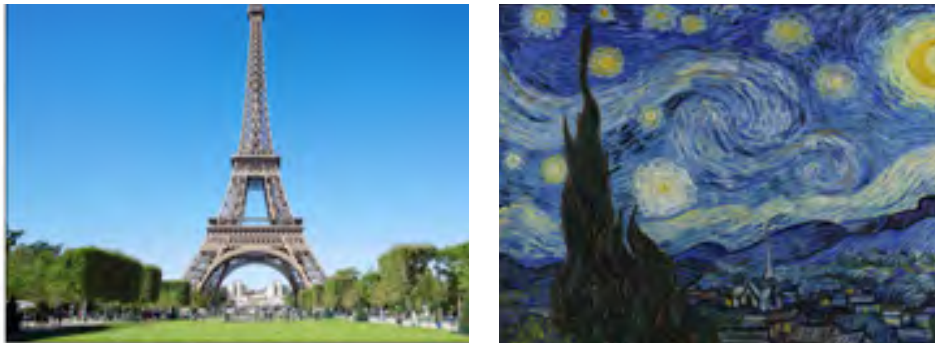
Business impact:

The current landscape demands intricate customization in virtual content creation. Harnessing HPC accelerates style transfer, expediting content personalization. This not only enhances competitiveness but also drives efficiency, enabling faster turnarounds and broader creative exploration in the industry.

In the realm of Manufacturing & Engineering, the fusion of HPC and AI sparked a revolutionary leap in design customization. This integration expedited intricate design alterations, slashing lead times significantly. Moreover, envisioning this innovation within VR environments amplifies the potential impact, as Style Transfer techniques, powered by HPC and AI, promise to redefine customization possibilities in the immersive world of Virtual Reality. This success narrative highlights how HPC and AI, when embedded in VR environments, reshape workflows, fostering unparalleled design personalization and efficiency.

Benefits:

- Enhanced Customization: Tailored Virtual Reality (VR) environments boost user engagement and satisfaction
- Streamlined Design Iterations: Rapid style transfer expedites design alterations
- Reduced Production Timelines: Quick customization minimises lead times
- Amplified Immersive Experiences: Personalized VR encounters deepen user connections



Content Photo and Stylized Photo

Keywords:Neural Neighbor Style Transfer, Data Parallel, Virtual Reality
Industry Sector: Manufacturing & Engineering, VR Environments
Technology: HPC, AI

Contact:
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Smart Sensors: Mapping Temperature – Kriging and Floorplan Analytic

NCC Cyprus

Industrial organisations involved:

EMBIO Diagnostics is a tech company and device manufacturer that shapes the future of diagnostics by designing and developing innovative, rapid, portable, biosensor-based digital devices, leveraging on Artificial Intelligence and Machine Learning. Their airbeld™ indoor air quality monitoring system, equipped with advanced sensors and AI, delivers real-time insights on air pollutants, empowering users to maintain a healthy and comfortable environment

Technical /scientific challenge:

EMBIO Diagnostics was interested in tackling the challenge of predicting temperature distribution across large, complex floorplans using the Universal Kriging interpolation method , a computationally intensive process, especially on extensive grids. Running these calculations on high-performance computing (HPC) systems allowed the company to efficiently process the large datasets involved. By parallelizing the experiments, the time required to generate accurate predictions was significantly reduced, making real-time sensor placement recommendations feasible.

Solutions:

To solve this challenge, a combination of image processing and statistical techniques was recommended. First step was the pre-processing of the floorplan to highlight essential features like walls, doors, and windows. Random points within the floorplan were generated, while distances from these points to key features was calculated using Euclidean distance grids. For temperature prediction, Universal Kriging was utilised, which accounts for spatial relationships and trends in the data. By running these computations in parallel on HPC systems, the company was able to process large grid data and thus find the correct variogram model that resulted in accurate temperature distribution maps and optimized sensor placement.

Business impact:

Currently, predicting temperature distribution within a building relies heavily on manual sensor placement, which can be both time-consuming and prone to inaccuracies due to limited data coverage. Traditional methods struggle to capture the spatial variability influenced by features like walls, doors, and windows, leading to suboptimal sensor configurations.

By leveraging HPC, temperature prediction was significantly enhanced. The computational power allows EMBIO Diagnostics to run complex algorithms like Universal Kriging on large grids, capturing detailed spatial patterns that would otherwise be computationally prohibitive. Parallel processing further accelerates this analysis, making it feasible to generate real-time predictions and adjustments.

As a result, HPC enables the creation of more accurate and reliable air quality distribution maps, which directly inform better sensor placement. This improvement not only enhances environmental monitoring but also optimizes energy efficiency in buildings by ensuring that sensors are strategically placed where they are most needed.

Benefits:

- Cost Efficiency: Optimized sensor placement minimizes the need for excess sensors, cutting hardware costs.
- Product Optimization: Enhanced accuracy in temperature predictions improves building energy management.
- Waste Reduction: More efficient sensor deployment reduces energy waste, contributing to sustainability.

Keywords: Seismic-resistant infrastructure
Industry Sector: Construction
Technology: HPC, AI, Machine Learning

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EURO²

Use of Cloud-Computing for rebar cutting optimisation

NCC Spain

Industrial organisations involved:

Schnell Software is a company specialized in software tools for steel cutting and bending companies (a sector in constant technological evolution and growth). The company has focused its activity on the program development of process optimization of iron for reinforced concrete.

The BIFI is one of the most relevant e-science centers in Spain, both as resource providers and for scientific users. Composed mainly by engineers and physicists, the Computing & Data Science Area includes a wide range of activities such as technological research, user support, applied research, technology transfer and/or dissemination.

The BIFI houses the Aragón Supercomputing Centre (Cesar), a computing infrastructure that encompasses a wide range of technologies: HPC (distributed and shared memory), grid, cloud, voluntary computing and dedicated computers

Technical /scientific challenge:

The challenge faced was to modify a software to run in an HPC-Cloud environment instead of using a local PC. The goal was to reduce the number of computing hours to minutes even for large-scale optimizations.

An additional goal was to develop a graphical user interface to guide the optimizations. The modified software would serve as a database portal to optimize functions in the Cloud and customers would be able to carry out cutting process simulations with minimal cost and effort.

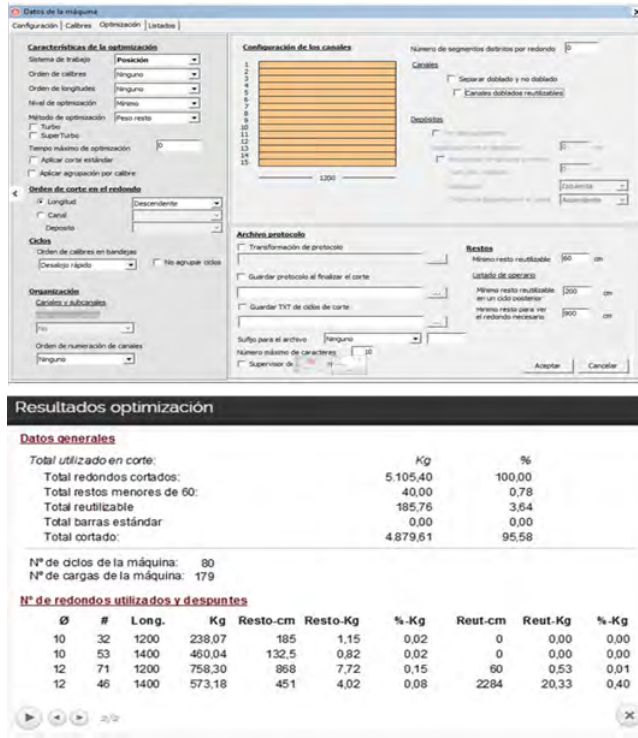
Solutions:

The optimization software has been adapted to run in a distributed HPC-Cloud infrastructure. Using a graphical user interface, it is easy to define and optimize the cutting and bending operations and bending operations, hiding the complexity of the Cloud.

Launching optimizations is as simple as sending input files with appropriate parameters and receiving the results after a reasonable processing time.

Business impact:

A large foundry produces two thousand tons of steel bars per month. By using high-level optimization based on the use of the Cloud, steel waste can be reduced by 2% (480 tons per year). Given that the average price of steel is 500 € per ton, this represents a saving of 240.000 € per year, compared to a saving of only 60.000 € per year using low level optimizations on PC. optimizations on PC. Additionally, by using high-level optimizations, there is an associated saving in personnel costs of 30.000 € per year.



GUI of the software optimized, and the results obtained when running the solution in the HPC-Cloud infrastructure

Benefits:

- Steel waste reduction (which means cost savings)
- Personnel cost reduction

Keywords: HPC, grid, steel fixing, Montecarlo simulation, steel cutting

Industry Sector: manufacturing & engineering, metals, mechanical engineering

Technology: HPC

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EURO 4SEE

Section 6

Finance and Mobility

Personalized banking software solutions

NCC Montenegro

Industrial organisations involved:

Fleka is an interactive design studio, specialized in web and mobile platforms and fintech products. Fleka designs and implements digital products through the design, development and maintenance of websites, mobile applications, fintech products, e-commerce platforms, as well as numerous other interactive concepts for the clients from various industries and areas of business.

Technical /scientific challenge:

Montenegrin company Fleka and Faculty of Information Systems and Technologies (FIST), UDG, worked on the project „Personalized Banking Software Solutions», partly funded by Innovation Fund of Montenegro. The project is centered around the development of a set of SaaS solutions, based on machine learning (ML) and data collection, which will enable financial institutions and other companies to significantly improve personalized banking and payment services for their clients. Fleka previously developed SKEN mobile application, a personal expense tracker that helps users keep track of their spending by scanning fiscal receipts.

Solutions:

The consortium has jointly developed ML classification algorithm based on NLP. The Algorithm analyses gathered data and classifies them into predefined categories (food, drinks, services etc.) according to previous annotated data (dataset collected through the SKEN app). Generated reports will provide assembled and detailed overview of expenses by itemized categories, customers, and companies. Instead of seeing it as just a chronological list, users will be able to have purchasing items grouped in categories, including category-specific expenditures breakdown, without requiring any additional effort on user's behalf. The advanced AI/ML system will manage to categorize each transaction automatically using available public information, crowdsourced inputs and ML models intelligence.

Business impact:

The project is based on the development of SaaS solutions, based on machine learning, HPC resources and data collection, which will enable financial institutions and other companies to significantly improve personalized banking and payment services for their clients. Fleka has also created mobile apps and services specifically designed for Montenegrin banks, where this reporting can be implemented. These tools aim to assist users in obtaining valuable information, recommendations, and analyses to enhance their financial management. Datasets will be basis for the analysis and prediction of behavior and purchasing habits of Montenegrin customers, uncovering business opportunities for financial institutions and business clients in data-driven promotions, marketing campaigns, loyalty programs etc.

Benefits:

- Enabling financial institutions to significantly improve personalized banking and payment services
- Offering business clients, the categorized and analysed data, with valuable insights supporting decisions related to product offerings, marketing campaigns, customer targeting, financial management etc.
- Enabling end users to optimize spending habits and improve financial discipline

Keywords: Fintech, m-Banking, Machine Learning, HPC, NLP

Industry Sector: Finance/Insurance, IT/HPC systems, services & software providers,

Technology: AI, HPC, HPDA

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EURO²

Understanding the Impact of Product Discounts

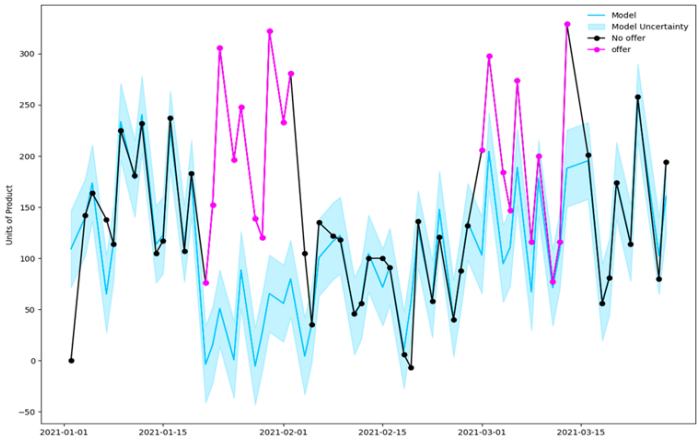
NCC Cyprus

Industrial organisations involved:

Charalambides Christis is a leading dairy company in Cyprus and a top leader in food production and distribution. They supply supermarkets, bakeries, and convenience stores across the island with milk and other dairy products. The quality of Charalambides Christis is internationally recognised with the company actively exporting in more than 32 countries, making it the largest exporting company in the food industry in Cyprus.

Technical /scientific challenge:

Charalambides Christis apply product offers frequently to their supermarket products, but do not have the visibility and clarity to the effect that these discounts have on sales. Their requirement was to understand the average treatment effect of an offer so they can subsequently do a cost-benefit analysis using reliable modelling data. They were also interested in understanding whether there was negative effect on sales after the offer expires. This a problem that requires understanding the effect of an intervention and therefore goes beyond standard machine learning analyses that makes use of correlations only.



Solutions:

The primary goal was to identify the average treatment effect (ATE) of a product offer, defined as the difference between actual sales and what sales would have been without the offer. To estimate ATE, we recommended developing a regression machine learning model tailored for time-series data on supermarket sales. The model would use features like seasonality, weather, and milk sales (a non-promotional benchmark). By training on non-promotional days, the model can then predict sales during promotions, allowing comparison with actual sales to estimate ATE. To develop this model, hyperparameter tuning and model selection are necessary, particularly to optimize the number of Fourier coefficients without overfitting. This process can be efficiently performed on an HPC by running parallel searches of the hyperparameter space.

Business impact:

The suggested methodology offers Charalambides Christis an opportunity to have an estimate of ATE and its uncertainty. Having an estimate of the ATE uncertainty is a crucial component of the cost-benefit analysis and it can be estimated using Monte Carlo simulations.

Our proposed method also included the use of permutation feature importance in order to be able to compare the purely data-driven analysis with the expertise in the company.

Lastly being able to estimate the ATE from past data is the first step toward a future what-if analysis whereby the company can have predictions of the impact of a proposed product offer. This capability can lead toward cost savings and more efficient supply chains.

Benefits:

- Data driven cost-benefit analysis of product offers
- Ability to use Explainable AI for model validation with domain experts and other stakeholders
- Groundwork done for future what-if analysis and more informed business decisions

Keywords:HPDA, Machine Learning, R&D, Average Treatment Effect, Counterfactual
Industry Sector: Finance (Retail), services & software providers
Technology: HPC, HPDA, AI

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Deep Code: Deep Learning system for customer characterisation, prediction and decision making in the insurance industry

NCC Spain

Industrial organisations involved:

Codeoscopic is part of a group technology companies with in-depth knowledge of the insurance sector. They offer their clients (insurers and brokers) the technological platforms and solutions that lead to a significant improvement in their productivity.

BIFIis one of the most relevant e-science centers in Spain, both as resource providers and for scientific users. Composed mainly by engineers and physicists, the Computing & Data Science Area includes a wide range of activities such as technological research, user support, applied research, technology transfer and/or dissemination.

The BIFI houses the Aragón Supercomputing Center (Cesar), a computing infrastructure that encompasses a wide range of technologies: HPC (distributed and shared memory), grid, cloud, voluntary computing and dedicated computers.

Technical /scientific challenge:

The challenge was to develop a Deep Learning system for the insurance sector to improve the data analysis needed in the actuarial process. Insurance companies use complex statistical and mathematical models to estimate the different types of risk associated with an insurance policy and therefore to determine the possible premiums, with a whole science behind it, actuarial science. In the case of automobile insurance, the risk estimation models can include from the variables most directly associated with the insured risk itself (characteristics of the vehicle, age and experience of the driver) to any other information, such as the probability of non-payment or the number of kilometres that the insured is typically going to drive. There is also the possibility of using statistical information, indirectly linked to the customer, but which has a direct impact on risk.

Solutions:

The models to be developed must work with a large volume of data, as more than 200 million records are generated annually, so it is necessary to work with multiprocessor systems, either High Performance Computing (HPC) or Cloud Computing.

Deep Learning models for premium estimation, price trends and alerts have been developed to form a system that will provide the insurance sector with an analytical environment to support decision-making. The use of a Cloud Computing environment allowed the training and efficient execution of the models.

Business impact:

This system allows the company to offer insurers a technological platform to position themselves in the market and visualise their current situation, detect premium variations in the market, perform portfolio qualification through premium prediction or estimation systems, anticipate market variations.

Benefits:

- Make decisions and strategic changes based on data
- Creation of artificial intelligence models for the prediction of car insurance premiums
- Creation of social impact models and brand image for insurance companies
- Prediction models for variations in the premium market

Keywords: deep learning, premium insurance, data scraping, big data, market trends

Industry Sector: Automotive, service & software providers

Technology: AI, HPDA

Note: This success story was performed in a business experiment of the Fortissimo (*) project involving the NCC member CESGA; the success story was included in this EUROCC booklet as it provides inspirational material for the take-up of HPC by SMEs.

*The Fortissimo project has received funding from the European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement No 609029.

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EURO²

Development of Self-Driving Technology

NCC Estonia

Industrial organisations involved:

Bolt is an Estonian mobility company that offers vehicle for hire, micromobility, car-sharing, and food delivery services headquartered in Tallinn and operating in over 400 cities in over 45 countries. In partnership with the Autonomous Driving Lab of the University of Tartu, the company developed self-driving technology for a Level 4 autonomous car.

Technical /scientific challenge:

Autonomous cars acquire up to 357 GB/hour of data during test drives. Autonomous car engineers needed a system to store and easily access those test logs.

Lexus RX450h equipped with the sensors that are a prerequisite for basic autonomy

Solutions:

Acquired test logs are copied to HPC storage, into appropriately guarded directory. Regularly Cron job processes those log files into metadata stored in MongoDB database. Processing is distributed over cluster and happens in parallel. Longest logs can take up to 24 hours to process, so processing them sequentially would be very time-consuming. On top of MongoDB sits custom-made application that allows filtering of test sessions and browsing them using Webviz visualization tool. Visualization tool accesses the raw sensor data from HPC storage.

Business impact:

People's needs for different means of transport are on the rise, which is why self-driving cars are a very good alternative to current modes of transport. HPC solutions offer the company an indispensable opportunity to develop the maps, car camera, radar, lidar and sensor analysis needed for self-driving vehicles, as well as the ability to detect the surrounding situation and make decisions. Quick results, in turn, improve the company's competitiveness.

Benefits:

- Custom database application and visualization tool enables easy analysis of the logs
- Thanks to distributed processing in the cluster, the metadata about the drives usually shows up already next morning
- Thanks to custom database application and visualization tool, the team members can easily analyse the logs and share their findings with each other
- Thanks to petabytes of storage at the HPC Centre, the company can keep all the data they need

Keywords: Autonomous cars, Autonomy software, Lidar, Human-vehicle interaction, High-definition maps

Industry Sector: Automotive

Technology: HPC, HPDA, AI

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EURO
4SEE

Section 7

LLMs and Communication

EURO²

Training Large-Scale Models for Speech-to-Text Recognition

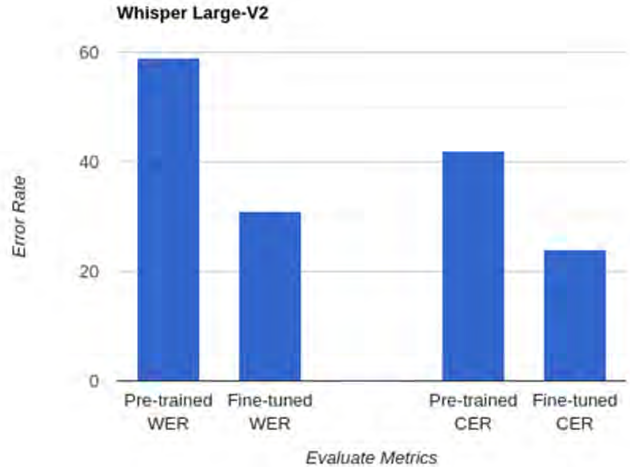
NCC Türkiye

Industrial organisations involved:

Erste located in Ankara, is a software engineering SME created in 2017, focusing on international R&D projects. It has a wide range of expertise in mobile-device management, predictive maintenance, digital twins, Internet of Things (IoT)-based intelligent port management, smart-software-powered manufacturing environments, blockchain-based ID management, etc. Sample projects Erste was involved in can be seen at https://www.ersteyazilim.com/en/projects-products-and-services/.

Technical /scientific challenge:

Although state-of-the-art speech-to-text models work well in English, they do not have the same performance for most of the other languages. Fine-tuning these models can be a solution, and using HPC systems for this purpose is the most cost-efficient solution. Erste requires the NCC's consultancy to get support in training and using large-scale models for speech-to-text transcription in Turkish. The developed tools will be utilized in an international ITEA project called InnoSale (https://www.innosale.eu/), which focuses on advancing state-of-the-art technology in the retail industry.



Solutions:

Despite Erste's prior experience with a Proof of Concept study (PoC) using HPC resources for training traditional ML models, the company lacked of expertise on large-scale models and how to work with them. EuroCC's training sessions and TRUBA User Documents proved to be quite informative. The model chosen for fine-tuning was the largest Whisper model. Working with the HPC expert, memory-efficient training approaches, Parameter-Efficient Fine-Tuning (PEFT) and Low-Rank Adaptation (LoRA), were implemented. Thanks to the TRUBA HPC Centre's help, the SLURM scripts that can work on multiple GPUs were prepared and the parameters for effective and efficient fine-tuning were set. We observed significant reductions in the character and word error rates of the pre-trained Whisper even after only 4-8 hours of training sessions.

Business impact:

Training a large-scale ML model is a highly demanding task, requiring significant computational power and financial resources. Despite numerous research and efforts to alleviate these demands, access to the computation power remains inevitable. The TRUBA resources provided through the EuroCC-2 project have been instrumental in supplying the necessary computational capabilities to Erste. Moreover, using the NCC's expertise on these models also enabled us to yield an effective training process with less time.

Benefits:

- Reduced training time with multiple GPUs and efficient training methods
- Marked reduction in transcribed text errors, though further improvement is possible
- Gain of expertise in large-scale model training
- Model improvement and development of other cutting-edge tools using the acquired knowledge

Keywords: xxx
Industry Sector: Manufacturing
Technology: HPC, AI, speech to text, GPUs, LoRA, PEFT

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EURO²

Building a family of multilingual open-source large language models

NCC Finland

Industrial organisations involved:

SiloGen is a large-scale initiative with the aim of building generative AI technology for Europe's digital sovereignty. As Silo AI's generative AI arm, SiloGen combines some of Europe's leading generative AI and large language model (LLM) experts with access to data sources, powerful computational resources and infrastructure to train, run and operate LLMs. SiloGen has been operational since 2022.

The TurkuNLP group of the University of Turku was founded in 2001 and has been carrying out research in natural language processing for over 20 years with a focus on machine learning applications to the automatic analysis and generation of text. TurkuNLP is the leading Finnish research group in large generative language models and is one of the partners in the Horizon EU High Performance Language Technologies project, which is currently creating the next generation of European language models on the LUMI supercomputer.

Technical /scientific challenge:

TurkuNLP and SiloGen are building multilingual open-source LLM models with the aim of strengthening European digital sovereignty and democratizing access to LLM models. The development of foundational models in line with European values is crucial in order to ensure that they are based on data and information that represent the different languages, citizens, organizations and cultural landscape of the European Union.

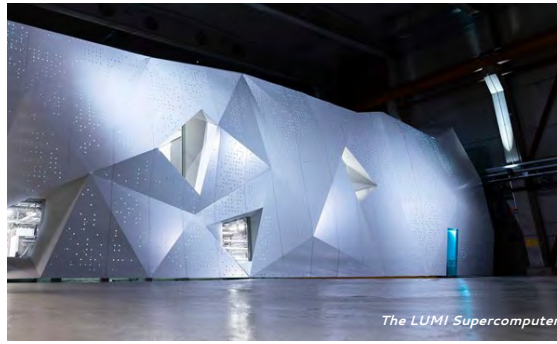
Solutions:

The Poro open-source large language model (LLM) outperforms all existing open Finnish language models, including the FinGPT models previously published by TurkuNLP and the previous BLOOM model with 176 billion parameters. The group has tried to define the optimal data repetition frequency for low-resource languages and included translation pairs of Finnish and English text in the training data. With this approach, the cross-language signal improves the model's understanding of cross-language connections, and has been shown to be crucial for achieving high performance for low-resource languages without compromising performance in English.

The completion of Poro is proof of TurkuNLP and Silo AI's commitment to the development of artificial intelligence models for low-resource languages. Releasing Poro as an open-source model facilitates large-scale availability and collaborative improvement, especially for smaller European languages. This approach enriches the global AI community by providing a valuable resource for research and product development, and demonstrates a conscious effort to increase linguistic diversity in AI applications.

Business impact:

Poro is the result of a collaboration between Silo AI's generative AI arm SiloGen and the University of Turku's TurkuNLP Group and HPLT project, bringing together cutting-edge research and industry expertise. Poro was trained on the EuroHPC pre exascale LUMI supercomputer operated by CSC – IT Center for Science and supported by CSC experts. The consortium, distinguishes itself from other initiatives through its diverse capabilities and resources for developing Large Language Models (LLMs). The approach encompasses a top-tier team comprising of top level scholars supplemented by the expertise of over 150 PhDs and 300 AI specialists affiliated with Silo AI. Furthermore, the consortium has access to a large array of data resources spanning all European languages, including High-Performance Language Technology (HPLT) data, meticulously gathered and curated. Access to cutting-edge computational infrastructure, including the software framework for LLM training and access to the LUMI supercomputer, alongside CSC support and other hardware and cloud services, has provided further synergies. Poro is trained using 512 AMD MI250X GPUs.



The LUMI Supercomputer

Benefits:

- Poro 34B is 34.2 billion parameters and uses a BLOOM architecture with ALiBi embeddings
- Poro is designed to process English and Finnish, and has proficiency with a variety of programming languages.
- Poro is freely available under the Apache 2.0 License
- The model is trained with a dataset of 1 trillion tokens, with English, Finnish and a variety of programming languages represented
- Poro is trained using 512 AMD MI250X GPUs on the LUMI supercomputer

Keywords: Large language models, AI, ChatGPt, OpenAI, Llama, Mistral

Industry Sector: Artificial Intelligence solutions providers, HPC systems, services & Solution providers

Technology: HPC, HPDA, LLM, AI

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Fine Tuning Large Language Model (LLM)- based matching platform

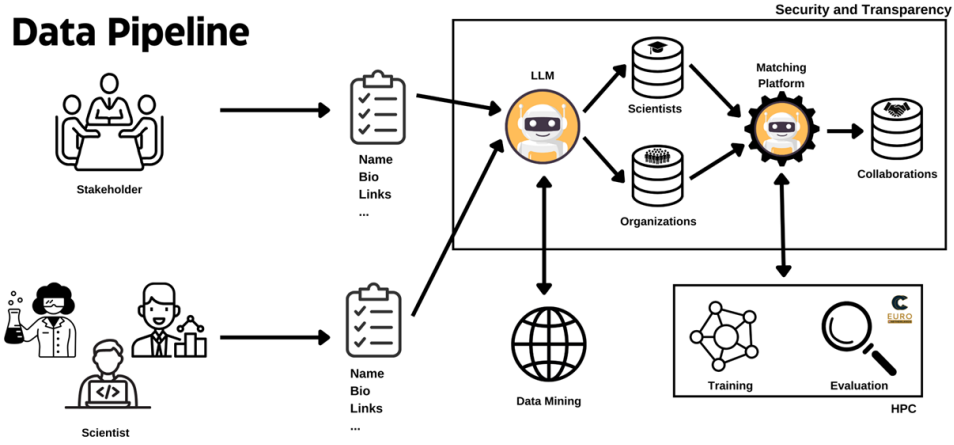
NCC Netherlands

Industrial organisations involved:

The Good Scientists are a team of dedicated volunteers comprising MSc, PhD, and PostDocs across diverse scientific fields that recognise the need for efficient and precise matchmaking between scientists and organisations striving to make a positive societal difference.

Technical /scientific challenge:

The Good Scientists are focusing on the training and fine-tuning of Large Language Models by making use of High-Performance Computing to allow high scalability and consequently access to larger models. The ultimate goal is the production of expert-findings with improved accuracy. Several challenges are addressed. However, the focus is on the reduced response time for the recommendation by handling efficient workload balancing and the efficient use of GPU resources.



Solutions:

To address the challenge of developing a comprehensive platform to allow an efficient matchmaking between scientists and organizations, The Good Scientists elaborated a decentralized online ecosystem composed of two main components: A Social Impact Project Marketplace and a Scientific Expert Network. The developers are focusing on expert-finding algorithms to build an efficient matching and candidate evaluation. Large Language Models are presented as an alternative to enhance algorithmic challenges, allowing a dynamic analysis of textual data from different sources, extracting the relevant information with a high level of personalization, and generating high-quality semantic comprehension.

Business impact:

To foster collaborations among scientists and non-profit initiatives, The Good Scientists introduces a Large Language Model (LLM)-driven matching platform. This tool represents a notable advancement toward the objective of making science accessible for societal advancement. With a dedicated group of volunteers proficient in diverse scientific fields, The Good Scientists recognize the necessity for precise and efficient connections between scientists and organizations and are devoted to foster significant societal change and improve the transfer of technology for social good. By applying High Performance Computing knowledge and resources, their platform is expected to have a significant business impact by making it possible to use technologies able to improve the accuracy of expert-finding and reduce the response time, generating high-quality and fast results.

Benefits:

- Description of the software deployment in a supercomputing environment
- Fine-tuning of the specific Large Language Model for the matching platform
- Improved accuracy of the results (expert-findings)
- Improved efficiency and performance of training models

Keywords: matching platform, Large Language Models, High Performance Computing, Artificial Intelligence, GPU, data efficiency

Industry Sector: Services & Software Providers

Technology: Artificial Intelligence for an improved matchmaking platform

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Austria, the Czech Republic and Germany introduce EuroCC to the international community

NCCs Austria, Czech Republic, and Germany

Industrial organisations involved:

EuroCC Czech Republic – represented by IT4Innovations

National Supercomputing Center at VSB – Technical University of Ostrava, www.it4i.cz

EuroCC Germany – represented by SICOS BW GmbH, sicos-bw.de

FFG – Austrian Research Promotion Agency, www.ffg.at

Vienna Business Agency, viennabusinessagency.at

Topic of collaboration:

High-Performance Computing (HPC) for digital businesses and industrial innovators: the workshop of EuroCC National Competence Centres (NCCs) from Austria, the Czech Republic and Germany took place on May 12, 2021 at the 6th International SoftwareDays – the biggest software b2b event in central Europe. The speakers Andreas Wierse, Harald Grill, Markus Stöhr, and Tomáš Karásek presented the EuroCC initiative to support European users in the uptake of HPC and provided valuable insights into the supercomputing infrastructure, successful HPC applications and benefits that help solve complex problems, e.g. in software development, engineering and manufacturing.

Results of collaboration:

The workshop on High-Performance Computing attracted 60 participants from more than ten countries and facilitated productive networking with the b2b sector. In essence, it became a great platform for promoting the uptake of HPC, explaining the European HPC landscape to the international audience and offering access to the technical know-how available in AT/CZ/DE in particular.

Apart from conducting the joint workshop, each speaker held one-on-one meetings with industrial stakeholders. For the NCCs this proved to be a great opportunity to forge meaningful connections with potential HPC users, and for the latter to gain a deeper insight into general as well as specific advanced computing solutions for their businesses.

Business impact/Benefits:

Being part of the EuroCC network, which extends over 33 countries, often proves challenging for participating NCCs when it comes to communication with each other and gaining insight into the processes of fellow competence centres. Joining forces for SoftwareDays thus became an excellent opportunity for the NCCs AT/CZ/DE to exchange perspectives and establish a closer relationship. Moreover, the joint appearance surely helped to convey the interconnected nature of the large and intricate system of European HPC initiatives including EuroCC, CASTIEL, EuroHPC JU, and PRACE.

The collaboration between AT/CZ/DE was not only a desired undertaking but also a necessary one, since the participation at SoftwareDays is only possible for entities with an international outreach. Therefore, the three NCCs accomplished a multifarious task pushing forward both internal and external goals, coming out as one and offering threefold value to the public.

Going forward, it would be advantageous to have NCCs collaborating with each other on a regular basis – a practice that aims to benefit international stakeholders as well as EuroCC, in line with the objectives of the project and the values of the European Union which promote international cooperation, exchange of expertise, and technological literacy.

Keywords: High-Performance Computing, HPC, Supercomputing, Engineering, Software Optimisation, EuroCC

Industry Sector: IT/HPC systems, services & software providers, manufacturing & engineering, natural science

Technology: HPC, HPDA, AI

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EURO²

Automated Voice Processing with Artificial Intelligence at Scale

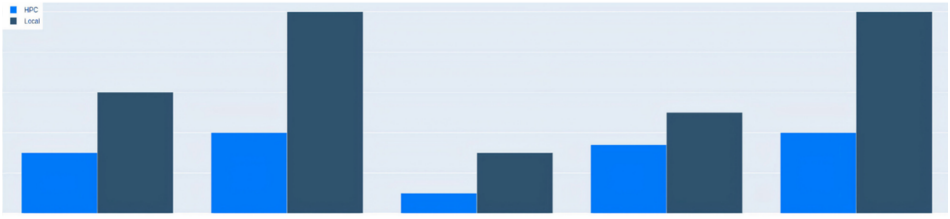
NCCs Romania and Netherlands

Industrial organisations involved:

RepsMate is developing a SaaS solution that integrates AI & Data Analytics technologies to understand customers' needs and behavior; to assist companies' representatives in their communications with customers. RepsMate aims to provide companies' representatives with automated and tailored guidance, simulating a real-time, always available virtual coach for agents.

RepsMate

Processing time comparison
(HPC compared to RepsMate-Cluster)



Text Preprocessing (CPU Intensive)	Text statistical-LM training (CPU Intensive)	Text dataset tokenization (CPU intensive)	Speech to text finetuning (GPU intensive)	Masked language modeling pre-training on large dataset (GPU intensive)

Technical /scientific challenge:

The RepsMate technical solution is based on different functionalities, such as automatic speech recognition and spoken emotion recognition, together with behavioural segmentation and enhanced with contextual real-time guidance. All of these elements make extensive use of recent machine learning technologies that allow processing raw information and extracting additional extensive details from the speaker's emotions and behavior, which is key to improving service quality. The main challenge is to ensure the optimal implementation for all the elements and to test the cohesion of the building blocks of the application to run on large-scale computing machines.

Solutions:

This collaboration focused on analyzing RepsMate's audio processing workflow and exploring parallelization on general-purpose GPUs. NCC Romania consultants initially evaluated RepsMate, identifying it as a potential candidate for supercomputing. RepsMate developers gained access to the Dutch national supercomputer Snellius for medium-scale testing on Nvidia GPUs, with support from NCC Netherlands experts. The analysis demonstrated RepsMate's scalability and efficient utilization on large-scale systems with Nvidia GPUs. Scalability analysis on AMD and other major GPU vendors is ongoing. Once completed, RepsMate will be able to apply for development access on Europe's best pre-exascale system for production-ready runs (funded by EuroHPC-JU). Further analysis is being conducted for systems with AMD GPUs to ensure scalability on both major GPU vendors. This step will guide RepsMate's application for development access on Europe's most suitable pre-exascale system, enabling production-ready runs.

Business impact:

The need for supercomputing power was proved to be justified by the high level of parallelization required by current artificial intelligence solution using deep learning (based on large convolutional neural networks with specific classifiers), as well as the large amount of audio files that require processing. With this concrete assessment, RepsMate proved to be a well-implemented code that can make optimal use of high-performance computing (HPC) systems, which will definitely help to reduce the time-to-solution in the processing of audio files. In particular, the thorough analysis of the application helps to clarify the optimal way of running RepsMate on heterogeneous systems with minimum costs, both in terms of money and sustainable use of the computing system.

Benefits:

- Concrete description of how the application runs on a large-scale computing system
- Verification of the optimal processing for the application
- Efficient use of compute resources on medium-scale test runs
- Guidance for the use of large-scale test runs for future use of the largest EuroHPC pre-exascale systems in Europe

Keywords: artificial intelligence, speech recognition, conversation, emotion recognition

Industry Sector: Services & Software Providers

Technology: Integral AI solution for the processing of conversations

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