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Leveraging HPC to Drive Innovation in AI
HLRS’ Strategy towards a Convergence of HPC and AI

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CHALLENGES OF AI
European Strategy for AI — Three Pillars [1]

• Boosting the EU's technological and industrial capacity and *AI uptake across the economy*
  – Supporting AI research excellence centres across Europe
  – Bringing AI to all small businesses and potential users

• Preparing for *socioeconomic changes*
  – Focus on jobs that are likely to be transformed or to disappear; leverage chances of new job creations

• Ensuring an appropriate *ethical and legal framework*
  – Citizens and businesses alike need to be able to trust the technology they interact with

Current AI Initiatives in Europe

• **European AI Alliance** [2]
  – Involve all stakeholders within Europe that are affected by AI
  – Dedicated platform where they can offer input and feedback to the high-level expert group on AI

• **High-Level Expert Group on Artificial Intelligence** [3]
  – Works on ethic guidelines towards “Trustworthy AI”
  – Steering group of the European AI Alliance

• **AI On-Demand Platform** [4]
  – Comprehensive European AI-on-demand platform to
    • lower barriers of innovation
    • boost technology transfer
    • catalyse the growth of start-ups and SMEs

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Why does AI need HPC? Why does HPC need AI?

- **AI solutions require immense compute-resources**
  - CPU, network, storage, accelerators, ...
- **Simulations** such as climate models are **hitting the wall**
  - Computing physical processes right down to the last detail is very compute-intensive
- **Information overload** will continue to increase
  - 5G, IoT, autonomous driving and flying, ...
- **HLRS addresses these challenges through different channels**
  - Economy, Society, Research
AI@HLRS

• **Economy** (with focus on SMEs)
  - Lacking AI expertise
  - No in-house AI hardware
  - Security concerns / data mgmt. (GDPR)

• **Society**
  - AI is seen as a blackbox model
  - Low acceptance rates of AI solutions
  - Security concerns (privacy intrusion)

• **Research**
  - Support of hybrid HPC/AI workflows on HPC systems
  - Resolve multitude of complementary requirements (e.g. software)
  - Interdisciplinarity: AI experts are no HPC experts
Combining HPC and HPDA for Academia and Industry

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The Catalyst Project [2016–2021]

• Our customers tend to run more and more data-intensive applications resulting in vast amounts of output data
  – A single turbulence & acoustics simulation of an axial fan with just four rotations results in 80 TB of data
  – Domain experts are no longer able to analyse data manually
• Close cooperation between HLRS and Cray (→ HPE)
• Evaluate requirements that arise when combining AI and HPC
  – Hardware + software environment
    • Cray Urika-GX (DA/ML), CS-Storm (DL), HPE Apollo (HPC)
    • Build upon open-source software stack
  – Perform case studies with both academia and industry

https://www.hlrs.de/bigdata
Case Studies

- Speech2Text models for German language (LandesCloud)
- Formal verification of neural networks (Fraunhofer IPA)
- Deep reinforcement learning for robotics (Festo)
- **Material characterization for metal forming** (University Stuttgart)
- Smart alerting system for freezers (CHECK)
- Identification of trends in scientific publications (Leichtbau BW)
- “3D City over Night“ (nFrames)
- Data analytics summer school (HS Alb-Sig)
- Prediction of S-Bahn delays in Stuttgart (HLRS)
- **SmartSHARK** (University of Goettingen)
- Performance variations in HPC jobs (HLRS)
- Turbulence detection in air flows (RWTH Aachen)
- Complications with biomechanical devices (HLRS)
- ...

:: HLRS@ISC-21 :: 07/01/2021 :: CATALYST – Convergence of HPC and AI
Scenario A: Processing of Massive Datasets

• With the improvements in system performance, HPC users are able to run
  – more simulations in the same time,
  – more complex simulations (e.g. finer meshes),
  – and thus **produce massive amounts of data**!

• Data produced can no longer be manually analyzed
  – requires domain experts and manual inspection

➢ **Let AI and DA automatically analyse data** to reveal interesting insights hidden within the data!
Case Study: “3D City over Night” (nFrames)

The illustration shows a textured 3D mesh of San Francisco. The data was provided by courtesy of Geomni. Copyright nFrames.

Scenario B: Parameter Sweeping via Feedback Loops

- Let AI models optimize the parameter space between simulations to reduce the overall number of required application runs [6]
  - Use output data from previous simulations to predict “better” input parameters to be used in future simulations
  - Drop simulations that are likely to yield similar results

• Advantages for the
  - User
    • saves time and resource costs
  - HPC center
    • saves energy
    • frees up resources to be allocated to other users

Scenario C: AI at the Edge

- Leverage full potential of Internet of Things via edge computing
  - Edge devices are becoming more powerful
  - Collect, preprocess, and analysis of (streaming) data
  - Avoid delays from sending everything into the Cloud

- Eliminate most communication with Cloud/HPC by making edge devices smarter: AI@edge
  - E.g. detect anomalies, generate predictions on the fly
  - A perfect fit for tasks such as predictive maintenance

- Typical workflow
  - 1) Run compute-intensive training of AI models on HPC
  - 2) Perform light-weight inferences at the edge
Scenario D: Mixed Workloads

➢ Let AI speed up simulations
  - AI-based models are able to replace computationally intensive-tasks in simulations
    • e.g. compute-intensive Monte Carlo simulations can be exchanged with a more light-weight trained AI model [7]

➢ Let AI improve simulation accuracy
  - Exploit AI methods to model physical aspects that are currently too complex to be understood entirely
    • e.g. effects of cloud formation are such a complex problem
    • meshes used for simulations are too coarse to model clouds
    • automatic grid optimisation during simulations through AI [8]

Why does Artificial Intelligence require HPC?
How can simulations benefit from AI?

CONVERGENCE OF HPC AND AI
Technical Challenges

• User needs
  – Combine and/or integrate AI into typical HPC workflows

• We should have an **unified software stack** and, ideally, a **single resource manager** to deploy AI workloads onto HPC

• Challenges and drawbacks
  – cf. next slide
Technical Challenges (cont’d)

• Allow DA/ML/DL frameworks to run on HPC systems
  – **Containerization** is the way to go (e.g. via Singularity)
  – Provide an **holistic resource manager** to run HPC, data analytics, machine learning and deep learning jobs
    • integration with PBS Pro, for example
  – Introduce **streaming processing** to HPC (IoT)

• **Large-scale AI**
  – Improve acceleration and scalability of AI on HPC
    • e.g. via offloading through RDMA (e.g. TensorFlow, Spark)

• Work on specific examples coming from the engineering domain to **showcase benefits** of the convergence of AI and HPC
Examples of Hybrid HPC/AI Workflows

- a) Synthetic data generation
- b) Define parameters for the simulation
- c) Initial solution is given by an AI model
- d) optimise the parameter space of simulations
- e) Iterations are alternating between AI and simulation
- f) Surrogate models (functions; equations)
Case Study: Distributed Learning on GPUs

• Problem: Material Characterization of Sheet Metals
  – Sheet metal forming processes require material parameters as input
  – Validation is very time-consuming (inverse parameter identification)

• Solution: Combination of FEM and DNN
  – Replace the time and compute-intensive inverse approach by DNN model to perform material parameter validation much more efficiently

  • **Phase 1:** FEM simulation generates synthetic data
  • **Phase 2:** Train a DNN model on the data to predict material parameters
Take Away Message

- **AI Strategy of HLRS** aligns well with the European one
  - Address societal challenges (e.g. ethics)
  - Support SMEs to work together on research problems
  - Push the convergence of AI and HPC; hybrid workflows

- The future of HPC requires a system architecture to run HPC, data analytics, machine and deep learning workflows **on the same system as part of a complex workflow** [9]

- Advancements of the AI software stack is required to leverage the full potential of HPC
  - Incorporation of container technologies into HPC (e.g. singularity)
  - Scaling of frameworks such as Spark (e.g. via RMDA support)
  - Interplay with shared file systems (e.g. Lustre) since AI frameworks are optimized for data locality

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Thank you!

Questions?

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