HPC, HPDA and AI Applied to Industrial Use Cases

Mentoring Path First Workshop

Summary Report

Date and time: 25 November 2021, 9am – 1pm CET
Location: Virtual via Zoom
Organiser: CASTIEL WP3 – Training, Twinning and Mentoring

Background

In the digital era greater volumes of data are being generated and the need for using HPC capabilities to enable their efficient processing and to deploy emerging analytics and AI workflows is indisputable. Centre managers need to optimise their HPC infrastructure to handle the variety and complexity of the large workloads of big data, as well as complex analytics, various advanced AI approaches and methods, accelerated data visualization, and modelling and simulation workloads that are deployed.

CASTIEL WP3 organised together with National Competence Centre (NCC) UK and other NCCs that have experience in this field, the mentoring workshop on topic: **HPC, HPDA and AI Applied to Industrial Use Cases**. The aim of this workshop was to bring together representatives from industry, academia and public sector across all over 33 NCCs to present case studies, exchange views and ideas, transfer knowledge and foster further closer collaboration between the NCCs.

Agenda

09:00 – 09:05 **Welcome from CASTIEL WP3** – Martina Blazkova, BSC, CASTIEL WP3

09:05 – 09:10 **Welcome from NCC UK** – Vassil Alexandrov, NCC UK, Hartree Centre

09:10 – 09:50 **Engagement with Industry**:

- Dominic Richards, Hartree Centre, NCC UK – "***HPC and AI for Finance – View from the Trenches on Both Sides Investment Banks and Hartree***"
- Svetozar Margenov, Stanislav Harizanov, IICT, NCC Bulgaria – "***Supercomputer Applications in Biomedical Engineering – From Simulation to PoC and Production***"

09:50 – 10:30 **Engagement with Industry and the Public Sector**:

- Duncan Sime, Hartree Centre, NCC UK – "***Hartree Centre Strategy of Working with the Industry – Sectorial Approach***"
- Vassil Alexandrov, Hartree Centre, NCC UK – "***Partnerships in the Public Sector – UKAEA – Hartree Centre (STFC) Collaboration***"

10:30 – 10:40 *comfort break*

10:40 – 11:20 **Engagement with SMEs**:

- Soner Steiner (VSC/TUW, NCC Austria) and Jürgen Zechner (TAILSIT, NCC Austria) – "***Electromagnetic Simulations with the Finite/Boundary Element Method for Large Systems Using HPC***"
- Pedro Alberto, UC, NCC Portugal – "***Tooling4G – Minimize the Airflow Generated Noise on Automotive HVAC System***"

11:20 – 11:30 *comfort break*

11:30 – 12:30 **Open Discussions**:

- Discussion room 1

moderator: Vassil Alexandrov (NCC UK)
How can we facilitate advanced HPC, HPDA and AI adoption by industry and public sector for societal advantages?

- Discussion room 2

moderator: Martina Blazkova (CASTIEL WP3)
Added value of HPC for Industry

- Discussion room 3

moderator: Sven Karlsson (NCC Denmark)
Added value of HPDA for Industry

- Discussion room 4

moderator: Pedro Alberto (NCC Portugal), Dominic Richards (NCC UK)
Added value of AI for Industry

12:30 – 13:00 **Wrap-up with main points to take out and which way to go forward**

Participants

The EuroCC Mentoring Workshop on HPC, HPDA and AI Applied to Industrial Use Cases was held on 25 November 2021. This was a very well attended workshop with 7 speakers, 2 additional discussion rooms' moderators and over 115 attendees from different National Competences Centres from, e.g. Bulgaria, Germany, Finland, Turkey, Belgium, Austria, Lithuania, Romania, Czech Republic, Spain, Portugal, Croatia, North Macedonia, Sweden, Poland, Slovakia, Greece, Latvia, Luxembourg, Norway, Slovenia, Hungary, Montenegro, United Kingdom, Netherlands, Italy, Estonia, Switzerland, France.

Speakers/Moderators:

- Vassil Alexandrov, Hartree Centre, NCC UK
- Dominic Richards, Hartree Centre, NCC UK
- Duncan Sime, Hartree Centre, NCC UK
- Stanislav Harizanov, IICT, NCC Bulgaria
- Soner Steiner, VSC/TUW, NCC Austria
- Jürgen Zechner, TAILSIT, NCC Austria
- Pedro Alberto, UC, NCC Portugal
- Sven Karlsson, DTU, NCC Denmark
- Martina Blazkova, BSC, CASTIEL WP3

Content of the Workshop

The mentoring workshop presented an update around the state-of-the-art and best practices in HPC, HPDA and AI. After short presentations, there was a set of discussion groups that investigated how attendees could encourage uptake of HPC, HPDA and AI by industry, particularly SMEs, and the added value of HPC, HPDA and AI for industry.

Summary of the presentations:
Dominic Richards, Hartree Centre, NCC UK – "HPC and AI for Finance – View from the Trenches on Both Sides Investment Banks and Hartree"
The main focus of this presentation was on application of AI for finance aiming to better understand and predict market risk (financial crises, flash crashes, volatility spikes, etc). Numerous challenges were outlined, such as:

- datasets present certain challenges,
- markets are usually slowly changing in their behaviour, occasionally large "regime switches" occur,
- statistical significance is rare,
- financial data is very noisy,
- large, adverse events are surprisingly common,
- financial markets are very complex,
- huge number of exchange traded instruments exists.

Further, challenges and opportunities of AI in financial institutions and AI in research institutions were outlined (availability of market data, know-how).

Svetozar Margenov, Stanislav Harizanov, IICT, NCC Bulgaria – "Supercomputer Applications in Biomedical Engineering – From Simulation to PoC and Production"
Focus was on mathematical and computer modelling in the area of biomedical engineering. A highly parallelised approach was presented that was implemented and used by an SME. Some challenges and opportunities dealing with Big Data and need to perform real-time processing were outlined.

Duncan Sime, Hartree Centre, NCC UK – "Hartree Centre Strategy of Working with the Industry – Sectorial Approach"
The focus was on Hartree Centre's strategy of working with industry outlining the importance of sectorial approach. The talk stressed the importance of: addressing industrial, scientific, economic or societal challenges, segmenting the market into sectors and working with sectorial bodies, selecting a small number of strategically important organisations, delivering solutions to a particular challenge, platform as a service, creating digital assets, and the importance of training and skills.
It was outlined that this should be a clearly structured engagement and sales process:

- Notice - Identified potential
- Qualify - Opportunity, identified challenge, purchase timeframe, purchase process, identify decision maker and influencers
- Develop – Understand customer needs, identify sales team, develop solution, identify competitors, understand IP position
- Propose - Develop proposal, complete internal review, present proposal
- Close - Present final proposal, deal with objections, negotiate contracts
- Win - Contract signed, deliver
- Generate referrals

Hartree's priority engagement sectors, such as automotive, aerospace materials, agriculture food and agri tech, health and healthcare, life sciences, energy, utilities were given as examples.
It was stressed that Business development works in tandem with other teams, all functions.
In the discussion it was outlined that, if starting, it is important to have the processes in place, to know what works to grow.

Vassil Alexandrov, Hartree Centre, NCC UK – "Partnerships in the Public Sector – UKAEA – Hartree Centre (STFC) Collaboration"
Hartree Centre's research framework was presented and it was explained how as such enables efficient collaboration with industry, the public sector and academia. Examples outlining collaboration in Exascale Computing in partnership with Exascale Computing Project in USA, MetOffice UK and UKAEA (UK Atomic Energy Authority) were given. In particular, UKAEA – Fusion modelling and simulation – a long established exascale simulation challenge, for modelling plasma turbulence, designing materials, etc was given as more detailed case study.
It was outlined that for such large scale collaborations it is essential to have clear processes in order to collaborate with colleagues from other departments and institutions.

Soner Steiner (VSC/TUW, NCC Austria) and Jürgen Zechner (TAILSIT, NCC Austria) – "Electromagnetic Simulations with the Finite/Boundary Element Method for Large Systems Using HPC"
The focus was on efficient use of Boundary Element Methods for electromagnetic simulations by an SME. In addition to advanced expertise in HPC and domain specific areas it was outlined the importance of the access to HPC resources, consulting from HPC experts, access to courses and training material as well as getting to know each other, clear specification of the objectives and goals and having regular meetings.

Pedro Alberto, UC, NCC Portugal – "Tooling4G – Minimize the Airflow Generated Noise on Automotive HVAC System"
Presentation about a SHAPE project explaining what HPC can do to shorten the development time of new products in the plastic and mould industry and also addressing particular design problem – devise a more silent ventilator for car HVAC systems in view of the reduced noise produced by electric motors. The requirement was not to use open-source software. It was stressed that it is important to have a well-defined existing problem and having in place the knowledge to perform the simulation as well as HPC resources and expertise. The main challenges mentioned were having in place the required ISV licenses and dealing with data confidentiality issues.

The last part of the workshop focused on open discussions covering the following four topics:

- How can we facilitate advanced HPC, HPDA and AI adoption by industry and public sector for societal advantages?
- Added value of HPC for Industry
- Added value of HPDA for Industry
- Added value of AI for Industry

The workshop finished with each group presenting the main conclusions and highlights and with an online survey to find out what further topics the participants were interested in.

Next Steps

- Upload all the material – slides, discussion notes, etc. in the internal sharing workspace and distribute it to all NCCs.
- There was a lot of interaction, interest and opportunities to foster collaboration. It was decided that NCCs would interact as per their interests and arrange further bi-lateral and multilateral meetings to advance on particular collaborations. (bilateral collaborations ongoing).
- It was discussed to arrange a second workshop to follow the progress and see how we can further enhance possible collaborations.

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