Date Submitted: 01/16/2015 Project Title: High Performance Processing Chain - HPPC Name: Open Ocean Address: 27 rue du chemin vert, 75017 Paris, France Website: www.openocean.Fr Name: Laborbe Position: CTO Email: renaud@openocean.fr Phone: +33 9 7239 0165

What does the company do? (300 words)

Open Ocean develops the Metocean Analytics, the first on-demand meto-ocean study offer.

It is an online support decision making tool for offshore project management and operations

This tools analyse in details atmospheric and oceanic conditions in a simple and intuitive way and provides services such as :

- Resource and energy assessment
- Design loads calculations
- Maintenance planning
- Those services are based on Open Ocean numerical expertise which gathered knowledge in:
- Ocean numerical expertise
- Offshore project requirements
- SaaS provider

Ocean numerical expertise required experience in high performance computing as it needs numerical simulations.

The ocean is discretized on a grid with hundreds of meters of spatial resolution. On each point of the grid, hydrodynamics equation are solved using ocean models developed in worldwide research centres.

Those numerical tools are parallelized (MPI) and generated hundreds of gigabit of data per area of interest. In deed, 20 years of data need to be simulated if you want to capture extreme phenomena.

It can take several months to simulate those data on Open Ocean cluster (2 nodes). Open Ocean is actually involved in the European programme FORTISSIMO to estimate the possibility of BULL cluster on our simulation.

Once the simulations are performed, the bloc of data is then analysed by Open Ocean

statistical toolbox.

In order to provide an on line, on demand tool, the whole Processing chain has been automatized.

This processing chain includes:

Preprocessing

Daily download format of input ocean data (satellite data, in-situ data)

Numerical grid generation

Processing

Ocean data forcing fields format (wind, tide…)

Numerical simulation itself

Post–processing

Numerical simulation Output files format

Statistical analyses of output files. It take several hours to extract a time serie of 20 years of data at a single point of interest. Clients can require an analyse on hundreds of points in case of offshore wind farm for instance. Fast Data access is vital for Open Ocean

Visualisation

Those statistics are then access by the Metocean Analytics user through an user-friendly web interface. It needs to be fast to be a convenient tool.

Project Abstract (150 words)

Ocean can be the answer of today's challenges : Energy (marine and fossile Energy), Food (Fish and Algues) and Health (marine biology).

However, offshore projects are always more challenging (bigger, deeper, and should last longer). On other hand Those projecst are always under budget constraint. Human safety error is no longer acceptable.

Furthermore those projects are continuously evolving with time. This is why Open Ocean

clients need fast and reliable on-line tools.

HPPC project will enable Open Ocean to proposed an online support decision making tool for offshore project management and operations.

This tool will meet offshore project requirements thanks to HPC facilities and will be adress worldwide.

Industrial relevance and potential business impact (250 words)

Offshore projects are always more challenging (bigger, deeper, and should last longer). On other hand they are always under budget constraint and human error is no longer acceptable.

Furthermore those projects are continuously evolving with time. This is why Open Ocean clients need fast and reliable on-line tools.

Open Ocean challenges to meet its client needs are

-Heterogeneous data storage

- Challenging quantity of data
- -long numerical simulation
- long data post processing
- Difficult access to those data through the web interface

Proposed high-level Work Plan (500 words)

Today, Open Ocean needs a global profiling of its whole processing chain This profiling is needed to identify the bottlenecks. Once those bottleneck will be identify, enhancement configuration should be proposed and test.

Hence, Open Ocean will be able answer client constraints from on online solution.

Open Ocean processing chain enhancements includes

- Better parallelisation of numerical simulation (hybrid MPI and openMP for example)
- Parallelised file system
- Adequate databased storage (Hadoop, flat file, NOSQL…)

This program will be splited into 3 phases

Phase 1: Profiling

The profiling of Open Ocean processing chain will be performed on Open Ocean infrastructure. This work is needed to identify the major bottle necks.

Once the bottleneck are identified, sample data and code will be installed on PRACE HPC Cluster to see how they can be solved.

Phase 2: Enhancing

HPC experts will tackle those bottlenecks in order to propose and validate enhancements on PRACE HPC infrastructure

Phase 3:

Those enhancements will be implemented in Open Ocean processing chain which can eventually be moved to better infrastructure.

Final test will be performed

Technical Requirements

- -5 TB of disque space
- parrallel file system
- -diferente file storage system(file, hadooop, NOSql...)
- the possibity for Open Ocean to install in houses codes (scripts and compiled codes)
- Open Ocean has no experience in remote visualisation.
- ssh acces

Business requirement

All the enhancement proposed shall be compatible with a Cloud based SaaS offer. This is required by the innovative Metocean Analytics offer.

Date Submitted: 01/15/2015 Project Title: HPC for Hydrodynamics database creation Name: Principia Address: 215 Voie Ariane Zac Athelia 1 13705 La CIOTAT Cedex France Website: Name: Mr. Rochon Position: Deputy General Manager Email: <u>michel.rochon@principia.fr</u> Phone: (044) 298-1612

What does the company do? (300 words)

PRINCIPIA is a scientific engineering company that performs for large industrial companies, engineering studies and develops and industrializes added-value numerical software solutions.

Principia has about 130 people worldwide, including 100 in France.

Core expertise focus on simulation of complex physics phenomena such as Structural Mechanics, Fluids Dynamics, including hydrodynamics, and coupling such as Fluid/Structure.

PRINCIPIA offer cover the system life cycle: basic design, detailed design, fabrication, installation, operations and dismantling and most of them are done according to appropriate code check.

PRINCIPIA realizes also monitoring project and basin tests campaigns.

PRINCIPIA develops added-value products that capitalizes know-how and R&D results. These products are used internally to perform projects and also distributed with associated services such as training, support, expertise, maintenance and specific developments.

Project Abstract (150 words)

The objective of this experiment is to port and optimise one of our code Diodore on HPC infrastructure in order to improve our Deepline HPC product line which is under construction. DIODORE is a fluid mechanics software designed to solve a large number of problems in ocean engineering (offshore, marine applications ...)

Indeed, Deeplines uses HDB files (Hydrodynamic DataBase) produced by Diodore to make these calculations. By parallelizing this generation, the user would take full advantage of the HPC resources and save time in these studies.

To achieve this project, we will rely on access to PRACE machines, but also on PRACE experts associated to the project for optimization and parallelisation.

Depending on the time remaining, we will apply the same methodology to another of our code Eole, an expert CFD tool able to simulate very complex physics such as multi-phase flows, thermal fluid/solid coupling, fluid/mechanic coupling,...

Industrial relevance and potential business impact (250 words)

Today Principia is in the process of establishing a commercial offer around Deeplines HPC to be available in 2015. In order to enrich some of the key functionalities of this package, we would add the ability to generate the HDB files directly on the cluster. The benefits for the users will be to make best use of their HPC resources by directly calculating HDB files on the cluster, rather than doing it on a separate machine and then transfering it to the cluster (the current generation can take time since calculations are sequential, but also can have a large file).

Principia is strongly motivated by this project and will provide internal resources for working with PRACE experts in order to take benefit and develop internal HPC skills.

Proposed high-level Work Plan (500 words)

Task 1: Profiling and audit of the Diodore Code (HDB module) (PRACE 0,5 PM – PRINCIPIA 1 PM)

Task 2: Definition of the best strategy, optimisation and parallelisation of the modules (PRACE 1PM – Principia 3PM)

Task 3: Performance test on PRACE HPC infrastructure (PRACE 0,5PM– PRINCIPIA 1 PM)

Task 4: Reuse of experience in tasks 1 and 2 for the Eole code in the time available (PRINCIPIA 1 PM)

Hardware needed:

- Access to a x86 based cluster allowing computations using 50 to 100 cores with storage capacities of around 600 GB, with 256 GB ram

- OS : Linux

Software needed :

-The Diodore code is written in Fortran, the HDB files generator of Deeplines is written in Fortran

- Eole is written in Fortran

Technical Requirements

Cluster:

Secure access

Support from PRACE experts for audits and support in optimisation and parallelization

NDA will establishes between Principia and experts who will have access to the code For Eole, use a remote data visualization : Paraview, teclpot, ..

Date submitted: 01/15/2015 Project Title: RAPHI Name: Optimad Address: Via Giacinto Collegno 18, Turin, Italy Website: www.optimad.it Name: Haysam Telib Position: CEO Email: haysam.telib@optimad.it Phone: (347) 958-7410

What does the company do? (300 words)

OPTIMAD develops software for aerodynamic analysis, design and optimization.

The company has been founded in 2006 by a group of researchers in fluid mechanics and enjoys since then the status of being a Spin-Off of the Department of Mechanical and Aerospace Engineering of the Politecnico di Torino. Currently all our technical staff holds a Ph.D. in fluid mechanics, aerospace engineering or similar fields or are enrolled in joint industial-accademic Ph.D. courses.

Nearly every CFD solution nowadays on the market has been originally designed for workstation-like hardware, which are equipped with limited memory and CPU. In order to address complex real-life applications, vendors came up with extremely optimized algorithms, which in turn introduce an overhead in complexity in usage and maintainability. With the advent of HPC resources, the vendors tried to adapt these algorithms to achieve sufficient scalability, not always with satisfactory results.

Within OPTIMAD, we believe that the opportunity provided by large-scale HPC resources, is not simply an (important) increase of computing power in order to address bigger problems. We believe that the real opportunity lies in a change of simulation paradigm:

In this sense Optimad is developing a family of Computational Fluid Dynamics (CFD) solvers, which uses Level Set functions to describe the geometry, adaptive Octree grids and an Immersed Boundary Method. By combining these technologies, a highly automated workflow may be adopted, which in turn enables Cloud-based computations, as no or little user interaction is required, in contrast with the canonical CAE workflow. On the other hand this approach requires superior computing power provided by underlying HPC resources.

Project Abstract (150 words)

When the flowfield is rarefied, for example in atmospheric re-entry vehicles, the continuum hypothesis is not valid any more, and we are obliged to solve the Boltzmann equations (or an approximated version). We chose the BGK equations, which are valid up to moderately rarefied flows. A critical issue is that the solution space is six-dimensional for monoatomic gases and even higher for more complex or reacting gases. The use of HPC resources is mandatory, but still the overall cost is prohibitive.

The structure of the numerical scheme to solve the BGK-equations is of mixed type: stencil type in the physical space and a completely local dependency in the phase space.

Within this project we would like to realize a proof-of-concept with the help of PRACE experts. We aim at demonstrating that through a mixed type of parallelization, a competitive solution in terms of computational time and cost may be derived.

Industrial relevance and potential business impact (250 words)

Rarefied flows are a niche within the entire CFD market and Optimad is one of very few solution providers in this field world-wide. A large number of applications exist, where this type of simulation could play a role analogous to what canonical CFD is for the mechanical industry: space technology (re-entry and satellites), vacuum industry and scientific instrumentation design, to mention just a few.

Nevertheless, the numerical solution of the BGK equations is extremely computational intensive. Due to prohibitive cost of the simulations often alternative paths have been taken in the past in industry. Often the problem has been simplified in order to apply theoretical results, but of course these approaches have a limited span of applicability.

Our preliminary analysis showed that through the adoption of coprocessors (GPUs or Intel Phi) the overall computational cost of the simulations has the potential to be reduced drastically. Optimad however has a limited expertise on co-processors, and therefore the support of PRACE experts will be crucial to progress in this direction.

If a significant performance improvement may be obtained, a unique service may be provided to the industry world-wide. We envisage to develop a cloud based service hosted on HPC-centers, where end-user may connect and upload their geometry and launch their simulation.

To our knowledge no such service is available on the market and consequently this would provide a competitive advantage for Optimad in the field of this advanced application in CFD.

Proposed high-level Work Plan (500 words)

What we need from PRACE is: (i) Access to an infrastructure equipped with the necessary hardware (ii) support in porting the code to the target architecture, and optimizing performances to provide a significant boost towards the assessment of the feasibility of this application.

Although a complete analysis would require comparing what may be obtained with the two competing technologies on the market (NVIDIA GPU and Intel Phi), the necessary effort would exceed the resources available for a SHAPE project, and therefore we will concentrate on porting to Intel Phi, having a simpler instruction set and enhanced portability. If possible, preliminary investigations with GPUs will be made also.

The workplan will be structured in three tasks:

1. Identification of porting strategy (PRACE 0.5 PM)

Together with the PRACE experts the available (C++) code will be analyzed in order to identify the most promising porting strategy to Intel Phi. Furthermore advantages and disadvantages of this architecture will be analyzed in terms of performance, costs, maintenance and

portability.

2. Porting to identified platform and validation (PRACE 1 PM)

The code will be ported to the platform. The work will be done by our developers with the support of PRACE experts. The results of the hybrid code will be compared to the baseline code in order to verify the correctness of the implementation.

3. Benchmarking, analysis and exploitation plans (PRACE 0,5 PM)

The performance characteristics in terms of computational time, and their related costs when going on the market, will be analyzed for a set of different industrial test cases. Based on these results the feasibility of the envisaged cloud-based platform will be verified and a concrete exploitation plan will be identified.

Technical Requirements

1. Hardware

We need a linux x86 cluster, equipped with Intel Phi coprocessors. To our knowledge at least one computing center (CINECA) within the PRACE consortium is equipped with a large scale Phi cluster.

2. Software

In-house C++ code.

3. Remote visualization

Remote Visualization is surely an important asset if available, but it is not strictly necessary for the success of this project. Data are being exported in the VTK format and if a remote visualization facility is readily available we will make use of it. Anyhow the data for visualization are order of magnitudes smaller than the ones used for computation. This is why the data can be transferred and visualized locally.

<u>4. NDA</u>

End-users (Thales Alenia Space and Agilent Technologies) have been contacted in order to have access to real-life test cases within this project. These two companies agreed on providing support to this hopefully successful proposal. In any case, non-disclosure of information and security of data need to be discussed with all partners involved.

Date submitted: 01/14/2015 Project Title: High performance to simulate electromagnetic disruption effects in embedded wiring Name: ALGO'TECH INFORMATIQUE Address: Technopole Izarbel 45 allée Th. Monod 64210 BIDART FRANCE Website: www.algotech-informatique.com Name: Jacques Pere-Laperne Position: CTO Email: j.perelaperne@algotech.fr Phone: ((055) 901-5960

What does the company do? (300 words)

Algo'Tech Informatique proposes:

A full suite of applications dedicated to Electrical CAD. Built around a graphical core tool very powerful, flexible, easy to use, doted with full symbol library and automatic design functions, it proposes dedicated modules as:

-Intelligent recognition of paper diagram,

- Automatic diagram generation

-Embedded wiring and Harness design

This application suite is evolving to support all the product life cycle management from the conception phase in the design office to the manufacturing and maintenance for all electrical and automatism part of the system. It addresses the SMEs market

We propose innovative modules to automate main tasks of the design office. It is based on the formalisation of the key expertise of the design office to produce automatically electrical and automation design from the first requirements.

Algoâ€[™]Tech Informatique also proposes electronic document management system particularly fitted for maintenance operations for facility managers.

Algo'Tech Informatique spend a significant effort in research & development and have always based its success on innovation.

Today one axis of our research is about simulation and mostly around simulation of electromagnetic disruptions in complex systems. In fact Electrical devices have taken on a major role in all types of electrical, automated and embedded systems. Today, the decision to shield or not a cable in response to electromagnetic effect is complex. Simulation became mandatory to obtain a first level of decision.

Thanks to HPC we are able now to compute very large and complex matrixes we have to manipulate to solve these problems.

Project Abstract (150 words)

As mentioned above Electrical devices have taken on a major role in all types of electrical, automated and embedded systems. Cables have thus become a serious issue in terms of safety, on-board weight and hence performance and consumption, as well as cost and reliability.

We are developing a cloud based service that will be accessible simply and directly from user's computer. And we want to go further multiplying variety of wires, increasing their numbers and diversity of environment to get closer to reality. For example in satellite industry electromagnetic specialist has generally to face 10.000 cases of unconformity or risk in term of electromagnetic disruption and to decide how to handle them in less than 2 months Reducing cases by ten or more is the objective thanks to simulation.

That will passed necessarily by an intensive use of HPC

Industrial relevance and potential business impact (250 words)

Electromagnetic effects have very serious consequences in electrical and automatic devices. These problems are growing as total reliance on electrical devices becomes increasingly common in every area: automatic machines, vehicle design, commercial buildings and public facilities, aircraft, trains, drones, robots, etc. In all these fields, European SMEs are offering more and more solutions and are therefore confronted to these problems of electromagnetism.

And the more we will be able to simulate precisely the reality the more impactful the simulator will be. That means an ability to integrate a very large diversity of wires conditions and environment, and to increase significantly their numbers.

All the SMEs working in the field of electricity and/or automated embedded systems face electromagnetic problems that disturb their systems. The problems are not constant; they arise from one to 10 times a year. Today the solutions for overcoming them tend to be empirical. Most often they consist in redesigning the cabling, adding shielding, separating signals, etc.

Using a system that can model electromagnetic effects on PCs connected to HPC centres will make it possible to identify and solve these problems.

The impact will involve:

- Reducing the time required to solve problems (50% improvement)
- Reducing the costs of solving problems (30% improvement)
- Improving customer satisfaction, company image and product reliability.

If we can evaluate that risks during the design process and anticipating them, the time and costs savings will be considerable and impact in term of image and customer satisfaction strongly improved

Proposed high-level Work Plan (500 words)

Today we are working on the following concept:

- The same tool will be used locally on a PC and when remotely connected to a computing centre.

- To users, switching from PC-based computing to remote computing must be virtually transparent.

This implies several consequences:

- ALGO'TECH must review and redesign its simulator so that it can operate just as well locally on a PC as in remote mode.

- ALGO'TECH must develop means of communication between PCs and the remote computing centres (with INRIAâ€[™]s help).

- ALGO'TECH must encompass the entire functionality within Windows-compatible software.

INRIA:

- Provides the Libraries or software elements to be used by ALGO'TECH

- Modifies those Libraries to meet the requirements of (sparse) equation systems in resolving electromagnetism issues.

- Allows FAST access to those Libraries from a PC.

In parallel we are trying to go further to get closer to the reality, modeling a large diversity of cables, included in different environments (more or less conductive wall with variable distance from cable to wall, $\hat{a} \in \{...\}$).

For that we will work in improving models to reduce calculation time on one hand, but use of HPC will be absolutely key. We will have to improve our knowledge, expertise on

- Solver and libraries

-Our Cloud expertise

-Parallelism mechanism

to integrate that in our software to maintain performances at an acceptable level. We will keep the same concept as PC remain the standard display for SMEs.

The work to upgrade the first tool we are working on will consequent

Then later we will need to access to massively parallel machines with the ability to align thousand of cores. It will be in 2 or 3 years from now.

Task 0: Project management

Task 1: To set up based on the different simulation models all requirements in term of hardware and software

Task 2 : Evaluate the modifications to be performed on the current tools

Task 3 : Select right solvers and librairies and specify evolutions needed, evaluate modifications impact on the current tools architecture

Task 4: specify user interface to go transparently from PC to HPC

Task 5: Implement and integrate

Task 6:Start testing and launching measure campains on HPC

Task 7: Package and integrate last simulation models.

Technical Requirements

HW state of the art X86, Os windows, maximum cores will be around 2000

We will need :

Support, expertise, training and know how transfer to really become able in a first phase to

-Mesure all impacts of cloud and master how to develop cloud based applications

-Master parallelism and all its impacts on software architecture

-analyse how to implement most effectively the different models

- Improve our use of HPC in our development

Then we will need HPC time machine and access to very powerful platform where we could access "easily" to thousands of cores to perform our tests and run effectively the simulation.

Date submitted: 01/14/2015
Project Title: HPC-based Design of a Novel Electromagnetic Stirrer for Steel Segment Casting
Name: Ergolines s.r.l.
Address: Area Science Park, Padriciano 99, 34016, Trieste (Italy)
Website: www.ergolines.it
Name: Isabella Mazza
Position: Physicist (R&D Department)
Email: isabella.mazza@ergolines.it
Phone: (040) 375-5417

What does the company do? (300 words)

Ergolines s.r.l. is an Italian SME expert in the design and development of advanced technologies for process control in steel continuous casting. Established in 1998, Ergolines is based in Area Science Park, Trieste (Italy), one of the most important multi-sector Technological and Scientific Parks in Europe. Our mission is to satisfy specific process requirements and to establish a durable technological and strategic partnership with our customers.

Ergolines' core business is represented by the electromagnetic stirrers (EMSs), special electrical machines used in various sections of continuous casting to minimize surface and internal defects of the steel and to increase productivity. Other innovative products for the steel industry include sensors for mold level control, breakout prediction, mold oscillation measurement and ladle-to-tundish slag carry-over monitoring. To guarantee highly reliable results, the Ergolines team has developed a new design and simulation software based on electromagnetic, fluid-dynamic and thermodynamic analysis. These specific tools allow the designers to accurately predict all influences caused by any variation in electric parameters (e.g. current and/or frequency) and process parameters (e.g. casting speed, type of entry-nozzle, etc.).

The philosophy that makes Ergolines unique in its market is its custom-made approach, meaning extreme design flexibility aimed at satisfying the specific engineering requirements of each individual customer, thus offering a technological and strategic partnership. The competitiveness of the company relies on its focus on product customization and growing investment in research and innovation, key factors which determine Ergolinesâ€[™] success at the international level: at present, Ergolines is in fact the third producer of EMSs in the world after the multinational corporations Danieli-Rotelec and ABB.

By drawing on its long-standing expertise in EMSs design and advanced FEM simulations of liquid steel magnetohydrodynamics, Ergolinesâ€[™] profile perfectly matches the proposal tasks and constitutes a robust premise for successful completion of this innovation project.

Project Abstract (150 words)

Electromagnetic stirrers (EMSs) are special electrical machines which improve steel quality by non-contact stirring of liquid steel during continuous casting. The design of EMSs for extremely large formats (diameter > 1000 mm) currently represents a challenging research frontier, addressing the emerging market of "segment casters†: by combining the advantages of ingot end continuous casting, these new-generation steelworks enable high quality casting of huge sections. The design of dedicated EMSs relies on advanced FEM simulations, requiring

very fine discretization and exceptional computational loads, which cannot be managed by Ergolinesâ€[™] internal resources.

SHAPE would provide Ergolines with the HPC technology and specific expertise needed to achieve an ambitious goal: designing a thoroughly new EMS specifically dedicated to the segment casting of very large blooms. The successive engineering and commercialization of this new technology would have a crucial impact Ergolinesâ€[™] growth and competitiveness, while opening key business opportunities at the international level.

Industrial relevance and potential business impact (250 words)

This proposal is envisioned to be of absolute business relevance for Ergolines: participation in the SHAPE would in fact enable the Company to design a new, highly competitive product by taking advantage of state-of-the-art HPC resources, specialized technical expertise and highly reduced R&D costs and time-to-market. Ergolines will also define a business plan addressing the commercial exploitation of the projectâ€[™]s results, including dissemination measures and IP protection issues. Designing an innovative EMS for huge cast sections will in fact represent the premise for the successive industrialization and delivery on the market of a novel technology, featuring a high commercial potential in the growing segment casting industry. Ergolines has in fact been encouraged to develop this novel technology by leading European steelmakers, representing key potential clients. EMSs for very large cast formats are huge and complex custom machines, relying on high-added-value research and technical know-how. The estimated price of one machine being about 0.5 M euros, an envisioned selling volume of one EMS per year would imply a 10% increase of the Company's annual turnover, which currently ranges about 5 M euros. This increase would promote Ergolinesâ€[™] growth and R&D investment, including an increment of 20% in R&D personnel (2-3 units). Successful completion of this project is therefore envisioned to have a decisive impact on Ergolines' growth and competitiveness, opening key business opportunities at the international level. By providing the EU steelmaking industry with high-added-value EMS technology, this project would in turn significantly contribute to boost European competitiveness.

Proposed high-level Work Plan (500 words)

A most critical stage of the steel continuous casting process is represented by the initial solidification of liquid steel: the molten metal is continuously poured into a special, water-cooled copper mold, enabling a highly efficient heat exchange and the consequent formation of a first solidification skin, whose thickness progressively grows along the casting line until complete freezing. Solidification dynamics has a dramatic impact on cast steel quality and therefore needs to be reliably controlled. Electromagnetic stirrers (EMSs) are dedicated electrical machines enabling non-contact stirring of the liquid steel during casting: the EMS generates a varying magnetic field which induces eddy currents into the liquid metal, causing it to rotate along specific paths. EM stirring significantly improves steel quality by enhancing homogeneity and reducing inclusions, thus preventing the formation of defects in the solidified product. Given the complexity of the system and the impossibility to experimentally assess liquid steel fluid dynamics during casting, EMS design necessarily relies on finite elements magnetohydrodynamics (MHD) simulations.

While employment of EMSs in standard cast formats (diameter < 400 mm) is a well-established industrial practice, EM stirring of very large blooms (> 1000 mm) is still in its initial stage and thus requires dedicated R&D investments. In fact, as an alternative to traditional ingot casting, the most recent advancements in the steelmaking industry are paving the way for novel

"segment casters†: by combining the advantages of ingot and continuous casting technologies, these new generation steelworks enable high quality casting of extremely large sections. Designing EMS for these huge formats proves very challenging: a thorough technological customization must be attained by dedicated MHD simulations. Accurate simulations of large formats imply a very fine discretization, requiring exceptional computational times. While having the technological know-how and the scientific competencies to design these special EMSs, Ergolines currently lacks the resources needed to manage the related computational load. Participation in the SHAPE would enable Ergolines to overcome these barriers: by accessing powerful HPC resources and cooperating with expert HPC specialists, the Company would in fact be able to design a new, high-added-value, technological product, while effectively addressing its successive engineering and commercialization. The goal of the project is to design and optimize a highly innovative EMS for the stirring of very large blooms by means of dedicated, HPC-based, MHD simulations. After collaborating with HPC specialists to define a workable solution, Ergolines will elaborate the EMS design following an iterative, multiple-simulation process including: 1) analysis of the geometrical constraints, 2) calculation of the EM performance, 3) fluid dynamic simulation 4) parameter optimization, 5) iteration of steps 2 to 4 until the required EM performance is achieved. Aside the activities related to the simulations, Ergolines will also elaborate a specific business plan, aimed at addressing key commercialization and business issues. This project will thus create the premise for the delivery on the market of a high-added-value, technological product displaying a high commercial potential, which is envisaged to significantly boost Ergolines' competitiveness at the international level while opening unique business opportunities.

Technical Requirements

Technical requirements: as preferred application software, Ergolines uses OpenFOAM for the fulid dynamic simulations and COMSOL Multyphysics for the electromagnetic ones. As the use of HPC for this project is basically required for the fluid dynamic computations, the priority is on OpenFOAM. Concerning hardware architecture, about 100 cores will be required for the simulations, the estimated standard load being 10M elements with 100k elements per core. Ergolines proposes to adopt an ssh-based data transfer protocol, because this choice would conveniently meet basic requirements of speed, ease-of-use and safety. It is envisaged an overall data storage capacity not exceeding 500 GB. No remote data visualization will be required.

Business requirements: as the projectâ€[™]s outcome is the design of a highly innovative product, IP protection measures will be necessary in order to safeguard projectâ€[™]s foreground including key know-how. For this reason, elaboration of a Non-Disclosure Agreement will be required.

Date submitted: 01/14/2015 Project Title: Numerical simulations for plant breeding optimization Name: CybeleTech Address: Campus Teratec, 2 rue de la Piquetterie, 91680 BRUYERES LE CHATEL Website: http://www.cybeletech.com Name: Christian Saguez Position: President Email: contact@cybeletech.com Phone: 33238698028

What does the company do? (300 words)

CybeleTech is a young SME that aims at developing the use of numerical technologies in agriculture. The core products of CybeleTech are based on numerical simulations of plant growth through dedicated biophysical models. This new technology can bring added values at different stages of the agriculture and food chain: in varieties breeding, simulating plant growth can help reducing the amount of field trials by approximately 50% and consequently reduce the time needed to produce a new cultivar. Plant growth simulations are also used to optimize cropping practices, helping farmers to save resources and to maximize yields. Another application is the forecast of yields and production at large scale in order to better anticipate storage and market variations. CybeleTech provides a range of software as a service dedicated to each step of the food chain described above.

One important aspect of the technology of plant growth modeling is its genericity and adaptability to various species. CybeleTech services are already available for the major field crops in Europe (corn, wheat, rapeseed). The company has the ambition to broaden its field of expertise in the near future to market gardening (tomatoes and cucumber mainly), arboriculture and to forest management.

CybeleTech works with various academic partners including INRA for soil and plant databases, Ecole Centrale Paris for plant growth modeling continuous development and CEA for sensors usage. HPC technologies are nowadays becoming essential for CybeleTech in order to be able to process the accumulating amount of soil data, climatic data and plant data together with numerical simulations.

Project Abstract (150 words)

Breeding a new variety is a long process that requires a decade and thousands of experimental trials in fields so as to select the most robust and efficient traits. In order to help seed companies to reduce the duration and development cost of a new variety, we propose to simulate the growth of the tested genotypes instead of running experiments in the field. For this purpose, HPC technologies are then critical. In a first step, the plant growth model used in numerical simulations must be calibrated with plant phenotypes data. The present project aims at defining the optimal experimental protocol to be followed for calibrating the model, i.e. to answer three questions: What observables to measure? In which quantity? In which environments? To address these issues, computer simulations are run to compare the precision derived on the model parameters as a function of the data used in input. Optimization techniques are then used to identify the best protocol offering a balance between quality of the final result and experimental costs.

Industrial relevance and potential business impact (250 words)

The present project on the development of simulation techniques for varieties breeding protocols optimization dwells in a context of strong competition between seed companies enhanced by the repositioning of historical chemical companies on the seed market. Moreover, thanks to the recent development of new technologies from molecular biology in modern plant breeding and the digitizing of increasingly larger data sets, seed companies are prone to invest in research and innovative technologies. For these reasons, numerical technologies to simulate plant growth and thus to save time and to reduce costs are in line with the needs of seed companies. We estimate that the outcome of the project could bring an economy of about 50% on the costs of developing a new cultivar, and reduce the time of the process by two or three years.

For CybeleTech, the project will be a valuable tool to better quantify the added value delivered by our services to our client and will strongly enhance the attractiveness of our offer of software as a services. We expect to at least double our business related to seed companies at the end of this project. Beyond that, this project is the opportunity to develop the use of HPC in the company and to introduce it to the agricultural world. The ambition is to follow the same change of paradigm that occurred for instance in the car industry with the introduction of numerical simulations of car crash, by substituting numerical simulations of plant growth to field trials.

Proposed high-level Work Plan (500 words)

The project is divided in three parts.

- 1. T0 -> T0 + 4 months : Implementation of optimization algorithm
- 2. T0 + 4 months -> T0 + 7 months: Tests of software on machines
- 3. T0 + 7 months -> T0 + 10 months: Running of numerical simulations

1. The optimization algorithm that will be used is implemented, taking care to provide a parallel framework. The algorithm should be able to find the best set of plant measures to take on a variety in order to calibrate the model with enough precision, under economic constraints that limits the amount of data that can be taken. For this purpose, genetic algorithms will be considered. The cost function that is used to constrain the amount of data taken will be defined in coordination with seeds companies to ensure its suitability.

In the end, a software is then delivered that can be run in a parallel environment.

Risks : The degree of precision that is desired cannot be reached even with a very large data set. In this case, a worse degree of precision will be set. The quality of the results consequently achieved will be estimated.

2. The software is tested on the machines and its performance and scalability to a high degree

of parallelism are studied.

A report on the performance of the algorithm and on the degree of parallelism that can be achieved is delivered.

Risks : the degree of parallelism that can be achieved by the optimization algorithm is not enough. In this case, the parametric estimation that measures the parameters and uncertainties for a given data set will be parallelized.

3. A complete run is performed and a report on the results is provided. A first rough estimation of the computation time is that 100,000 hours of core CPU time would be enough for the optimization algorithm to converge toward an adequate solution. This estimation will be refined during phase 2 before starting the run.

In the end, a report on the results is delivered.

Risks : The estimation of the computation time required made during phase 2 may underestimate the time needed for convergence so that at the end of the run, an adequate solution is not yet found. To address this problem, the implementation of the algorithm (phase 1) should be such that the run can be restarted at the point where it was stopped for additional iterations.

Technical Requirements

The output data that will be stored are the uncertainties on the plant model parameters derived as a function of the experimental protocols tested. This does not represent a huge amount of memory and should be limited at the scale of 100 MB.

The computation will mainly be based on simulations so that no proprietary data will be involved, but the original detailed idea as well as the potential results should remain confidential so that we would prefer to include a non-disclosure agreement.

Date submitted: 01/14/2015 Project Title: Automatic Optimal Hull Design by Means of VPP Applications on HPC Platforms Name: Hydros Innovation Address: EPFL Innovation Park C / 1015 Lausanne - Switzerland Website: www.hydros.ch Name: Stephane Dyen Position: Head of design team Email: stephane@hydros.ch Phone: (021) 508-0382

What does the company do? (300 words)

Hydros Innovation is an Engineering & Research Swiss company founded in 2007 with several patented designs in the field of marine and sailing yachting. Hydros Innovation service portfolio includes:

- Boat development: Hydros Innovation offers a boat development service ranging from the deck plan to the choice of customized technical solutions. Focused on the nautical industry, the scope of this service ranges from yachting to motor boating.

- Project management: through its activities, Hydros Innovation has developed the ability to manage projects combining several players in different fields, coordinating the many required skills with a pre-defined common goal.in-house tools for performance prediction and dynamic simulation.

- Measurement, performance analysis: from the outset, we thought of Hydros.ch as a laboratory boat. Since 2010, Hydros Innovation has made use of a large quantity of data collected from this extraordinary flying catamaran. This expertise is now available to everyone to optimize boat efficiency and carefully analyze all the parameters that come into play.

- Manufacturing: Hydros Innovation has relationships with many shipyards in which the boats and prototype designed by the company are built, and has also facilities to do fast prototyping and modifications on the parts that need to be optimized.

Hydros Innovation most famous projects are:

- HydroptÃ" re: two world speed records in 2009 and absolute sailing speed record (51.36kts);
- Hydros.ch: laboratory boat which breaks all the records on Geneva's lake;
- C Class: first yacht built in TPT, 2nd place at Little Cup 2013;
- HY-X: first hybrid « Fly and Float » motorboat.

In recent years Hydros is exploring new market segments such as yachts and super-yachts hull design.

Project Abstract (150 words)

The main scope of the proposed application is to evaluate, with the help of PRACE experts, the feasibility of automatic optimal hull design on HPC infrastructure and the impact of such a workflow on the day-by-day work of Hydros personnel.

Thanks to hardware and software improvements, today it is possible to perform yachts design using high fidelity 3D Computational Fluid Dynamics computations, driven by optimizations tools, to feed Velocity Prediction Program (VPP) applications.

The usage of open-source software, such as OpenFOAM, joined with automation procedures and highly efficiency scalability performances (HPC) may allow the user to customize his design workflow to match time-to-results and budgets constraints. OpenFOAM is already considered today an effective tool in CFD applications based on HPC infrastructures during VPP feeding process. A real-life industrial case study will be used.

The outcomes will be used to eventually drive the novel design of the selected hull industrial case.

Industrial relevance and potential business impact (250 words)

Yachts and super-yachts are until now mainly conceived to suit design and architecture clientsâ€[™] needs, and few time is used for performance investigations. Builders only use towing tank to estimate the resistance and then choose the motorization. Hydros wants to show yacht companies that technology can provide them more efficient hull shapes that fits their design needs, and have less impact on environment.

Hydros is working with yacht builders, providing resistance values such as towing tank, but also analyzing the flow and pressure to propose shape modifications. Stability evaluations are also performed with modern VPP and dynamic simulator tool, which need RANS CFD values to be calibrated for the hull shape. Classic optimization procedure based on the analyze of the previous geometry results is time consuming for engineers, because it require a manual analyze, new geometry definition and preparation before new calculation is performed. During this time, computers are not used.

Design process has to be done in short time. Automation of the global procedure, from the hull shape modification to the result would reduce the engineer time, and use computer possibilities to the maximum. Optimization could also drive the geometry modification, in order to converge to the goal fixed in the optimization.

If the optimization workflow is effective then the bottleneck to become competitive in this market is only related to the computational power. So that, the more the HPC infrastructure is performing the more the time-to-optimal-design can be reduced and the most Hydros can achieve optimal hull designs.

Proposed high-level Work Plan (500 words)

As introduced earlier, the main scope of the proposed application is to evaluate the feasibility of automatic optimal hull design on HPC infrastructure and the impact of such a workflow on the day-by-day work of Hydros personnel.

Therefore, in short the proposed workflow is as follow: sitting on top of the HPC infrastructure provided by PRACE the optimizer is driving the changing CAD hull design according to the outcomes of 3D CFD results that can be processed to obtain synthetic hydrodynamics indices of hull performances. This workflow, once instructed and properly settled, is therefore totally automatic and is able to obtain an optimized version of a starting hull design.

In order to exploit the perspectives offered by the proposed workflow the most interesting scenario is the design of Palmer&Johnson yachts. In particular PJ42m hull is a good candidate, it's a semi planning hull with sponson. When a new design is conceived, the number of CFD runs required can easily rise to hundreds for a single hull (usually the number of hull designs considered can range from 5 to 10) in order to take into account of basic parameters (hull speed, leeway, pitch, and so on). The time to results is also another important constraint in PJ42m hull design since is usually very limited (3 to 5 months). In order to deliver thousands of 3D CFD RANS computations in such a limited amount of time the use of HPC infrastructure coupled with robust automation is mandatory, but the adoption of open-source softwares business model is also healthy and can make the difference when also budget limitations comes in to play.

Hydros is strongly committed in evaluating the PRACE-enabled workflow in its production environment, and in providing the necessary effort, in term of personnel and software, to accomplish the work plan tasks here below listed.

Task 1: Requirement analysis

- 1.1: assessment of objectives and workflow
- 1.2: assessment of hardware&software requirements
- 1.3: elaboration of detailed workplan and milestones
- Estimated effort (in work months): PRACE: 0,25 Hydros: 0,25

Task 2: Modelling of starting hull design with CFD tools

- 2.1: set-up of tools and workflow on PRACE HPC infrastructure
- 2.2: set-up of first complete workflow
 - 2.3: testing and benchmarking

Estimated effort (in work months): PRACE: 2 Hydros: 1,5

Task 3: Optimization of design parameters

3.1: evaluation of computing resources and ease of access to PRACE infrastructure

3.2: production campaign and hull optimization

Estimated effort (in work months): PRACE: 0,5 Hydros: 0,5

Task 4: Testing of new optimized hull design

4.1: validation of the new hull design with Hydros in-house tools

Estimated effort (in work months): PRACE: 0 Hydros: 1)

Task 5: Analysis and reporting

5.1 analysis of the business case

5.2 final reporting

Estimated effort (in work months): PRACE: 0,5 Hydros: 0,5

Total estimated effort (in work months): PRACE: 3,25 Hydros: 3,75

Technical Requirements

<u>SoftWare</u>

- OpenFOAM: http://openfoam.org; open-source.
- Paraview: http://paraview.org ; open-source.
- Caeses: https://www.caeses.com/ ; license provided by Hydros.
- Python programming language: http://python.org; open-source.
- VPP and dynamic simulator: developed and provided by Hydros.

Hardware:

- HW: state-of-the-art X86_64 architecture

- Os: linux

- Disk space requirements (estimated): 0,5 TB
- Maximum level of parallelism per single run (estimated): 256 cores
- Remote visualization facility is required

Non-technical:

- Optimized hull designs should not be disclosed

- Preferable HPC center: CINECA – SCAI Dept. since in 2014 we performed a feasibility study for a Class-C hull CFD study using openFOAM.

Date submitted: 01/14/2015 Project Title: Transonic cfd Analyses with openFOam and Rbf mesh Morphing (TRANSFORM) Name: Dâ€[™]Appolonia SpA Address: Viale Cesare Pavese n. 305, 00144 Rome Website: <u>www.dappolonia.it/en</u> Name: Emiliano Costa Position: Project Engineer Email: <u>emiliano.costa@dappolonia.it</u> Phone: 0039_0659450300

What does the company do? (300 words)

Dâ€[™]Appolonia (DAPP) is a team of engineers, consultants, designers, planners and specialists supporting public and private Clients from concept to decommissioning, through consultancy, design, management, operation and maintenance. The company operates in the markets of Energy, Transport and Infrastructures, Industry and Investor Support. We provide a wide range of services such as feasibility and specialized studies, design, Project Management, site engineering and operation & maintenance management. In addition, we offer technical capabilities to cover all aspects related to the environment, health and safety, geosciences and innovation for specific applications.

With a staff of about 700 engineers, scientists and associated professionals located in 20 offices worldwide, Dâ€[™]Appolonia offers high-end services to investors, promoters, operators and contractors, as well as to insurers and public administrations, to support their initiatives. All Dâ€[™]Appolonia services are performed at the highest professional level, understanding and complying with Clientâ€[™]s needs and requirements while taking into due consideration sustainability and health, safety and environmental goals.

Relating to the Aerospace sector, Dâ€[™]Appolonia aims to develop and adapt innovative technologies for industrial applications to meet the final usersâ€[™] need. Then virtual prototyping requirements as well as system modelling and numerical simulation endeavours bring the Company to face with challenging solutions to optimize computer resources and SW tools required to deliver engineering design in a more demanding industrial planning framework. The current applications of interest mainly deal with external aerodynamics (aircrafts and rockets) and shape optimization.

Project Abstract (150 words)

Due to strong competitiveness and considerable increasing of technological demand in terms of performance and reliability of constituting components in the aeronautical sector, designers are constantly urged to invest in innovative technologies to enable manufacturers to reduce aircraft development costs and delivery times. In such a context, CFD (Computational Fluid Dynamics) open source technologies, especially at transonic and supersonic regimes, still show deficiencies, at least in terms of efficiency, if compared to well-established and validated commercial solvers.

The proposed project aims at testing a wide range of real world aeronautical applications coupling an open source CFD compressible flow solver with a RBF mesh morphing tool and improving their performances on HPC systems, with the help of the PRACE experts.

Industrial relevance and potential business impact (250 words)

The TRANSFORM project is a key item for DAPP and is of strategic importance in the field of numerical modelling and simulations capability. DAPP will enjoy both short- and long-term benefits of the application. At first, DAPP will enrich its R&D know-how to later turn this experience of methodological assessment and engineering evaluation applied to industrial aeronautical applications into engineering services. DAPP will also gain the instruments necessary to reliably approach the top-level aeronautical design, namely the availability of a very competitive computational tool and related knowledge. As a matter of fact, DAPP is planning to expand its commercial offerings to its clients and to reduce, at the same time, the high costs sustained in the past due to use of commercial codes. In particular, DAPP envisages being able to discount its current sell hourly rate of CFD services up to 10%, thus producing more competitive offering and accessing a wider range of revenues, at least in the range of 20%.

With regard to medium-term impacts, this project is strategic for opening a new front of potential clients by giving opportunity to promote more specialized consultancy services. Moreover, DAPP will gain more chances to reinforce its presence in EU research dealing with aeronautical design and optimization, started in 2013 with RBF4AERO (www.rbf4aero.eu). Finally, concerning the methodological approach for design, the remote access to cloud-based HPC resources for CFD simulation will facilitate the development of promotional activities and scientific disseminations towards an industrial audience, thus generating an indirect beneficial effect.

Proposed high-level Work Plan (500 words)

The proposed project is specifically conceived to evaluate the accuracy and computing performance of a numerical platform able to perform multi-objective shape optimization analyses through the use of existing open-source CFD library OPENFOAM® coupled with the stand-alone version of the RBF Morph commercial tool.

The use of an open source based solver facilitates the deployment and parallel execution of CFD applications in cloud-based HPC systems without any license limitations, thus enabling the incorporation of additional computer power beyond in-house hardware capabilities at a reduced cost. On the other hand, the utilization of RBF Morph allows to parameterize the computational model via mesh so that multi-objective optimization (MOO) analyses are carried out through efficient procedures such to prevent the typical compromise of standard optimization procedures in terms of speed, accuracy and extent.

To get reference data for comparison with output obtained through the proposed numerical platform, two representative test cases with an incremental level of complexity will be simulated mainly using the most adequate compressible solver among those available in the OpenFOAM libraries, identified with the support of PRACE experts. These cases are the ONERA-M6 wing at Ma= 0.8395 (#1) and DLR-F6 model at Ma=0.75 (#2) employed in NASA DPW (Drag Prediction Workshop).

In particular, Test case #1 will be mainly used to support the identification of the solution setup guaranteeing the best trade off in terms of accuracy and numerical stability. This operation will be accomplished by comparing the Cp (pressure coefficient) variation on wing sections in transonic regime with the corresponding experimental evidence registered during the wind tunnel test.

At first, the appropriate strategy for the generation of a proper mesh, in terms of settings and

algorithm, is to be studied. Secondly, the suitable solver, the most reliable and consistent boundary conditions, discretization schemes as well as the turbulence model need to be identified. All such choices will be taken with the support of PRACE personnel expertise.

Then, the resulting set-up will be used to run the Test Case #2 in the baseline configuration (original geometry) to verify, by comparing the numerical results with experimental ones, its consistency towards a convincing and more complex model. Finally Test Case #2 will enable to perform massive MOO analysis considering several shape modifications of interest for aircraft optimization. Those modifications involve nacelle horizontal and vertical translation and the rotation around a horizontal axis (y according to aircraft aerodynamics) respect to the wing as well as the sweepback, the twist and dihedral angles of the wing.

Aircraft aerodynamic coefficients (Cd, Cl and Cm) will be simulated at steady cruise conditions identified by Ma=0.75, Re= 4.5 E+06 and altitude=9000 m. As far as geometrical constraints are concerned, in the case of nacelle the modifications will be limited to the pylon only, whilst wing modifications will be performed by keeping the leading edges straight and preserving the wing area.

The design points will be defined with objective to maximize aircraft efficiency (E=Cl/Cd) considering limitation on pitching and bending moment.

Technical Requirements

SW requirements:

- OpenFOAM 2.3.0
- Paraview 4.1.0
- RBF Morph 1.6 (commercial license of the stand-alone version provided by RBF Morph)

HW requirements:

- Linux cluster, Intel processors, software required does not support accelerators
- Expected scalability > 200 cores
- 3 TB disk space
- Remote visualization for pre/post processing

Non-technical requirements:

- use of RBF Morph tool requires a LNDA (license non-disclosure agreement) to be signed by DAPP and PRACE personnel involved in the TRANSFORM project.

- we express the wish CINECA be our support center because of their current relevant experience with RBF Morph.

Date submitted: 01/13/2015
Project Title: HPCWelding
Name: Ingenieurbüro Tobias Loose
Address: Herdweg 13, D-75045 Wössingen
Website: www.tl-ing.eu
Name: Tobias Loose
Position: President
Email: <u>loose@tl-ing.de</u>
Phone: +49 176 6126 8671

What does the company do? (300 words)

Ingenieurbüro Tobias Loose is an engineering office specialized on simulations for welding and heat treatment. Welding simulations and heat treatment simulations aim on the one hand to determine the final state of the assemblies after these manufacturing processes: Distortion, residual stress, material properties and microstructure. On the other hand these simulations aim to optimize the processes.

Loose provides consultings for industrial customers, training and software for customer applications.

Moreover, Loose is involved in own reseach projects concerning welding and heat treatment simulations.

Loose has over 10 years experience in welding and heat treatment simulation. Loose started in 2014 with LS-DYNA with the aim to use a FE-code which has good performance in parallel computation. The welding simulations from Loose done in the past were successfully performed with LS-DYNA but only on one CPU.

Project Abstract (150 words)

Welding simulation models need a fine discretisation in the weld area. Further the industry has been requesting the analysis of large assemblies as well as the analysis of thick plates with multilayered welds. Furthermore, welding is a transient process and its numerical analysis involves a large number of time steps. These circumstances lead to welding simulation models for industrial cases with a large number of elements and a large number of time steps. This yields the problem of long simulation times on small computing clusters which poses an obstacle in the acceptance.

High performance computing can provide a solution to this issue. The Finite Element Code LS-DYNA provides good performance and permits parallelized computation using domain decomposition. The common method for welding is the implicit analysis.

This project will check the feasibility of parallelized welding analysis with LS-DYNA and its performance.

Further tasks will be:

- work out optimized solver parameter for parallelized analysis
- test the result quality using high level parallelization

Industrial relevance and potential business impact (250 words)

The duration of simulation time for welding analysis is a high barrier for the acceptance of this simulation technique in the industry. A welding simulation needs to be performed within one week which requires calculation times within one day. Consultings about welding simulation can be performed in reasonable manner if the issue of calculation time is resolved.

The demand for the determination or pre-calculation of welding distortion and the implementation of the welding simulation analysis in the manufacturing simulation exists and is forced by industry.

Thus the results of this project have an high impact on industrial relevance. Consultants who are in charge with welding simulation need a solution for fast simulations to be competitive.

Small companies can not invest in High Performance Computers. Supercomputing on demand enables small companies to participate on the benefits of HPC and its impact on the competitiveness. Finally, it enables small companies to become a respectable consultant in welding simulation.

Concerning this points above, this project promises to yield a high business impact. Loose expects a significant increase of consulting assignments.

Proposed high-level Work Plan (500 words)

The LS-DYNA licenses will be provided by Loose. Loose works actually close together with DYNAmore (Stuttgart), the provider of LS-DYNA, to realize welding and heat treatment simulation with LS-DYNA. Loose provides the request from the model technique and DYNAmore realizes necessary improvements in the DYNA source code.

LS-DYNA is a well parallelized Fine-Element-Code. Parallelization is used in explicit crash analysis up to 2048 cores. Welding simulation is a new field for the LS-DYNA solver. Welding simulation is a high specialized FEM-application with a lot of challenges for the FEM-Solver, for example the issue of high gradients in temperature and Young-Modulus.

It is not clear now how the solver reacts if welding analysis is set up highly parallelized. It is an open question how is the performance, how is the scaling related to number of cores or model size. Welding simulation is used to be done implicit (state of the art). It has to be checked out if explicit analysis leads to shorter simulation times or not.

These open questions demonstrate that parallel welding analysis is not yet ready to use. The project shall discover existing issues. The close collaboration between Loose and DYNAmore will guarantee that Loose gives feedback on discovered issues to DYNAmore and DYNAmore takes care on the improvement of the LS-DYNA code.

Loose is an one-man operation with no experience in HPC and needs support by HPC experts in order to run the LS-DYNA simulations on a highly parallelized system.

Workpackage 1 – Simple model

Set up a simulation model with simple geometry (T-Joint single layered weld).

Investigate the performance on various number of cores with different number of elements.

Investigate the performance of contact problems.

optimize time stepping and solver parameters (convergence criteria).

Evaluation of the result quality.

Workpackage 2 – Multi layered welding

Set up a simulation model with a large number of layers – multi layered weld with 100 layers.

Investigate the performance on various number of cores.

Workpackage 3 – Modelling methods

Compare models with several modelling methods especially in meshing:

- solid model with hexaeder and pentaeder meshes
- solid model with tetraeder mesh
- shell model
- shell-solid model

Evaluation of the calculation performance.

Evaluation of the result quality.

Workpackage 4 – Industry cases

Check the performance on industry cases (automotive, rail),

multiple components, large number of welds.

Workpackage 5 – explicit analysis

Check if it is possible to perform welding simulation with explicit analysis.

Check the result quality of explicit analysis.

Solver settings and time scaling.

Check the performance of high parallelized explicit analysis versus low parallelized implicit analysis with larger time steps.

Technical Requirements

Technical requirements:

HPC-resource up to 1024 cores.

Temporary file storage up to 16 TB.

Software: MPI, LS-DYNA .

Business requirements:

The predominant part of models have the copyright of Loose and are not protected by a NDA. Industry cases will be modelled with the copyright of Loose, similar to real cases but without any NDA. Date submitted: 01/13/2015 Project Title: Coupled sail and appendage design method for multihull based on numerical optimization Name: Design Methods Address: Viale Regina Elena 207, 98121 Messina (Italy) Website: www.designmethods.it Name: Ubaldo Cella Position: Senior research engineer and owner Email: ubaldo.cella@designmethods.it Phone: +39 339 3970006

What does the company do? (300 words)

Design Methods is the name of the engineering firm created after around fifteen years spent gaining competences and experience within European research projects in the aerospace field. The mission of Design Methods is to provide multidisciplinary engineering consulting and design services to industries and design teams supporting them with highly specialized competences on aerodynamic design, CAE analysis, software development, CAD modeling, numerical optimization environment and customized design tools development. We operate in aerospace, automotive and marine fields.

We have many years of expertise derived from the use of CFD commercial and research codes in the aerospace field. We are specialized in the creation of design tools based on CAE methods integration, in multidisciplinary numerical optimization environments development, in codes coupling, in the definition of geometry parameterization procedures and the identification of appropriate optimization strategies. We have the expertise to develop and efficiently use state of the art technologies in aerospace design. We can provide assistance in all phases of the design process with services as conceptual definition, preliminary design, software development, development of preliminary design codes, aerodynamic design, experimental tests in towing tank and wind tunnel.

Project Abstract (150 words)

The project consists in implementin on a HPC system, with the help of PRACE experts, a numerical optimization workflow, for sailing boats sail plans and appendages, to be tested on the design of an A-Class catamaran sail. The criterion is to integrate a parametric geometric module, an automatic mesh generator and a VPP based on CFD computations and analytical models. The VMG is evaluated solving the 6DOF equilibrium system iterating between VPP and sail CFD analyses. The hull forces are modeled by empirical formulations tuned against a matrix of multiphase CFD solutions of the demihull. The appendages polars are estimated applying preliminary design criteria from the aerospace literature. The method can be adapted for the design of any sailing boat of any dimension. The task of this project is to develop the procedure, to optimize its computational requirements and to demonstrate its performance on a test case.

Industrial relevance and potential business impact (250 words)

With the exception of important competitions or research fields, sails are usually designed according to sailmaker experience with limited investment in aerodynamic design using high

fidelity tools. The reason is simple: the aerodynamic design is complex, it requires high skilled resources, expensive software and, therefore, a costly time to market which is unacceptable for normal customers.

The object of the project proposer is to develop an accurate design method, possibly using open source software, which, apart to the earliest investment in development, can be affordable to normal market. Its setup requires, however, large computational resources related to the number of possible design variables, to the CFD runs required per iteration and to the process of appropriate optimization strategy selection. In order to face these tasks, an HPC infrastructure is necessary. Furthermore, experts support in the selection and integration of the opportune codes within the HPC environment is essential.

When available, validated, optimized to limit the computational resources requirements and tested on a real case, the tool will give the proposer the possibility to provide a reasonably cheap design service to sailmakers, sailing teams and to any private shipowner who wish to improve the performance of its boat.

An important part of the activity will be the application of the design procedure on a test case of practical interest. The aim is to verify the practical feasibility of the tool and to provide a demonstration of its value to the market.

Proposed high-level Work Plan (500 words)

The methods is based on the integration, within a numerical optimization procedure, of a velocity prediction program (VPP) and a RANS solution of the fluid dynamic sail domain. The hull is modeled by analytical formulations both taken from literature and developed by a comparison with a matrix of isolated demihull CFD solutions at several attitudes and leeway angles. Dagger boards and rudders are modeled as wings. The polars are estimated applying methods from aeronautical preliminarily design literature. Sail forces and its aerodynamic center are obtained by a RANS analysis. The described analysis block is integrated in an optimization environment in which the optimal sail plan and appendage configuration, that maximize the VMG (Velocity Made Good) speed is searched.

The analytical models and the VPP have been already developed and tested using commercial codes. The project do not then start from scratch but several aspects need to be further developed. In particular, critical points are the implementation of the geometric parameterization strategy and the codes coupling in an efficient optimization environment. The methods (geometry generation, mesh updating, aerodynamic analysis and optimization strategy) have to be selected, validated and coupled in an efficient manner. The task of the project is then to implement, with the support of PRACE, the described optimizing procedure in the HPC environment, to define the most efficient optimization configuration (in term of variable and design space limits) to integrate the tools, to tune and optimize the procedure with the view of reducing the computational requirements. The setup of the CFD computation will require particular attention. The possibility to use an open source code has to be verified in term of computation stability, robustness and accuracy. A preliminary activity has to be addressed in validating and optimizing the CFD configuration against wind tunnel experimental measurement available in literature. The PRACE support in all this points will be valuable.

More in detail, the project will be divided in the following main parts:

- selection and assessment of the candidate CFD analysis tool against experimental data;

- definition of the strategy and implementation of the workflow for the automatic geometry parameterization, CFD analysis and objective function computation within the existing VPP;

- codes coupling and implementation of the optimization environment;

- application of the developed procedure on a test case with the double objective to optimize the workflow and to demonstrate its validity as design tool.

The proposed test case on which to apply the procedure is the sail of an A-Class catamaran. This class has relatively simple rules that enables the development of a high technological environment without excessive economical resources requirement. The analytical boat model is available and the design problem can be limited to the sail shape. Furthermore, the sail plan type involves the generation of a less critical flow field, from the CFD analysis point of view, respect to conventional displacement boats sail plan. This aspect permits to focus the attention on the efficiency improvement of the optimization environment.

Technical Requirements

To be economically affordable, numerically accurate and computationally efficient, the procedure must fulfill several requirements: it must use in-house developed and/or open source software, it must be optimized to reduce the computational costs and its strength must be demonstrated.

A first version of the procedure, developed in Scilab but coupled to commercial software, is already available. Several aspects, however, still need to be deepen. We require a particular support from PRACE for the setup of the procedure in the HPC environment and for the integration and validation of open source software in the workflow (DAKOTA, OpenFOAM, Snappy or any other tool considered appropriate). In order to mitigate the risks, however, the possibility to use well tested commercial tools will be offered by the University of Rome Tor Vergata which is our partner of research. At this point, CINECA would be the preferred supporting PRACE center. CINECA has, in fact, already collaborated with the University of Rome on activities that involved the use of RBF-Morph code, which is a candidate to perform the mesh parameterization, has experience in developing analyses with OpenFOAM and developed optimization procedures using DAKOTA in HPC environments.

All software run on standard linux cluster, we are interested in testing accelerators when supported by software. License for commercial software will be provided by Design Methods. Expected scalability > 200 cores. Estimated disk space: 3 TB. Remote visualization required for pre/post processing.

Date submitted: 01/13/2015 Project Title: VORTEX Name: VORTEX BLADELESS SL Address: C/ Pont de Molins, 21, esc. izda., 3ºD, 28038, Madrid Website: <u>www.vortexbladeless.com</u> Name: RaúI MartÃ-n Position: Founder and coCEO/Organization Email: <u>rmartin@deutecno.com</u> Phone: (066) 558-4568

What does the company do? (300 words)

VORTEX BLADELESS is a dynamic R&D company founded in 2013 and exclusively dedicated to the development and marketing of devices capable of capturing wind kinetic energy by vortex shedding, transforming it into other useful forms of energy.

The founding partners began its activity with the development of electronic devices and the manufacturing of small series according to specifications set out by our customers.

David J. Yáñez wrote his first draft about the wind turbine by vorticity in 2002. The idea was maturing during the following years until the application for the first patent in the summer of 2010. This initial patent is currently in its international stage.

In September 2011, VORTEX BLADELESS team achieved its first demonstration of the concept in a wind tunnel. Since September 2012, the team is fully dedicated to the development of the project with a sponsorship of the Repsol Foundation. The end of this incubation stage was due in September 2014. The Vortex team, apart from the founders, is comprised of four engineers and reputed external advisors giving technical support to the project, as well as a first line Advisory Board and shareholders adding great value to the Company. They invest their own money and are linked to powerful capital funds and energy companies, who can support us or become our future investors.

Since 2010, the founding partners have won numerous awards for the quality of their research. Among the awards obtained are the Entrepreneurs Foundation Award (EVERIS) in 2010, the Latin American Entrepreneurship Award 2011 or the 1st Prize for Entrepreneurs (REPSOL Foundation) in 2012.

VORTEX BLADELESS is dedicated exclusively to the development of this project. The philosophy of the team is to provide technological solutions that, in many cases, can repair the mistakes of technologies that have reached a high degree of maturity.

Project Abstract (150 words)

The project objective is to develop a new concept of wind turbine without blades, called Vortex or vorticity wind turbine. This design aims to eliminate or reduce many of the existing problems in conventional wind energy.

This device represents a new paradigm of wind energy. Due to the significant difference in the project concept, its scope is different from conventional wind turbines. It is particularly suitable for offshore configuration and it can be exploited in wind farms and in environments

usually closed to existing ones due to the presence of high intensity winds.

Given its morphological simplicity and considering that it is composed by a single structural component, its manufacturing, transport, storage and installation has clear advantages. The new wind turbine design has no bearings, gears, spools, etcetera, so the maintenance requirements could be drastically reduced and their lifespan is expected to be higher than traditional wind turbines.

Industrial relevance and potential business impact (250 words)

Computing simulations are the most important success factor before prototyping to scale. These are the best way to improve the technology before manufacturing.

Computer models could give us a clear idea of the model and its behaviour. We could also develop Vortex thoroughly before testing. Trial and error is not the most efficient way to achieve success in designing, in particular in the case of an undeveloped technology. With the help of supercomputers, the convergence to optimal design will be reached sooner. We have not reached any valuable results by computing our device and its characteristics with the help of experienced companies. Supercomputing is an opportunity to demonstrate that we are on the right track.

A successful completion of the project could lead to new customers and jobs. Our Vortex technology would offer two new and differentiated products:

Vortex Mini (4 kW rating) will cover the energy needs of household distribution in places without access to electricity grid. 4 kW power is enough to satisfy the energy needs of an average family unit in Europe and more than one in villages or farms in rural Asia, Africa, South America, etc. and at a very low cost. Selling is to begin in October 2016, with 275 units sold in year 1 and > 1000 in year 2.

Vortex Gran (+1 MW) targets traditional wind power customers: renewable energy investments, countries, large electricity utilities, etc. This expected global market is more than 600 GW in 2020 (over 0.5 million of wind turbines).

Proposed high-level Work Plan (500 words)

The project will have an initial set up and validation part, in which the numerical tool developed by Barcelona Supercomputing Center will be adapted to a study case. The results of this initial phase will be analysed together with the members of VORTEX BLADELESS and, depending on the success of this analysis, a short range parametric study will be carried out. Using these results, the industrial part of the project will be carried out by the company. The work plan is as follows:

1. Simulate the wind tunnel demonstrator for the Fluid Structure Interaction problem (FSI) with properties for certain wind speed. A comparison between the numerical simulations and the amplitude and oscillation frequency obtained in the tunnel tests will be used to determine the accuracy of the numerical results.

Collection and delivery data: drag coefficient, lift coefficient, oscillation amplitude, reactive forces, power generated, and lock-in region, etc.

Technical report: contour maps, images and video media, tabulated metadata.

2. Scalability studies. Depending on the success in the development of the FSI solver in point 1, a short range parametric study will be carried out.

Characterization of the new vortex shedding region as an effect of aero-elasticity. Study of influence of scalability in the behaviour of devices, variation of lift coefficient within 2s, 2p, p+s vortex configuration. Report of the above described.

Efficiency curve for a given wind speed.

Report of feasibility of the technology. Market target (micro-wind, mini-wind, wind energy, etc.)

3. Ultimately, all aerodynamics or/and mechanics effects to evaluate risks, lower losses, extreme conditions, life span, etc.

Technical Requirements

As far as we are concerned, computing capacity (time, complexity, etc.) is a critical part of our project. We have been working close to engineering services companies that tried to achieve the computation and idealization of our assumption. They have been unable to do so.

Since our device involves structures and fluid dynamics and their interactions, a coupled system is needed. Efficient independent solvers for the Computational Fluid Dynamics problem and the Computational Structural Dynamics problem are available in the Alya system (developed at Barcelona Supercomputing Center) and are able to couple in order to solve FSI problems.

Finally, and as an implementation of our project, we will need to simulate the generation of energy, thus electromagnetic simulations would be more than welcome in the future.

FSI simulations are prone to present divergence when solved with independent solvers (partitioned approach). Thus, a large amount of iterations per time step is required in order to achieve convergence and accuracy. Normally, the CFD problem alone needs a large amount of computational resources, and given the dimensions of the considered device and the wind speed to be simulated, we will require around a max of 1-2 million hours as the task is extremely complex and demanding in terms of resources.

(Currently, we are working with a WorkStation, 24 cores, 64GB RAM. Some simulations trials, with not expected results, are taking weeks even months).

Date submitted: 01/02/2015 Project Title: Simulation of sails and sailboat performance Name: WB-Sails Ltd Oy Address: Itälahdenkatu 22b Website: <u>http://www.wb-sails.fi/en</u> Name: Mikko Brummer Position: Manager, head of R & D Email: <u>mikko@wb-sails.fi</u> Phone: (358) 621-5055

What does the company do? (300 words)

WB-Sails designs and manufactures sails, specializing in top-end racing products. WB-Sails has from the beginning relied on technology, research and development, to become one of the very few sailmakers in the world present at the Olympic level. In London 2012 our sails, designed and manufactured in Finland, won a gold and a bronze medal in two different disciplines (boat classes).

WB-Sails have a long tradition in CAD and CAM, with computer based design since 1979, and computer aided manufacturing since 1988 (using an automated cutter). Recently, we have been doing increasingly design and consultation work in the nautical sector, in addition to our own R & D. The work has involved studies in mast or keel shapes and hull design. Traditional manufacturing work of sails is becoming more and more difficult, and less profitable within EU, due to rising labour costs. Consequently, our long term strategy is to expand in this direction, offering our design services to other sailmakers and the nautical industry in general.

Project Abstract (150 words)

We wish to implement in the project a HPC-based CFD-analysis of sails and sailboats, with the XFlow dynamic simulation code. The code allows 6-DOF (degrees of freedom) motion of the objects, for a realistic simulation of forces and moments around a boat moving in a seaway. Coupled with the Friendship Framework's code CAESES, XFlow can be used for optimizing sail shapes described by a parametric model. XFlow's ability to predict free surface flows is explored against known model test cases by the Delft model Basin.

Industrial relevance and potential business impact (250 words)

The use of CFD has been crucial to the success of WB-Sails. We are currently doing our R&D work on the desktop, with two workstations running 24/7 year in and out. As simulations are getting more complex (and realistic) the requirements on computational resources are becoming more demanding. For optimization work, the desktop is simply not sufficient. Optimization is not only about finding the "best" shape, it is also about providing options from which to choose, complementing the knowledge base for high-Âquality decisions.

Besides our own development work, HPC-based simulation would allow WB-Sails to expand into design consultation in the marine sector, which we see as our strategy in the years to come. The potential of simulation in the marine sector is constantly rising, as the codes get better and ROI on CFD is more and more outperforming traditional physical model testing. The project will allow WB-Sails to further develop their sails, to boost and ensure continued Olympic success in Rio de Janeiro 2016. In addition, it will promote diversification of our business from manufacturing towards simulation and consulting.

Proposed high-level Work Plan (500 words)

WB-Sails proposes to run several different studies which will fully benefit from the HPC-cluster:

Study #1

HPC will allow more demanding simulations than possible on the desktop. It allows true fluidstructure interaction (FSI), which is important for the sail simulation process. Sails are made of flexible material which distorts under the loading of the wind pressure. The distorted shape will alter the pressure field around the sail, which again will affect the sail shape. It's an iterative process, demanding lots of computer capacity. XFlow has a built-in structural model, but at WB-Sails its use has been limited to some simple test cases, because of the time/capacity limitations. One of the main objects of the project is to perform an FSI case involving motions of the boat in a seaway and deformation of the sail under varying loads caused by these motions.

<u>Study #2</u>

In the second instance, sailing yacht wave making (free surface effects) are simulated. The results are validated against model tests performed at Delft University in Holland, the SYSSER-series (http://dsyhs.tudelft.nl/dsyhs.php). Again, we have performed some analysis with the Sysser models, with encouraging results, but HPC would permit a larger domain and longer runtimes at high resolution. As opposed to modeling in the air only (1-phase), the 2-phase modeling of the air/water interface requires lots of capacity. If the results are good, CFD could indeed put tank testing with ship and yacht models into history. For a sample of a simulation performed on a SYSSER model by WB-Sails and XFlow see http://youtu.be/t7EPxD7ahX0.

<u>Study #3</u>

Parametric optimization by coupling XFlow with CAESES (https://www.caeses.com/products/caeses/). In the 3rd study, a parametric sail model created in CAESES will be analyzed using XFlow. Such a study will create overview and insight into the importance of various parameters on hand for the designer.

The above work plan is acknowledged to be highly ambitious. Should it prove too difficult to execute within the given resources or time frame, studies directly pertaining to sail performance will be prioritized.

Technical Requirements

Our preferred CFD code is XFlow (http://www.xflowcfd.com/). XFlow represents the next generation of CFD, beyond the industry standard Navier-Stokes RANS. It features a Lattice-Bolzmann particle based environment, with no meshing, and allows 6-DOF motion with no limit on complexity of geometry. The XFlow licensing scheme allows computations using HPC clusters. The distributed (DMP) solver makes use of MPI supporting both HPC clusters with a shared file system or a group of workstations with no shared file system. One of XFlow's partners is Teide HPC (http://teidehpc.iter.es/en), where the software is successfully deployed. XFlow is fully parallelized for multi-core technology with near-linear scalability. Its distributed solver scales efficiently even for a very large number of nodes.

However, WB-Sails would prefer to implement XFlow at CSC - Center for Science (https://www.csc.fi/csc), next to us in at Espoo, Finland. They don't have XFlow at the moment, but have declared their interest in implementing and supporting its deployment at CSC. CSC would be a viable technical partner for WB-Sails, expanding more into simulation in the future.

XFlowâ€[™]s data storage requirements are large, typically 0,5-1 Terabytes/run. However, since even all the post-prosessing is is done remotely on the HPC, very little data transfer is needed for the performing of an analysis.