## FF4EuroHPC Success Stories

SME Innovation Through HPC

1st Edition

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#### FF4EuroHPC Success Stories SME Innovation Through HPC 1st Edition, November 2022

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www.ec.europa.eu

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# www.ff4eurohpc.eu

## About the FF4EuroHPC Project

The FF4EuroHPC project 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. The total funding is 9.9 Million EUR. The project started in September 2020 and its duration is 36 months. The project is coordinated by the University of Stuttgart/HLRS (Germany) and supported by 5 other core partners: Arctur (Slovenia), CINECA (Italy), CESGA (Spain), scapos AG (Germany) and Teratec (France).

#### The Aim of the FF4EuroHPC Project

FF4EuroHPC helps facilitate access to High-Performance Computing-related technologies for European Small & Medium Enterprises (SMEs) and thus increases the innovation potential of European industry. Whether an SME is running high-resolution simulations, doing large-scale data analyses, or incorporating AI applications into its business or service workflows, FF4EuroHPC assists them to connect their business with cutting-edge technologies.

#### **SME** Participation

Two open calls were implemented through the project targeting the highest quality experiments involving innovative, agile SMEs. The focus was put particularly on





SMEs from the manufacturing and engineering sectors but also on other key European industrial sectors. Each experiment was centred on an end-user SME (or consulting SME) and the consortium was completed by technology or service providers such as ISVs, technology and domain experts, and HPC providers. The experiment partners identified and addressed a specific business challenge for the SME linked to a specific industrial sector (or in some cases for multiple industrial sectors). By implementing HPC, Artificial Intelligence (AI), Machine Learning (ML), High-Performance Data Analytics (HPDA), or other state-of-the-art technologies, the experiment partners were able to develop unique products, innovative business opportunities, and become more competitive.

#### **Experiments and Success Stories**

In total, 42 experiments met the open call requirements, successfully passed the evaluation process, and were selected for funding. During the 15-month duration of an experiment, the experiment partners jointly worked on the relevant use case and strove to overcome the challenges with the help of HPC. In the first Open Call, 16 experiments ran, involving 53 partners from 9 European countries. All 16 experiments from the first Open Call were successfully concluded and are presented in this booklet.

Each experiment had to address SME business challenges by using HPC and complementary technologies such as HPDA and AI. Therefore, each was an End-User-relevant case study demonstrating the use of HPC and the benefits it brings to the value chain from the end-user to the HPC-infrastructure provider. As soon as the experiment was successfully concluded, it generated a success story, which highlights the expected business benefits for the participating SMEs. The success story also presents the potential impact of the experiment's results in economic terms as well as with regard to societal or environmental challenges. Thus, it provides an inspiration to the broader industrial community.



FF4EuroHPC core partners supported participating experiment partners in accessing HPC-resources, as well as planning and promoting their experiments. The partners CESGA, CINECA and HLRS also acted as a provider of HPC resources and expertise in a number of experiments. Furthermore, FF4EuroHPC partners connected SMEs with the National Competence Centres (NCCs) and Digital Innovation Hubs (DIHs). NCCs closely collaborated with SMEs to implement appropriate actions to foster the use of HPC by SMEs.

#### ARCTUR



Arctur is a Research & Development oriented SME active in the field of Information and Communications Technology. Arctur is the main Slovenian commercial supplier of HPC services and solutions. Arctur has its own infrastructure to be used as the technological foundation for advanced HPC and Cloud computing solutions and innovative web services in a distributed, high-redundancy environment. The company has extensive experience in server virtualization and deployment, integration of disparate IT systems, IT support of project management, and server farm leverage for the deployment of SaaS specialized for SMEs.

### CESGA



Galicia Supercomputing Center's mission is to contribute to the advancement of Science and Technical Knowledge by means of research and application of HPC and communications, as well as other information technology resources, in collaboration with other institutions for the profit of society. In general, the purposes of CESGA are all those that promote the research in and use of HPC, advanced communications, and the development of information and communications technologies as an instrument for sustainable socioeconomic development.

www.cesga.es

#### **CINECA**

CINECA

HLRS

Cineca is the largest Italian supercomputing centre with an HPC environment equipped with cutting-edge technology and highly qualified personnel which cooperates with academia and industrial partners. Cineca's mission is to enable the Italian and European research community to accelerate scientific discovery using HPC resources in a profitable way, exploiting the newest technological advances in HPC, data management, storage systems, tools, services, and expertise at large.

www.cineca.it

#### **HLRS**

established in 1996 as the first German national high-performance computing center, building on a tradition of supercomputing at the University of Stuttgart that stretches back to 1959. As a research institution affiliated with the University of Stuttgart and a founding member of the Gauss Centre for Supercomputing — the alliance of Germany's three national supercomputing centers — HLRS provides state-of-the-art HPC services to academic users and industry. HLRS operates one of Europe's most powerful supercomputers, provides advanced training in HPC programming and simulation, and conducts research to address key problems facing the future of supercomputing.

The High-Performance Computing Center Stuttgart (HLRS) was

www.hlrs.de

#### Scapos AG

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Scapos AG is a German SME. Its business is the distribution of advanced software solutions, particularly from research and academic institutes. Its product portfolio includes optimisation software, computer-aided engineering, and libraries for HPC. Its worldwide customers range from industrial corporations and large research institutes to SMEs. Its activities in HPC R&D projects complement the above and target service provision and the development of new business opportunities. WWW.Scapos.com

#### TERATEC



TERATEC is a non-profit European pillar of expertise in HPC, numerical simulation, and Data Analytics, and brings together more than eighty technological and industrial companies, laboratories and research centres, and universities that wish to combine their resources in the strategic field of HPC and simulation. It forms the core of a Research & Development technology park and is a member of the "SYSTEMATIC Paris Region" industrial cluster.

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**price**intelligence

parsionate.



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## AI/ML Computer Vision for the Next Generation Poultry Farms

#### **Organizations**

Radinovic Company and Meso-Promet-Franca are well-recognised Montenegrin SMEs in the agri-food sector and poultry industry. DigitalSmart is a Montenegrin start-up SME targeting digital innovation and smart solutions based on AI. DunavNET is an ISV from Serbia and is an expert in implementing and integrating IoT/AI solutions in agriculture. The University of Donja Gorica is part of the NCC Montenegro and an HPC expert who provided support for experiment implementation and engagement of domain experts.



University of Donja Gorica is part of the NCC Montenegro.

#### The Challenge

Monitoring chickens on large farms is highly labor-intensive and costly. Raising chicken to ensure animal well-being as well as humane food production means to closely monitor environmental conditions: measuring air temperature, air humidity, CO<sub>2</sub>, and ammonia levels is required as a basis for successful production. Al and ML can be utilised to develop computer vision sensors that can monitor parameters. However, training, selecting, and calibrating the prediction models using only a standard computer was extremely slow and tedious.





#### **The Solution**

Al and ML algorithms were used to create prediction models, which could indicate the appearance of certain diseases. The involved organisations utilised HPC to efficiently apply DL to train and later calibrate prediction models. This led to the creation of a new type of precision agriculture sensor that combines cameras, edge computing, and an IoT platform. Models are calibrated for specific end-users and achieve an accuracy of over g0% for chicken detection and segmentation. Such IoT devices, enhanced with edge Al capabilities and new prediction models, represent new building blocks for advanced smart agriculture solutions for the poultry industry.

The smart agriculture solution developed within this experiment could boost the productivity of poultry farms by reducing both manual labor costs and chicken mortality rates by about 10% each. For SME farms such as Radinovic Company and Meso-promet these savings could exceed hundreds of thousands of Euros annually. This is accomplished because assessing the weight of chickens in real-time increases the uniformity of the finished product and reduces the impact of stress on both the chickens and manual labor. Furthermore, real-time insight into poultry barns allow the improvement of disease management due to early detection.

HPC provied the organisations DunavNET and DigitSmart with the technology needed to deveop smart agriculture solutions quickly and efficiently using ML and computer vision, in this case for the needs of the poultry industry. The computer kit has become a part of their PoultryNET platform offering, and there is an opportunity to sell such components to third-party vendors active in the market of smart agriculture solutions.

- Reduce both manual labor costs and chicken mortality rate by 10%.
- More than 10-fold speed-up of predictive model generation with HPC empowers SMEs to quickly commercialise customised solutions for customers.
- Quicker detection of disease or abnormalities led to improved animal well-being and better agrifood product quality.
- Better management of carcass disposal, dead chicken detection, and lower greenhouse gas emissions.

*f*fEuroHPC

Leveraging HPC for AI and Deep Learning Powered Solutions for Asset Management

#### **Organizations**

AXYON AI is an Italian fintech SME on a mission to bring AIpowered predictive value to the investment management industry. UNIMORE - AImageLab is a research laboratory of the Dipartimento di Ingegneria "Enzo Ferrari" at the University of Modena and Reggio Emilia. CINECA is the largest Italian supercomputing centre with an HPC environment equipped with cutting-edge technology and highly qualified personnel which cooperates with academia and industrial partners.

End User

Research Centre

🕅 AXYON.AI





HPC Centre & Provider

EUROCC

CINECA is part of the NCC Italy.

#### The Challenge

Optimising financial portfolios composed of assets like stocks, bonds, and indices with respect to revenue and risk is a core task in the financial industry. Banks, asset managers, and hedge funds face a continually increasing amount of data that needs to be considered for optimal results. Al-based methods offer a predictive power superior to commonly used purely quantitative approaches and represent a tremendous opportunity for highly innovative fintech companies to provide such solutions to the finance industry and bring portfolio risk assessment to a new level.





#### **The Solution**

The development of AI/DL-based models to support asset management brings rigorousness and automation to the models that guide better investment choices and support the creation of risk management tools. These tools in turn contribute to the entire system's stability and reduce investors' risks. With the HPC infrastructure boosting the computation scalability of the ML platform, Axyon IRIS® was further developed to support investment strategies with over 1,000 financial assets.

With the enhanced offering developed during the experiment, Axyon AI can expand its market reach to a wider array of customers, especially SME customers that need a complete, end-to-end solution. In detail, the following main business impacts for Axyon AI were achieved:

- Increased computational scalability of the company's ML platform allowed Axyon AI to train larger ML models on larger datasets (1 order of magnitude) and lower costs (approximately 25% of cost savings).
- Enhanced Axyon IRIS® risk management features for end-to-end portfolio construction resulted in a larger market target (approx. 150% increase of the serviceable obtainable market).
- Improved adaptability of Axyon IRIS® forecasting models decreased the time needed for the model retraining by around 30%, an important improvement in a fast-changing market scenario.

- Approximately 25% of product cost savings.
- Ability to train Al models with over
   1,000 financial assets instead of 100, resulting in a larger approachable market.
- Due to the enhanced product features, improved company positioning in the market:
- generation of new sales opportunities (a 30% increase in leads generation expected) and contributing to the completion of a €1.6m fundraising round in July 2022.



#### Organizations

Parsionate GmbH is a consulting company in the field of digitalization, data analytics/science and data management. Price Intelligence GmbH focuses on the collection and analysis of e-commerce market data and resulting actions, providing SMEs with data analytics for automated decision-making. German Top Secure provides industry-leading hardware infrastructures and software PaaS to organizations. HLRS, University of Stuttgart is one of the three national supercomputing centres in Germany. SICOS BW supports SMEs in accessing simulation and HPC as well as big data and smart data topics.



HLRS and SICOS BW are part of the NCC Germany.

GCS

#### The Challenge

The E-commerce market is growing rapidly. It is becoming increasingly complex to decide on the right assortment and pricing of products and to identify innovations, trends, and counterfeits. In the past, this comparison was done using unique identifiers like the EAN (European Article Number) or Manufacturer Part Number. Since many platforms have disabled the EAN or MPN search functions, a new product-matching method had to be found. For this purpose, image or textual data from product descriptions could be used, but the combination of both in a single search approach would enable the creation of a more reliable and powerful model for product identification and comparison.





#### **The Solution**

Pre-processing was done to transform product data into so-called embedding vectors. The key tool for computing embedding vectors is neural networks, and pre-trained networks based on generic data are an important and valuable building block. Price Intelligence created pre-trained networks for both image and textual data in isolation that could be employed to implement a synthesized algorithmic approach to build networks pre-trained with a combination of all data. For customers, pre-built networks will subsequently be customised using the customer's product data and also related product data to generate better embedding vectors, fitted to the specific use cases, and thereby producing better matching results.

The newly created matching service decisively expands the existing software of Price Intelligence and will be available to over 100 European manufacturers and retailers to help them optimize their pricing and, as an example of a new feature, even optimize their portfolio. The matching service is already being used productively by two retail customers within a web store and call centre to optimize their suggestion system for alternative products. Price Intelligence has already identified many other potential customers from various industries. The knowledge gathered in the experiment can be used to create other new services such as assortment analysis, detection of product trends, or detection of counterfeit products using similar techniques. Due to the wide range of projects in which the two partners Price Intelligence and Parsionate are involved, many companies in Europe will benefit from the capabilities developed in the experiment.

- End customers from retail and manufacturing use over 70% less time when searching and comparing items on the internet.
- With the new product matching service in the Price Intelligence software, an increase in sales of up to 30% is expected.
- The newly developed matching service for finding similar products in an assortment has already led to new sales at Parsionate.



Robust Power System Maintenance Planning via Stochastic Optimization and HPC

#### Organizations

Artelys is a French SME specializing in applying data science, artificial intelligence, mathematical modelling, and numerical optimisation to the analysis of power systems. INRIA-Aviz Team is a worldwide renowned research group specializing in big and unstructured data visualization. INRIA also provides the HPC resources for this project.



HPC & Technology Provider

**4** Artelys OPTIMIZATION SOLUTION:



#### The Challenge

Shutting down a power plant or transmission line for maintenance likely means having to rely on more expensive energy sources or external energy providers. Moreover, as the installed capacities of renewable energy sources grow and electric mobility options are deployed, the overall system becomes more subject to uncertainties. As such it is of prime interest to develop tools to ensure that maintenance plans are prepared for a number of scenarios.





#### Industry Sector: Energy Technology used: HPC, Monte Carlo Simulations



Find out more

#### **The Solution**

Solving the problem required creating a representative data set for the European power system. Massive scenarios were simulated and optimised. For every candidate maintenance plan, various plausible, yet unknown scenarios were generated. The results of simulations were combined to compute KPIs for maintenance plans. During computation, the KPIs were fed back into an optimisation model which computed the next candidate maintenance plan. This process was repeated until all potential plans in a greedy approach were exhausted or until convergence was achieved in the case of local optimisation.

This approach will help power producers and transmission system operators schedule their maintenance in a manner that is resilient to uncertainties. By finding optimal maintenance timing, they will reduce the risk of having to resort to external market players or minimize this cost and reduce the risk of potential demand curtailment situations. Optimal scheduling of maintenance can prevent the need to resort to more polluting assets to compensate for the limited availability of other power generation assets. Artelys gained the ability to conduct quantitative prospective studies on behalf of its clients for a large number of scenarios that cover uncertainties. It is expected that the results will contribute to as much as €4 million in revenue in the upcoming years through performing this new type of prospective study. Artelys bundle the HPC-based optimisation with their portfolio of optimisation software available to more advanced customers. This work also has societal impacts as it will help key players

make better use of the power system, which in the end sums up to better usage of renewable energy generation resources and a lower cost of electricity.

- Estimated additional sales of up to €4 million over the next 5 years.
- HPC-based computational tools enable 3 quantitative studies per year (previously infeasible) and accelerate and improve up to 5 other studies per year.
- Improved calculation capabilities in Artelys software for experienced users.



## HPC-Based Navigation System for Marine Litter Hunting



#### **Organizations**

Green Tech Solution s.r.l. is a Start-up focused on the digital integration of ICT, AI and UV. University of Naples Parthenope is a public Italian university with a background in the science of navigation, maritime economy, computer science, computer vision. BI-REX is one of the 8 Italian Competence Centres with a specific focus on Big Data, innovation processes, and the adoption of enabling technologies. CINECA is the largest Italian HPC centre and cooperates with academia and industrial partners.



#### The Challenge

Marine litter is a problem for the planet. Green Tech Solution sets out to automate the collection of marine litter by integrating Neural Networks and Deep Learning logic into its existing approach. The existing solution consisted of the use of an Unmanned Aerial Vehicle (UAV) to monitor the litter. The inaccuracy of the predicted litter speed and direction forced the UAV to remain close to the litter before its collection by a catamaran to monitor any possible changes in its position. The existing recovery strategy only focussed on one piece of litter at a time and led to long recovery paths and times for the catamaran.



#### **The Solution**

EUROCC

The new HPC-based approach "Litter Hunter" predicts the litter's various trajectories and thus calculates an optimised recovery trajectory through the use of two neural networks and a newly developed multi-objective optimization algorithm. The first neural network acquires the aerial images of waste objects as input, identifies the position, and classifies them in terms of size, materials, and buoyancy level, while a second neural network predicts the trajectories of the observed litter by combining this information with meteorological and oceanographic data. An algorithm uses the predicted trajectories to compute the 'best' trajectory to be followed by the catamaran to collect the most litter while minimising time and distance.

The service now allows an area of 1 km<sup>2</sup> to be covered in a single operation and about 100-200 pieces of waste to be collected. As the neural networks improve over the years due to Reinforcement Learning, the system is estimated to allow up to 1,000 floating objects (>25 mm) to be automatically collected per km<sup>2</sup> of the area in a single day of operation (expected by 2025). The following are the main identified guidelines of the business strategy:

- 4 sales packages (duration min. 1 month / max. 6 months) designed to optimize the cost per contact with the customer.
- Focussing on the investment in drones and boat systems in the 3rd year (reaching 25 available systems) will increase commercial activity.
- Optimization of the services, prices, and fleet management cost will generate a different value proposition in comparison to potential competitors.

Maritime municipalities will reduce cleaning costs by up to 80%. In the medium term, municipalities will benefit from a platform to predict floating waste on a local scale and improve their environmental planning. The new service will enable the recovery of tonnes of plastic or other materials from the sea for recycling.

- An estimated 60% reduction in energy consumption of vehicle batteries used per km<sup>2</sup> of operation.
- A reduction of 80% in time-to-planning, 50% in time-torecovery and 40% in maintenance costs.
- A price for services of €2k-3k per km of road.
- Market expansion outside Italy, reaching 2,000 km of EU coastline served (Greece, Spain and Norway) in the next 5-6 years.



## **AI-Aided Wind Flow** and Gas Dispersion Simulations in Cities

#### **Organizations**

Bettair Cities S.L. is a Spanish SME focused on deploying hyper-local real-time air quality monitoring networks in cities that identify the sources of pollution street by street to provide actionable information to the different stakeholders. Barcelona Supercomputing Center was established in 2005 and serves as the national supercomputing facility. Its mission is to research, develop and manage information technologies to facilitate scientific progress.



HPC Centre & Provider





EuroCC S P A I N

Barcelona Supercomputing Center is part of the NCC Spain

#### The Challenge

Urban air quality is influenced by complex atmospheric dynamics, urban geometry, land use, and traffic patterns, leading to very different pollutant distributions at microscales. As a consequence, any high-accuracy air quality map needs to use either a very dense network of sensors that measures pollution in real-time and/or high computational resources to process the data and model the distribution of pollutants with high spatial and temporal resolution.









Using 30 3D models of 1km<sup>2</sup> areas of real urban geometries from European capitals as a basis, a dataset of approximately 30,000 256 m x 256 m areas was built. These urban geometries were used to perform CFD simulations of the wind flow for three different wind directions and the pollutant dispersion generated by traffic with a high spatial resolution. Deep Neural Networks were trained to learn the results of these simulations at different heights. Using AI models, simulations of new urban geometries can now be performed instantaneously with high precision. These models have been added to Bettair's platform to provide information about air quality and local emissions in real time.

Bettair's ultimate aim is to help improve the air quality in local communities by providing accurate and actionable information. Organisations want to raise awareness and work together with stakeholders to create policies and push initiatives that improve air quality. As a result of this experiment, Bettair has created an energy and computationally efficient low-cost AI solution to model air quality in cities with up to 1 m<sup>2</sup> resolution, in near real-time. This type of precision and resolution is currently out of reach for any competitor due to the computational requirements of the CFD simulations with scientific software. The cost of the service provided by Bettair is up to 95% lower than the competitors with similar spatial resolution and runs in real-time. The expected revenue for this year will be two or three times higher because of the new service. Bettair is able to combine sensor measurements with AI simulations and extract precise information about the local emissions and pollutant concentrations in the cities. This information is then made available on Bettair's platform and enables individuals and communities to take collective actions to improve air quality for everyone. These solutions are already being tested in big cities (e.g. Rome) and smaller cities (e.g. El Prat de Llobregat).

- The simulation cost per km<sup>2</sup> is reduced from €1,850 to less than €1,00.
- The spatial resolution of the real-time modeling capabilities is enhanced from  $100 \text{ m}^2$  to  $1 \text{ m}^2$ .
- The experimental setup time for new cities is reduced by 80%.
- Access to new markets: municipalities and regional governments that could not afford classical modeling before.



## **A Pediatric Simulated Dosimetry Platform** for Clinical Use

#### **Organizations**

IKH is an SME and a regional leader in large-scale ICT solutions in the fields of: Digital Government, Digital Health, and Industrial Innovation & Robotics. **BIOEMTECH** is an SME in the field of biomedical engineering offering hardware solutions for medical imaging and dosimetry applications. **GRNET** provides networking and cloud computing services to a broad range of public and private sectors.



Domain Expert & End User



GRNET is part of the NCC Greece.

EURO

#### The Challenge

Radiation dose calculations from radiopharmaceuticals in nuclear imaging have been a challenge to the scientific community and clinicians, as no commercial solutions for personalised dosimetry existed previously. In clinical practice, there are only rough estimations of the administered dose that a child should receive. Obtaining improved dosimetry protocols for children is difficult through standard clinical practices such as experimental dosimetry and validation. Current solutions and the traditional approaches lack personalisation of dose assessment on a patient basis.





#### The Solution

The involved organisations exploited all the appropriate tools for creating a precise dosimetry software, which allow clinicians to assess internal dosimetry and optimise Nuclear Medical imaging clinical protocols toward personalised medicine. By employing HPC resources, a speedup by a factor of 80 was achieved, permitting a high level of accuracy in predicting the absorbed doses of radiation in organs. A predictive dosimetry model based on ML algorithms was developed and trained with computed results, permitting an individual dose calculation for each new patient, taking into account personalised anatomical characteristics.

PediDose is expected to strengthen IKH and BIOEMTECH in the EU industry of medical software and provide these SMEs with great advantages.

PediDose has been technically integrated into the evorad® suite, a competitive software for medical imaging. After further maturation and obtaining the CE Mark and FDA approval, this add-on is expected to generate additional net income for IKH of about €1,25 m within the next five years. PediDose will be offered on a license basis to other vendors of medical software. Further business opportunities are anticipated in an extension of the approach for adult patients or specific groups like obese patients or pregnant women. PediDose will permit BIOEMTECH to enter the medical software market through a business partnership with IKH and utilise the existing customers of BIOEMTECH's imaging devices for extending its portfolio.

Personalised dosimetry supported by PediDose can lower administered doses and minimize radiation's harmful effects for a very large number of treated children. The proposed solution provides a great potential for expansion to other patient groups.

- Significant strengthening of the value proposition for IKH's product Evorad® achieved.
- €1,25 m additional total income expected through increased sales of **Evorad**®
- Medical market entry for BIOEMTECH facilitated through a partnership with IKH.



## Advanced HPC Based Drug Discovery with Converged Deep Physics and Al



Industry Sector: Healthcare Technology used: HPC, ML, AI, Molecular Dynamics Simulations

#### Find out more



#### **The Solution**

The involved organisations conceived a drug discovery strategy and toolchain focused on small molecules targeting novel proteins. Al algorithms generated novel molecules, and high-end calculations predicted how the compounds bind to challenging targets. The combined technology can speed up the drug design process and improved the quality of the generated compounds, thereby improving the entire drug discovery process. The combined workflow was applied to a target USP7, involved in cancer pathways. Progress in the drug discovery stage for this target could lead to drugs for various kinds of cancer.

The newly developed in silico framework for drug discovery has the potential to cut drug discovery time and reduce overall drug development costs, which leads to savings of several million Euros. As time constraints and agility become crucial in the pharmaceutical industry, a new service offered through Iktos and based on this framework will be a competitive advantage in a challenging market and represent an unrivalled product especially for hard-to-drug targets.

Additionally, the novel hit families of drugs targeting USP7 already discovered during the experiment will support the two SMEs' internal drug discovery pipeline. An estimated €2 Million will further be invested to bring these hit families to the pre-candidate stage. Having successfully reached that stage, the SMEs will be able to enter into a licensing agreement with pharma companies. Qubit Pharmaceuticals intends to use the new toolchain in further in-house drug discovery programs promising high profit by exploiting considerably increased success rates (40% vs 10%) enabled by the newly developed technology.

- A unique physicsbased AI-assisted workflow cuts the drug discovery time by 25% and reduces the cost of drug development by 20%.
- Novel, highly profitable services to be offered by the SMEs.
- Discovered promising compounds which could lead to new cancer drugs, potentially generating substantial income for the SMEs far beyond the invested sums.

**Organizations** 

**Iktos** is a French start-up SME specialising in AI applied to drug discovery. Iktos has developed a retro-synthesis algorithm and generative AI for drug design. **Qubit Pharmaceuticals** is a French start-up SME specialised in physics-based simulations for drug discovery. Using advanced simulation software and AI-enhanced medicinal chemistry, the company develops novel drug candidates and identifies their modes of action against challenging targets.

End User

Domain Expert

IKTÔS



#### The Challenge

The discovery phase of new drugs can be costly, time-consuming and is often covered by specialised companies. Computer-aided drug design has emerged as a new in silico method for the discovery stage and many SMEs are competing in this field. The tendency is to outsource the research effort outside of pharma companies to contract research organisations. The SMEs Iktos and Qubit Pharmaceuticals, are part of this ecosystem and help many pharma companies advance their research projects.





Cloud-Based HPC Platform to Support Systemic-Pulmonary Shunting Procedures

#### **Organizations**

InSilicoTrials Technologies SpA is an SME that promotes innovation and commercializes in silico tools for healthcare through a cloud-based platform. RBF Morph is an ISV that develops the RBF Morph software and an expert in CFD and FEA. Fondazione Toscana Gabriele Monasterio is a healthcare public entity and a leader in the field of

cardiology. **RINA Consulting** provides a wide range of services covering the whole project life cycle, site engineering and maintenance management. **CINECA** is an Italian HPC centre equipped with cutting-edge technology and cooperates with academia and industrial partners.



#### The Challenge

The experiment consortium decided to work in the challenging field of Congenital Heart Disease. Without the ability to alter the prevalence of CHD, interventions and resources must be focused on improving survival and quality of life. In this context, the Modified Blalock Taussig Shunt (mBTS) is the most common palliative operation performed but is associated with significant morbidity and mortality. A simulation of effects could support the medical decision, yet this requires substantial know-how and computing power, in order to provide high-quality results and the subsequent surgery in a short timeframe.







Find out more

#### **The Solution**

The partners generated an affordable decision support web application Copernicus that, thanks to a medical digital twin (MDT), allows surgeons to optimally approach the mBTS medical intervention. Copernicus circumvents problems by generating the MDT through a Reduced Order Model of a patient-specific vascular district, condensing complex computations can be used interactively to vary its dimension and positioning. With a dedicated user interface, the medical staff is thus able to inspect the MDT of the patient and observe how the shunting layout influences the fluid dynamics of the involved impacted area, helping to finalise the decisions on surgical intervention.

The impact of the solution proposed by Copernicus at the clinical level is highly relevant: The combination of speed and interactivity permits surgeons to find the best treatment option for CDT, thus lowering the incidence of post-surgery complications and reoccurrence, leading to a decrease in the days of hospitalisation of treated patients and related costs. For Fondazione Toscana Gabriele Monasterio, this could mean savings in the order of over €100k per year. InSilicoTrials Technologies will add the tool to its portfolio, pursue certification for clinical use, and commercialise it on the market through a SaaS approach, with shares held by RBF Morph and RINA-C, and using CINECA's HPC system as a backend. In addition, both RBF Morph and RINA-C will use the results to increase their presence in the healthcare market: RBF Morph by offering new functionalities in their software library, and RINA-C by offering consulting services backed by hardware and software leasing to medical device manufacturers and medical research clinics.

- IST: Generating an increase in annual revenue of about €450k after 4 years.
- Clinicians: Surgery outcome improved, reducing hospitalization per patient by 5-6 days.
   FTGM: savings of more than €100k per year are expected.
- RBF: Expected increased annual revenue 4 years after the experiment is €250k, additional 2 qualified jobs/year.
- RINA-C: Expected increased annual revenue 4 years after the experiment is €200k.

High-Performance Computing Enhances Treatment Precision in Breast Cancer

#### **Organizations**

**CHOSA** is a UK SME developing techniques to predict outcomes of treatments with anticancer drugs in patients using molecular models based on data from cell cultures exposed to drugs and selling this as a service to health providers. **AH-HMU** from the Hellenic Mediterranean University has a deep experience in molecular pharmacology and cancer biomarker identification. **JADBio** is an SME developing the JADBio automated ML platform for biomedical tasks, providing life-science professionals with effective analysis of molecular and clinical data with an accessible user interface.

End User

CHOSA



Technology Expert

JADBio<sup>®</sup>

#### The Challenge

Breast cancer is a major health issue and many cancer patients fail to respond to the treatment. Lack of efficacy is mainly attributed to tumour variations at the genetic and molecular level, which clinical practice struggles to address. The emergence of new genomic technology combined with digitalization has delivered treatment regimens that assess the DNA, RNA, protein, and metabolites in the individual patient's tumour and integrate those into therapeutic decision-making. Current technologies focusing on just one or a few genetic biomarkers or using complex ex vivo laboratory tumour models are predictive of treatment outcomes only in highly selected cases.

### JADBio\*





#### **The Solution**

Using JADBio's tools and employing HPC resources, a huge amount of data on drug-like chemical compounds was processed to create ML models predicting the efficacy of drug candidates in cancer treatments. 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. After clinical validation, the models will be used to set up a complete platform to predict the efficacy of different cancer drugs for each individual patient, based on their biopsy readings. Clinicians will receive a report listing a number of relevant drugs that highlight those most likely to work for a given patient's cancer.

At the moment, no similar solutions exist and therefore the resulting product AIDA has the opportunity to become a firstin-market product that can truly revolutionize the way cancer patients are treated. With a breast cancer incidence of over 780,000 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 €3k per service. Beyond those initial targets, the business model is highly scalable and the system can be applied to any tumour 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 HPCbased 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.

- CHOSA targeting a USP in a market worth €69 million in Germany and Nordic countries leads to an expected additional revenue of several million Euro from mid-2024.
- More cancer patients with limited disease get the right treatment which could be lifesaving.
- More cancer
  patients with
  advanced disease
  live longer by
  avoiding ineffective
  treatments.



AI-Platform for Automated Training of Object Detection Models Based on CAD Data

#### **Organizations**

Gabler Engineering GmbH is a production SME working in the design and manufacturing of production machines, especially confectionery machines and pharma production lines. Kimoknow UG is an expert in object detection with cameras, based on deep learning models. SolidLine GmbH is a sales and engineering company for CAD products from Dassault Systèmes. The company is an expert in 3D CAD software, CAD model databases, and product lifecycle management solutions. Karlsruher Institute of Technology is one of the biggest science institutions in Europe and owns HPC infrastructure.



#### The Challenge

The manual assembly of devices consisting of many individual parts is a time-consuming, tedious and error-prone industrial process, which could be supported by automated recognition technologies. Currently, only a few specific industrial applications such as autonomous robots or mass production quality control can benefit. Applications such as warehouse part detection, where one is dealing with thousands of individual parts, are still not economically feasible. The part identification process could be assisted through automated object detection within an Augmented Reality (AR) application which outputs a list of potential candidates that limits the number of objects to check.





#### Industry Sector: Manufacturing Technology used: HPC, AI, ML



Find out more

#### The Solution

To make object detection for large datasets of industrial parts possible, Kimoknow maximized the automation of AI training. The approach for automatic AI training entails generating synthetic images from 3D CAD data and then using datasets to train an object recognition model. The solution is service-based and can be scaled modularly to available computing resources. The reduced time to generate an AI model allows very quick delivery to a customer and fast, cost-effective fine-tuning of the results.

End-users of the Kimoknow AI detection system can enable their staff to be more efficient and to work in increasingly complex environments. Therefore, jobs can be preserved as staff becomes more effective, and workers can be hired to do difficult tasks without extensive training. The infrastructure built during the experiment provides Kimoknow with a business model that is highly scalable and can be backed by a cost-effective and energy-efficient HPC backend for the batched creation of fine-tuned object detection models in reduced time. This serves the longterm business goal of Kimoknow to provide object detection services, where users can easily train object detection models based on their CAD data. Production and logistics companies such as Gabler Engineering benefit from Kimoknow services as they can generate object detection models for their own data with very low manual effort and implement object detection applications much more cost-effectively, thus creating AR tools to substantially improve their processes. Companies that are new to AI-object detection can see

results for their own use cases and therefore the entry

barriers to new applications are significantly lowered.

- Reduction of manual effort from more than 800 hours to less than 10 minutes for generation of an AI model of more than 1,000 parts.
- Kimoknow can
  offer AI applications
  previously economically
  unfeasible.
- Kimoknow is able to provide services to thousands of customers at once.
- Gabler can save several work hours each day through reduced search times, resulting in higher productivity and guality.



## **Multiphysics and Multiscale Modelling** of Aeronautical Components

#### **Organizations**

Manta Group is an Italian SME that operates in the aeronautical field and specializes in the production of composite aircraft parts. CETMA is the technology expert, a private Research and Technology organization, which has acquired skills and know-how focused on composite materials and numerical modelling of these advanced materials and their manufacturing processes. CINECA is the largest Italian supercomputing centre with an HPC environment equipped with cutting-edge technology and highly gualified personnel which cooperates with academia and industrial partners.



Technology Expert HPC Centre & Provider



CETMA



#### EUROCC CINECA is part of the NCC Italy.

#### The Challenge

Autoclave moulding is the main fabrication method for composites used in the aerospace field. Working with innovative materials and geometries and (or together with) the rising mechanical stresses during the curing process lead to an increased number of defects and voids in the finished components which then are rejected. During the curing process, the mechanical stresses in the various materials rise. Currently, an expensive trial-anderror approach is used to find the optimal process parameters to produce complexshaped components while minimizing the risk of voids or geometric distortions, which leads to long development times and high costs.





#### Manufacturing Technoloav used HPC. FEM Simulation



Find out more

#### **The Solution**

To optimize the autoclave process parameters, the different phenomena during the curing process need to be simulated to predict the parameters' effects on the quality of the components to be manufactured. To this end, two separate multiphysics and multiscale numerical models were set up and validated. Using the material properties, the lamination sequence, the geometry of the parts, and the specification of the autoclave curing cycle as input parameters, the HPC simulations proved to be able to provide the required information about the resulting part distortion and possible defects in the finished part in a very short amount of time.

Thanks to this simulation experiment called MULCOM, MANTA now uses HPC-based simulations to produce highquality composite components, reducing development time and costs while increasing its competitiveness. Since autoclave moulding will remain the main manufacturing technology of aerospace structures at least for the next 10 years, this significantly strengthens Manta Group's business position.

In addition, the improved autoclave process know-how can enable MANTA to profitably enter many other sectors besides aerospace (e.g. luxury boats, automotive, sport). All this helps to attract new customers by offering a full service, from design to the production of the component. The expected business impact has been quantified at €1million three years after the end of the experiment.

- MANTA: Design costs reduced by up to 50% (about €100k saving per year), material waste by 70% (about €60k saving per year), and raw materials usage by 15% (about €150k saving per year).
- CETMA: expects to join new R&D projects and consultancy services with an increase in its revenue of about €50k per year.
- CINECA aims to become MANTA's provider of HPC resources estimating its related increased revenue to €20k per year.



Multi-Head Additive Manufacturing with Optimal HPC Thermal Stabilization

#### **Organizations**

**Mikrotvornica Ltd.** is a Croatian SME that has extensive experience with different additive and digital manufacturing technologies and sells 3D printers.

**Ruđer Bošković Institute** is regarded as Croatia's leading scientific institute in the natural and biomedical sciences as well as marine and environmental research.



Ruđer Bošković Institute is a part of the NCC Croatia.

#### The Challenge

When using industrial machines for additive manufacturing, heat and its dissipation to individual structural elements of the machine play a major role. A heated workspace inside a 3D printer is important because most materials used in industry require heated work chambers to work with. Problems with the heat distribution inside the 3D printer can lead to void formation, geometrical deformation or poor interlayer bonding in the printed pieces. Mikrotvornica's aim was to understand what effect temperature distribution and different possibilities for generating a high temperature inside the chamber have on the printer itself and on the final 3D-printed pieces.





#### Industry Sector: Manufacturing Technology used HPC, CFD Simulation



Find out more

#### **The Solution**

The impact of heat on the structure and motion system of the 3D printer was predicted using a numerical simulation model for the 3D printer. The 3D geometry files for the different parts were generated and boundary conditions and material parameters were set up. Simulations were performed incorporating the unsteady process while the printer chamber heats up and different parts move. The CFD had a run time of 3-4 days and could be used in the development and production process of new machines or to find the correct temperature setting. Several tests on 3D printers were performed to validate the numerical simulations. During tests, the exact temperature values inside the chamber were measured and compared with the results of the numerical simulations.

By using HPC and numerical simulations, delivery times can be shortened significantly by 30-50% leading to a reduction of 15-30% in production costs. This amounts to savings of €150k over a period of three years.

Through the usage of numerical simulations, the accuracy of the 3D printing process is increased and Mikrotvornica can be more competitive on the market with the improved 3D printers. Therefore, it is possible for Mikrotvornica to achieve an increase in sales by 20-30% which can generate €600k more in revenue over a period of 3 years.

By using simulations in development and production Mikrotvornica will create jobs for new highly skilled employees, in order to generate even better results in the future.

- Shortening of product delivery time to the customer by 30-50%.
- Cutting costs in production by 15-30%.
- Greater accuracy of 3D printers expected to increase sales by 20-30%.
- Creation of jobs for new highly skilled employees performing simulations for even better results.



## **Topology Optimization** of Micro-Channel Heat Exchangers

#### **Organizations**

Aidro is an Italian high-tech SME specialized in the design and manufacturing of hydraulic parts and metal devices by both traditional technologies and Additive Manufacturing. **OPTIMAD** was founded in 2006 as a Spin-Off company of the Department of Mechanical and Aerospace Engineering of the Politecnico di Torino and is specialized in the development of numerical simulation codes for scientific computing. CINECA is the largest Italian supercomputing centre with an HPC environment equipped with cutting-edge technology

and highly gualified personnel which cooperates with academia and industrial partners. ISV



HPC Centre & Provider



OPTIMAD



EUROCC

CINECA is part of the NCC Italy.

#### The Challenge

The design of Micro Channel Heat Exchangers (MCHX) requires balancing many competing design constraints, including weight reduction and manufacturability. Topology Optimization (TO) is a promising design paradigm for finding an optimal design that meets all requirements. However, geometries resulting from TO are impossible to manufacture using standard techniques. Instead, the design and production paradigm of combining TO with Additive Manufacturing has enormous potential but requires the solution of key technical challenges to provide accurate results at speeds consistent with industrial design cycles.





Manufacturing Technoloay used: HPC. CFD Simulation





#### The Solution

The TOLOMHE platform was conceptualized and developed as a SaaS platform, which integrates a set of computational tools for topology optimization of MCHX in an HPCcentric framework. TOLOMHE represents the first step towards cloud services for topology optimization methods and generative design offered to SMEs specialized in AM for MCHX. An innovative solution is based on coupling a standard CFD solver, an ML model and a parametrized topology. Thanks to the synergic deployment of the ML model and the CFD solver, multiscale CHT simulations can be performed without the burden of simulating high-resolution models during the online phase.

TOLOMHE represents an easy-to-use platform for generative design and product optimization. The ultimate goal is to alleviate problems and barriers encountered by SMEs specialized in the design of high-performance MCHX. TOLOMHE has the potential to become a technology enabler and will allow a user to target high-value applications, improve the design of existing products, and ultimately increase market competitiveness. Thanks to the adoption of TOLOMHE, the end-users are expected to accelerate the transition from a build-to-print to a build-tospec business model by reducing R&D costs and time-tomarket for new products.

The first applications at Aidro foreseen for the TOLOMHE platform are an oil-air heat exchanger project for the transmission system of helicopters, and a sea water-natural gas heat exchanger project for off-shore gas platforms.

- Automation of the design workflow has the potential to reduce time-to-design by 75%, time-to-market by 50%, and time-toprototype by 90%.
- Aidro: End-user savings can potentially add up to €100k by redirecting skilled labor to other added-value activities.
- OPTIMAD: TOLOMHE can generate a stream of revenue of approx. €250k-500k in the first 36 months.
- CINECA: Sales of CPU cycles can generate up to €40k per year.



## High-Performance Computing for High-Value Weather Forecasts

#### Organizations

Aslogic is a Spanish Engineering SME that develops and co-creates solutions for highly efficient and safe air traffic management. University of Leon is an expert in developing numerical weather forecast models for the aeronautical sector. It has been a technology supplier for the Spanish National Institute of Aeronautical Technology for over 25 years. **CESGA** is a public foundation that provides HPC services for R&D, supporting SMEs to leverage their competitiveness through the usage of HPC.



#### The Challenge

Currently, aeronautical meteorological information is focused on providing the meteorological conditions at departure and arrival airports. Although this is sufficient for conventional aviation, it is not enough for Unmanned Aerial Vehicles (UAVs, so-called 'drones'). Due to their size and flying dynamics, drones are more vulnerable to their surroundings. Hence, one of the main factors to be considered in the operational safety of drones is accurate and reliable weather forecasting throughout the flight path.





Industry Sector: Transportation Technology used: HPC



Find out more

#### The Solution

The experiment addressed the challenge of creating reliable weather forecasts appropriate for drones without expensive ground equipment, creating a solution dubbed HERCULES. The specially equipped weather impervious Meteodrone collected weather information during 150 flights over key locations in Galicia to provide the necessary data for the building of the forecast models. 4 different parametrized Weather Research and Forecasting (WRF) models were provisioned to compute accurate weather predictions in the region of Galicia in a timely manner, using HPC. Lastly, tools and services through the newly developed HERCULES website were provisioned.

HERCULES' solution will enable safe and efficient drone operations by providing operators the capability to obtain dedicated weather forecasts at their flying altitudes without relying on expensive ground infrastructure. This service will be one of the keys to unlocking an emerging sector that is expected to grow by €10 billion annually until 2035. In addition, the live information provided by the Meteodrone could be used to support traditional manned aviation during landing procedures in aerodromes that cannot use ground infrastructure for weather predictions. HERCULES highresolution local weather forecast models have the potential for future business opportunities in other industries – for example, wind energy or fishing in which accurate weather prediction could positively impact safety and efficiency.

- High-resolution weather forecast without relying on ground infrastructure (saving €100k), providing capabilities to characterize atmospheric conditions at any location.
- A weather forecast optimised for UAVs can increase operational efficiency and safety.
- Using a subscription model, HERCULES could reach 2,000 users in the next 3 years with an expected revenue of €78k per year for Aslogic.



HPC Vessel Maintenance Optimization by Natural Language Assistance

#### **Organizations**

FIGAL Innova is a Spanish SME, a leader in marine surveying and maintenance engineering. FIGAL is specialized in assets such as maritime machinery, vessel hulls, containers, in more than 30 countries. SREC Solutions is an SME that offers an expert system platform for setting up Digital Assistants powered by AI and Natural

Language Understanding to use in any connected textual and voice interface. **CESGA** is a public foundation that provides HPC services for R&D, supporting SMEs to leverage their competitiveness through the usage of HPC.



#### The Challenge

In order to improve the maintenance process in the maritime industry and to better integrate it with their overall digitalisation approach, companies are calling for the integration of virtual assistants into their maintenance processes. FIGAL Innova and SREC Solutions developed a Vessel Predictive Maintenance System to monitor and assist a vessel's crew and operators with predictive maintenance of the ship's machinery. However, a virtual assistant must also work in highly noisy environments, increasing the complexity of such command recognition.





#### **The Solution**

A Natural Language Processing system was developed and adapted to a set of the most commonly used commands in the sector, which works reliably in noisy environments. The solution is based on a noise filter that uses a DL technique to identify and train the correct model. Once trained, the model was subsequently integrated with mobile devices for spoken command recognition. After HPC training, the Natural Language Understanding (NLU) algorithm can now correctly work with an accuracy superior to 95% in environments with a noise level of up to 80 dBm using only software.

FIGAL can offer a virtual assistant based on voice commands that have the potential to reduce up to 30% of maritime maintenance costs by shortening their duration by up to 15%, eliminating up to 30% of breakdowns, and reducing harmful maintenance gaps due to insufficient crew knowledge and awareness by up to 20%. SREC owns a proven technology that can be applied to many other sectors. CESGA will use the results for demonstration of the benefits for SMEs of using HPC. SREC and FIGAL are located in a small village far from the high-tech business centres of Europe. The results demonstrated that innovation can be driven by players in rural areas too, and thus that highly-qualified employment is possible in these areas. Marine transportation carries over 90% of the global merchandise trade, totaling 11 billion tons of cargo per year. Hence, the improvements in maritime logistical chains have tangible repercussions in every economic sector. In the short term, they reduce the risk of shortages of essential goods and can contribute to controlling inflation; in the medium to longer term, they could result in acceleration of economic growth, employment, and lower trade costs.

- New robust vessel maintenance assistant can reduce the maintenance costs by 30%.
- SREC expects to apply technology to other sectors, with an increase of incomes of 20% yearly in the next 5 years.
- FIGAL and SREC expect to create 10 jobs in the next 3 years.
- CESGA will use these results to leverage the usage of the HPC and Spanish NCC by Spanish SMEs, increasing the number of SMEs using its infrastructure and services by 10% annually.





EUROHPC Joint Undertaking eurohpc-ju.europa.eu



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For further information, please visit:



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## List of Abbreviations

Al	Artificial Intelligence
AM	Additive Manufacturing
AR	Augmented Reality
CAD	Computer-Aided Design
CFD Simulations	Computational Fluid Dynamics Simulation
CPU	Central Processing Unit
DL	Deep Learning
DNN	Deep Neural Networks
FEM Simulations	Finite Element Method Simulations
GPU	Graphics Processing Unit
HPC	High-Performance Computing
HPDA	High-Performance Data Analytics
ISV	Independent Software Vendor
MC Simulations	Monte Carlo Simulations
ML	Machine Learning
NCC	National Competence Centre
PaaS	Platforms as a Service
SaaS	Software as a Service
SME	Small and Medium Sized Enterprise

