Developing HPC for Luxembourg's R&I

BUILDING TOWARDS A NATIONAL COMPETENCE CENTRE

Valentin Plugaru
Parallel Computing and Optimization Group
High Performance Computing Team
University of Luxembourg

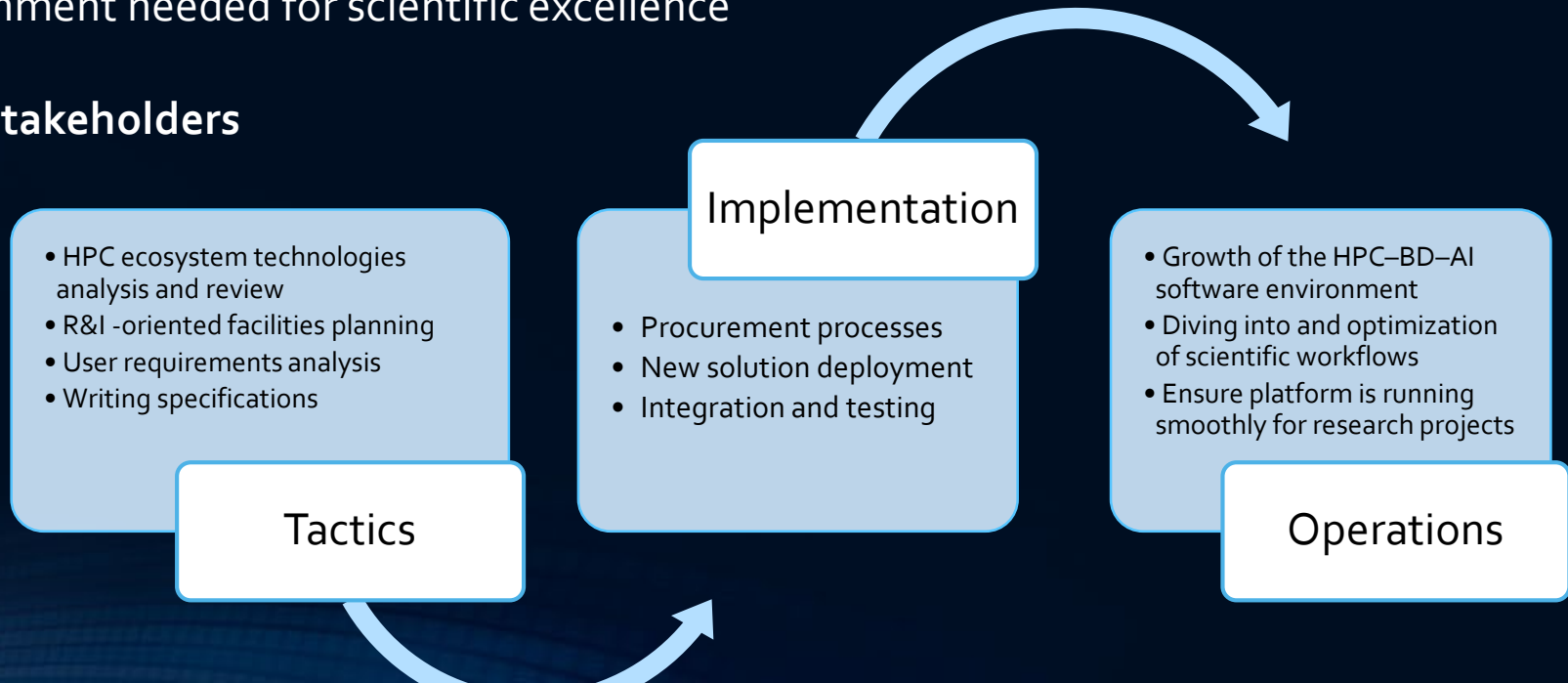
Context – the past four years

- **Overarching goal and responsabilities: growing Uni.lu HPC capabilities and software ecosystem**
  Bring in over a decade of expertise with HPC and cluster technologies to:
  - enable and accelerate research and innovation for national and international projects
  - drive change for the benefit of researchers facing evolving and challenging technology scene

- **Architecting solutions and integration of HPC technologies**
  - complete cycle from solution planning to implementation and operations
  - adapting leadership centers design choices to local needs
  - implementing the software environment needed for scientific excellence

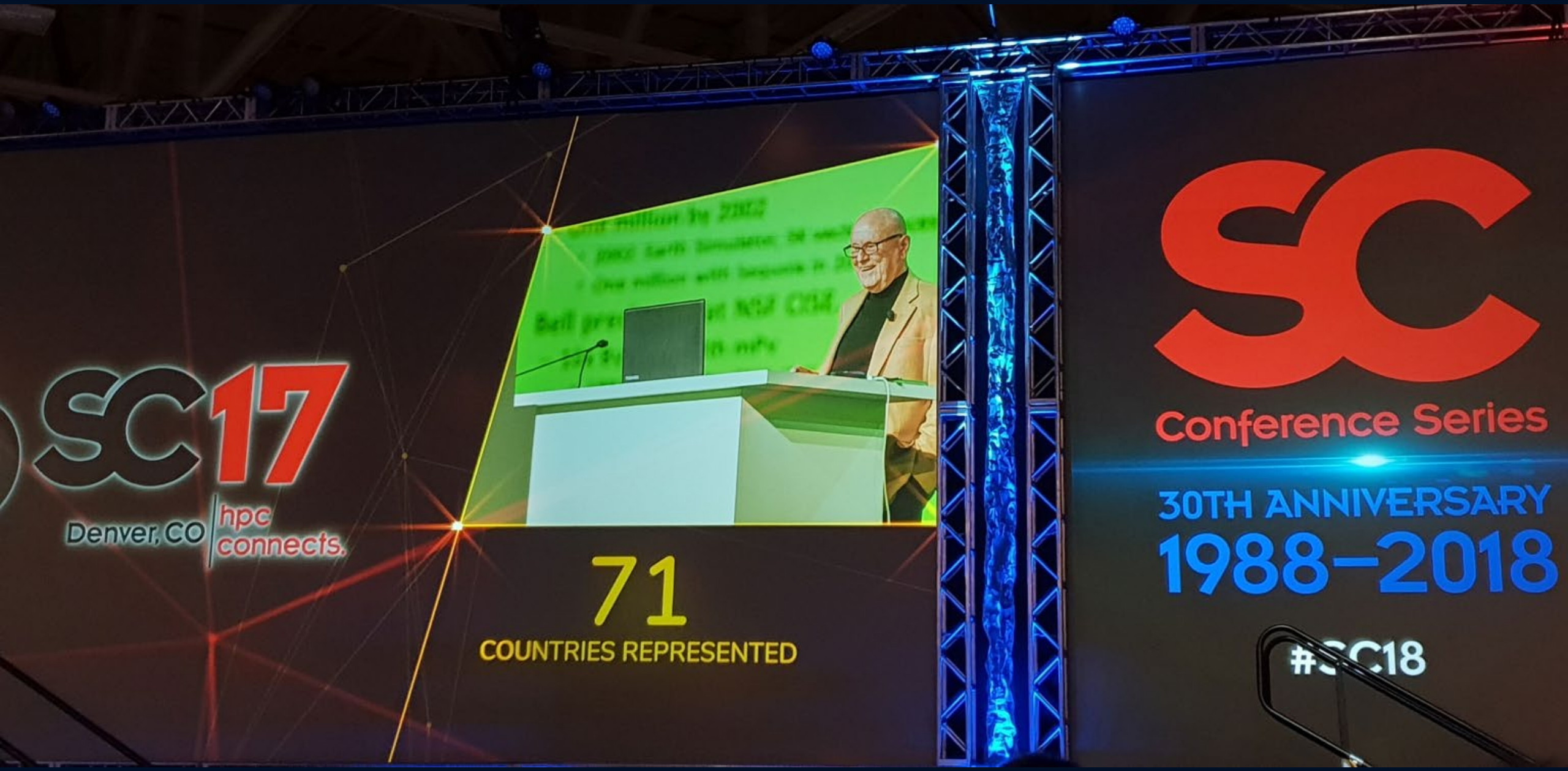
- **Building relationships and trust with stakeholders**
  - Top world HPC techology vendors
  - Industrial partnerships

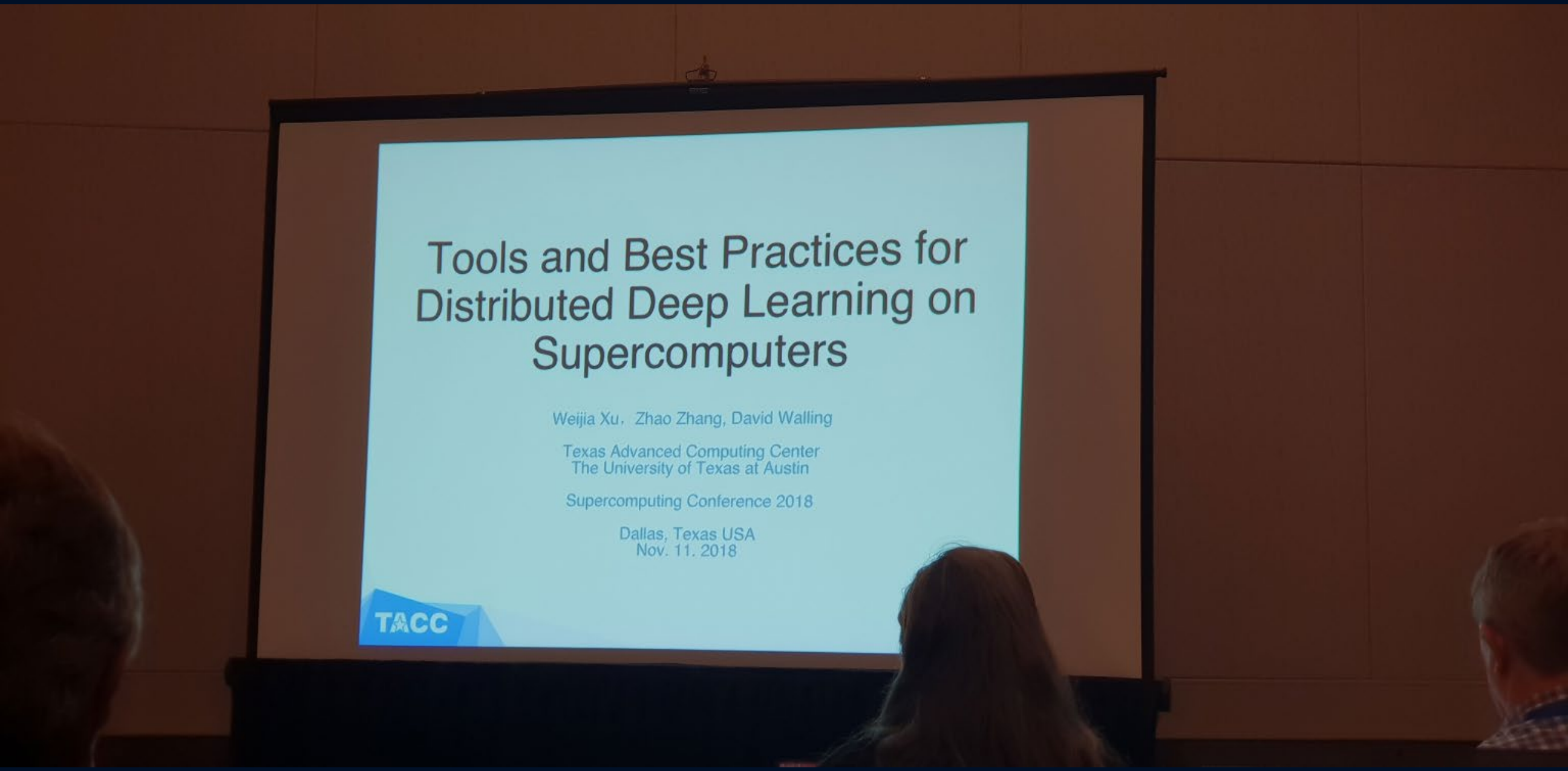
- **Knowledge transfer**
  - On-boarding new teams
  - Master-level teaching & projects
  - Organization of HPC workshops

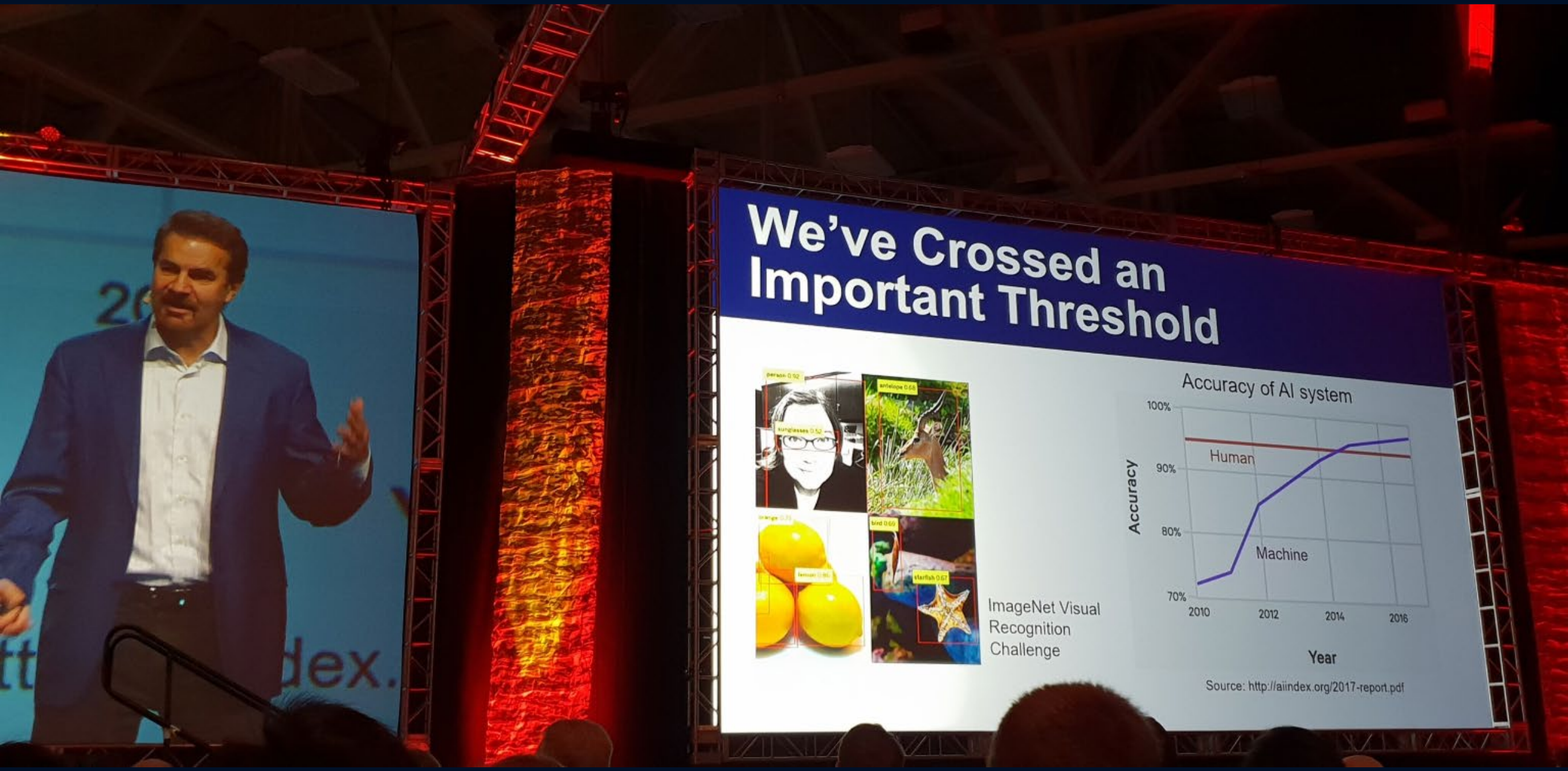


Spot the theme in the next slides
(short story time)

@Supercomputing
@SCconference
@SC_Conference
@sc_conference
SC18
Dallas, TX
hpc inspires.
@Supercomputing
@SCconference
@SC_Conference
@sc_conference


SC17
Denver, CO
hpc connects.
71
COUNTRIES REPRESENTED
SC
Conference Series
30TH ANNIVERSARY
1988–2018


Tools and Best Practices for Distributed Deep Learning on Supercomputers
Weijia Xu, Zhao Zhang, David Walling
Texas Advanced Computing Center
The University of Texas at Austin
Supercomputing Conference 2018
Dallas, Texas USA
Nov. 11. 2018
TACC


We've Crossed an Important Threshold
ImageNet Visual Recognition Challenge
Accuracy of AI system
100%
90%
80%
70%
Accuracy
Human
Machine
2010
2012
2014
2016
Year
Source: http://aiindex.org/2017-report.pdf

NVIDIA.
APPLYIN EP LEARNING
Bryan Catanz

FLOW BASED GENERATIVE MODELS
Laurent Dinh, et al., 2014, 2016
Generative model:
sample x from an unknown distribution: $x \sim p^*(x)$
Easy, if we only knew the distribution!
x is a multidimensional vector
Flow based model:
Training
This is a change of variables!
Simple distribution
z
network

NASA
NASA
EXPLORE
National Aeronautics and Space Administration
AISLE
2700/280
AISLE
2200
2200
AIST
Integration for Innovation
AIST
NASA@SC
GMAO
Global Modeling and Assimilation Office
Aerosol Extinction AOT [550 nm]
081 Forecast Hours
In the Beginning ...

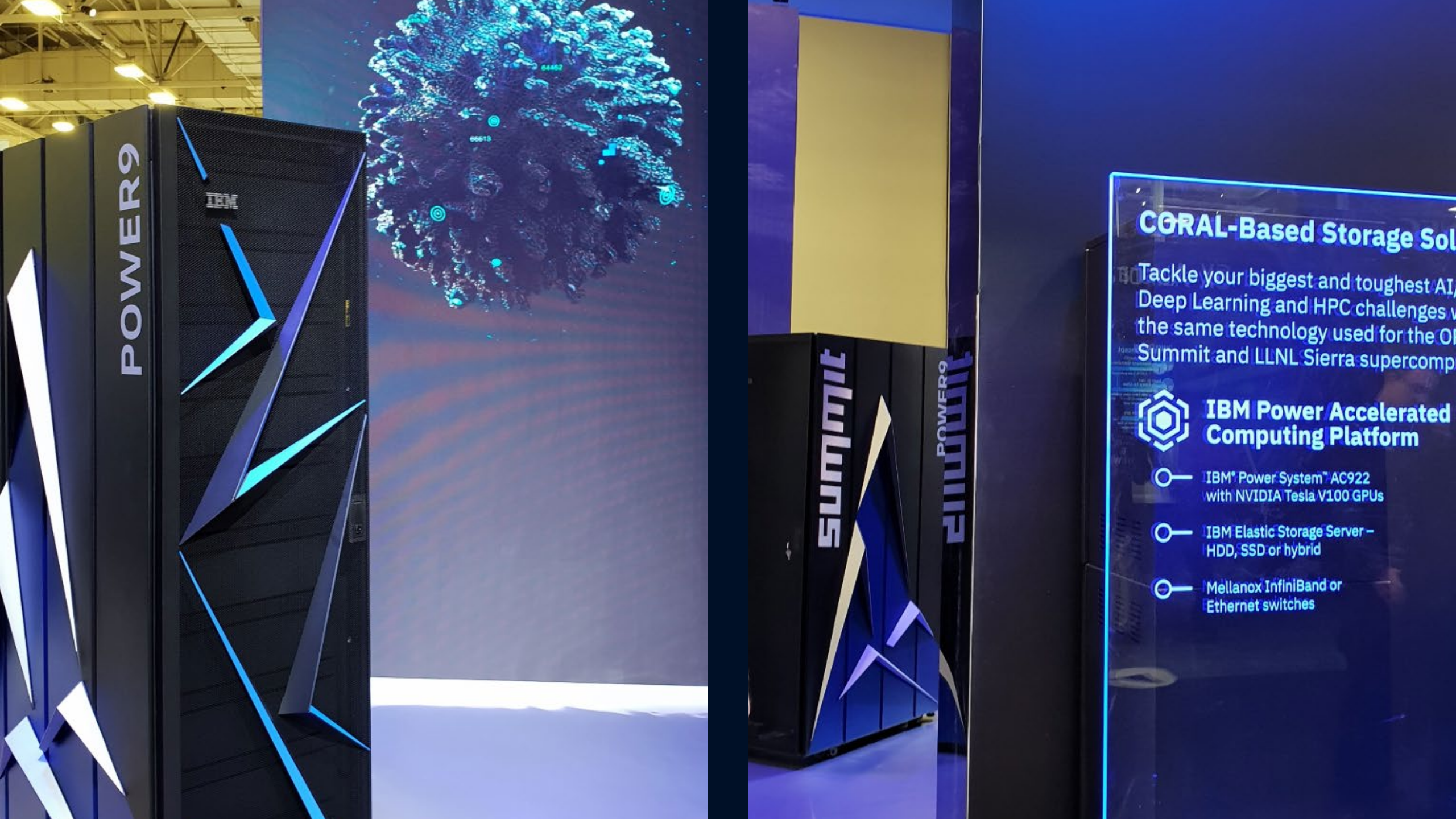
Hewlett Packard Enterprise
intel
Supercomputing in Space
Supercomputing in Space

BOXX
Built for Deep Learning &
APEXX NEUTRINO™
2nd gen 32-core AMD Ryzen™ Threadripper™ professionally overclocked
Four NVIDIA Tesla® V100 GPUs
Advanced liquid cooling for CPU and GPUs
NVIDIA
AI IMITATING ART
Real-Time Artistic Transfer
NVIDIA TESLA V100 GPU, PYTORCH, ONNX, NVIDIA TENSORRT
TYAN
TYAN
GOMI

TRANSFORMING THE FUTURE
intel
Flexibility
Energy efficiency
DELL EMC
POWEREDGE
R640 SERVER
WITH FPGA's
MEET THE EXPERTS
NVIDIA
atipa
TYAN
STULZ
MATLAB
ARI
HPC

Technologies
TRANSFORMING THE FUTURE
TYAN
TYAN
TRANSFORMING
NVIDIA
intel
STULZ
ARISTA
KEK
MEET THE EXPERTS
HPC 2018

ALE YOUR
OVATION
TECHNOLOGY
SHOWCASE
INTEL® RENDERING FRAMEWORK
IN ACTION!
Argonne
NATIONAL LABORATORY
ENERGY
National
Laboratories
Altair
arm


POWER9
IBM
summit
POWER9
CORAL-Based Storage Sol
Tackle your biggest and toughest AI,
Deep Learning and HPC challenges w
the same technology used for the OR
Summit and LLNL Sierra supercomp
IBM Power Accelerated
Computing Platform
IBM® Power System™ AC922
with NVIDIA Tesla V100 GPUs
IBM Elastic Storage Server –
HDD, SSD or hybrid
Mellanox InfiniBand or
Ethernet switches

ACCELERATE YOUR
INTELLIGENT TRANSFORMATION
ThinkAgile
ThinkSystem
THE BEST USE OF HPC
PHYSICAL SCIENCE
SciNet
Innovation in Storage
Book A Meeting
AI Infrastructure
Solutions
Best AI
Product or Technology
NGC-READY
THE UNIVERSITY OF TEXAS
Lenovo

NVXL
Polymorphic Acceleration
NVXL
X-ScaleSolutions
Comprehensive Solutions for HPC, Big Data, and Deep Learning
Custom Solutions
End User Training
Tuning and Optimization
THE OHIO STATE UNIVERSITY
HiDL
MVAPICH
Scalable and Distributed Deep Learning (DL): Co-Design MPI Runtimes and DL Frameworks
OSU Booth Talk (SC '18)
MVAPICH
High Performance Solutions for High Performance Systems
Parallel Programming Libraries
Benchmarks
Tools
THE OHIO STATE UNIVERSITY
Network Based Computing Laboratory
Accelerating Discovery
High Performance Big Data
Empowering Big Data using HPC Technologies
Scalable Big Data Frameworks
Benchmarks
Tools
High Performance Interconnects
Stream Processing

Carme
oves Your Machine Learning Tool Chain
o a HPC Environment
ww.open-carme.org
rme Key-Features:
en Source
ractive, Secure Multi User Environment
and Data Science users want interactive
access to compute resources
Management
rates into existing LDAP
ainer Management
luler
ates into existing SLURM
Management and I/O
d DS GUI → Interactive Web-Interface
le Framework
ted multi-GPU Deep Learning
Maintenance + Monitori
DEEP LEARNING
Accelerate and Simplify AI on HPC Systems
TensorQuant
A Simulation Toolbox for Deep Neural Network Quantization.
www.tensor-quant.org
Open-source Tensorflow plugin:
Simulates training and inference of DNNs on Hardware with sparse and quantized tensor operations.
Answers open questions like:
How accurate is a given model with 8-bit fixed point arithmetic?
How much sparsity can be enforced during training?
HP-DLF
Deep Learning without Memory Limits
Automatic Parallelization of Large DNN's (ONNX) across Heterogeneous Computer Cluster (CPU, GPU, FPGA).
Removing the Memory Limitations of Current implementations
Fraunhofer
ITWM
MEMORY DRIVEN COMPUTING
The Paradigm Change to User friendly Parallel Programming
GPI-SPACE
ALOMA
Next Generation Data Processing & QC For the Oil & Gas Industry
GPI-Space: The Technology behind ALOMA & HP-DLF
Application Independent Global Memory
Workflow Management using Petri Nets
Distributed Runtime
Fault tolerance
Project Carme
An open source software stack for multi-user GPU cluster

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QCT
www.QCT.io
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intel®

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CSCS
ETH ZURICH

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FIND THE BUNNYPEOPLE
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FPGA Accelerators
NGS Analytics Solution
AI Inferencing
UNIVA
Hewlett Packard Enterprise
NVIDIA
Optimize Your AI Solution Customized Recipes Using HPE Deep Learning Cookbook
Artificial Intelligence High-Performance Compute Services and Expertise

SETEK
ASET
RELIABLE PROVEN FLEXIBLE
HPE SGI
8600 System
arm
2600
DDN

Intelligent Computing Empowering AI
Full Stack AI Solution
Inspur FPGA Acceleration Solution:
Object Recognition Powered By F10A+TF2
inspur
Efficient AI Management Suite
AIStation
AI Deep Learning Cluster Management Software
Deploy deep learning environment
Teye
AI Application Performance Monitor and Analyzer
Parameters Monitoring: complete and in-depth data
Analysis and Diagnosis: Initial data visualized
System Optimization: Increase software and hardware combination efficiency
AGX-5
inspur
Inspur FPGA Acceleration Solution
Real-time Object Recognition Powered By F10A+TF2
inspur
PERFORMANCE
LATENCY
0.106 ms
THROUGHPUT
1465.8 FPS
EFFICIENCY
32.574 images/w/s
REMOTE CONTROL
AGX-2
inspur
AISLE
1400
DDN
STORAGE
1400
NCAR
Leading HPC Solution

SC18
BIRDS OF A FEATHER
TOP500 SUPERCOMPUTERS

#	Site	Manufacturer	Computer	Country	Cores	Rmax [Pflops]	Power [MW]
1	Oak Ridge National Laboratory	IBM	Summit IBM Power System, P9 22C 3.07GHz, Mellanox EDR, NVIDIA GV100	USA	2,397,824	143.5	9.8
2	Lawrence Livermore National Laboratory	IBM	Sierra IBM Power System, P9 22C 3.1GHz, Mellanox EDR, NVIDIA GV100	USA	1,572,480	94.6	7.4
3	National Supercomputing Center in Wuxi	NRCPC	Sunway TaihuLight NRCPC Sunway SW26010, 260C 1.45GHz	China	10,649,600	93.0	15.4
4	National University of Defense Technology	NUDT	Tianhe-2A ANUDT TH-IVB-FEP, Xeon 12C 2.2GHz, Matrix-2000	China	4,981,760	61.4	18.5
5	Swiss National Supercomputing Centre (CSCS)	Cray	Piz Daint Cray XC50, Xeon E5 12C 2.6GHz, Aries, NVIDIA Tesla P100	Switzerland	387,872	21.23	2.38
6	Los Alamos NL / Sandia NL	Cray	Trinity Cray XC40, Intel Xeon Phi 7250 68C 1.4GHz, Aries	USA	979,072	20.16	7.58
7	National Institute of Advanced Industrial Science and Technology	Fujitsu	AI Bridging Cloud Infrastructure (ABCI) PRIMERGY CX2550 M4, Xe[illegible]Gold 20C 2.4GHz, IB-EDR, NVIDIA V100	Japan	391,680	19.9	1.65
8	Leibniz Rechenzentrum	Lenovo	SuperMUC-NG ThinkSystem SD530, Xe[illegible]m 8174 24C 3.1GHz, Intel Omni-Path	Germany	305,856	19.5	
[illegible]	Oak Ridge National Laboratory	Cray	Titan Cra[illegible]K7, [illegible]16C 2.2[illegible]nini, NV[illegible]	U[illegible]A	[illegible]60,640	17[illegible]	8.21
10	Lawrence Livermore National Laboratory	IBM	B[illegible] BOC[illegible], C[illegible]	[illegible]	[illegible]64	[illegible]	[illegible].89

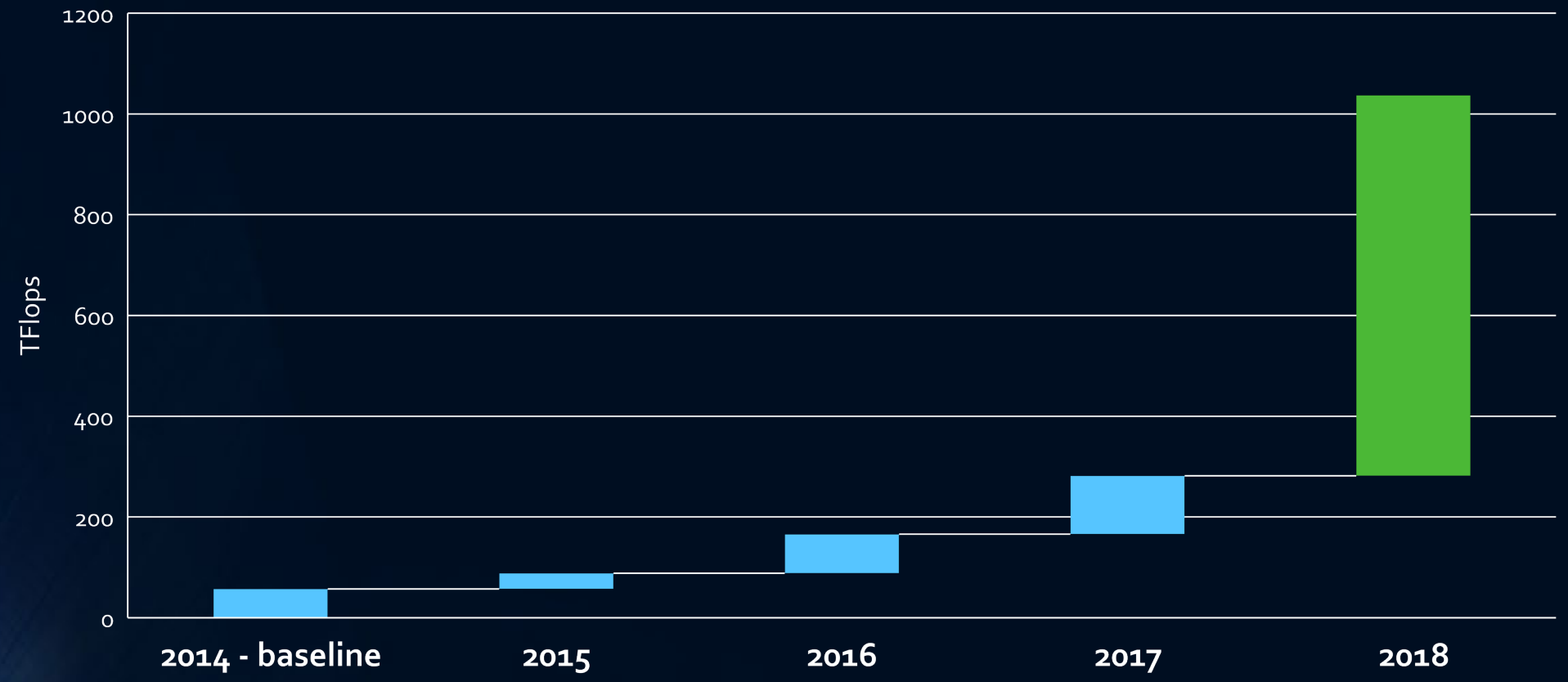
PRACE
Partnership for Advanced Computing in Europe
PROVEN
Altair
Hewlett Packa
Enterprise
DOE: Seven Decades of HPC Leadership
intel
SAGE Implemented System Stack
Tools
Use Case Access Methods
OBJECT STORE
www.prace-ri.eu
PRACE

EXIT
ETP 4
HPC
ROPEAN
CHNOLOGY
ATFORM
R HIGH
FORMANCE
MPUTING
The EuroHPC Joint Undertaking
Mission & Objectives
Mission: Establish an integrated world-class supercomputing and data infrastructure and support a highly competitive and innovative HPC and Big Data ecosystem
Objectives
1. An integrated world-class supercomputing and data infrastructure
– 2 pre-exascale + 2-3 petascale by 2020; 2 exascale by 2022/2023 (1 EU tech); post-exascale infrastructure by 2027
– federation of HPC infrastructures at European level
– hybrid HPC/Quantum infrastructure
2. Research and innovation for a HPC and Big Data ecosystem
– an integrated European HPC R&I agenda
– independent HPC technology supply
– excellence in HPC applications and use
– HPC Competence Centres, training/skills, outreach

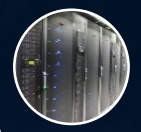
EXIT
ETP 4 HPC
EUROPEAN TECHNOLOGY PLATFORM FOR HIGH PERFORMANCE COMPUTING
EuroHPC in the next MFF (2021-2027)
Work in progress
Digital Europe programme
Commission proposal of 06 June
Investing in the future:
Digital Europe Programme
Digital transformation & Interoperability
1.3 € billion
€ 9.2 billion in total
Advanced digital skills
0.7 € billion
High performance computing
2.7 € billion
Cybersecurity & trust
Artificial intelligence
2.5 € billion

EXIT
ETP 4 HPC
EUROPEAN TECHNOLOGY PLATFORM FOR HIGH PERFORMANCE COMPUTING
DEEP Projects
Modular Supercomputing Architecture
• Address diverse user requirements in one system
– Data intensive
– Highly scalable parallel computing
– High throughput computing
• Modules shaped via co-design
• Achieve leading scalability & energy efficiency
– Extreme Scale Booster → Exascale
• Unified SW environment to run applications across all modules
CN
CLUSTER MODULE
EXTREME SCALE BOOSTER
NETWORK FEDERATION
SCALABLE STORAGE SERVICE MODULE
DATA ANALYTICS MODULE
SN
FE
DN
NAM
GCE
40

Uni.lu HPC core computational capacity



Software & Integration



Integration with Uni.lu high capacity storage system (now 3.3PB)

Expanding user software environment with ISV & community codes (200 pkg.)

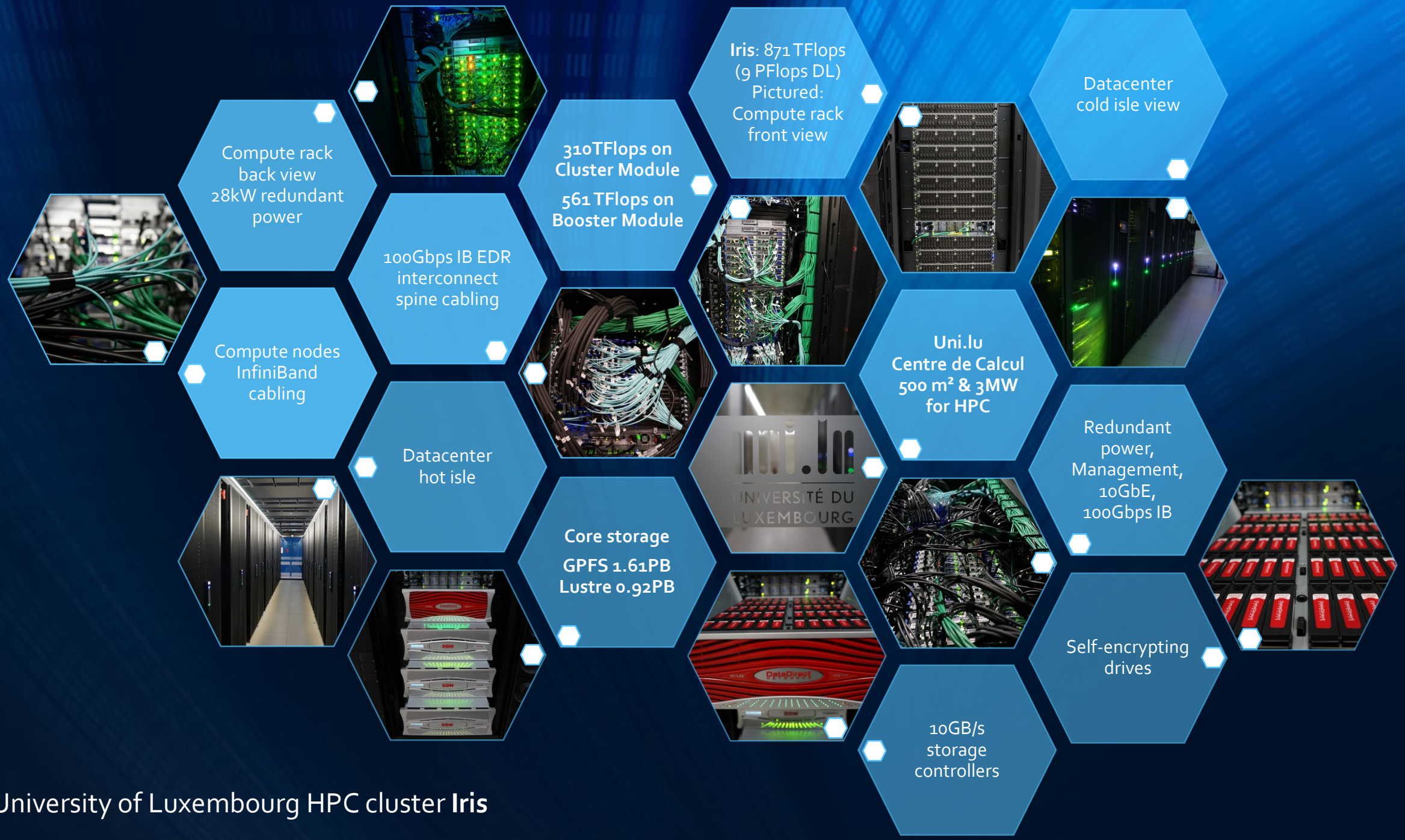
New core technologies in line with world leadership supercomputing centers

17x growth

... of computational capacity in 4 years

... with increasing capability, matched by software environment

2018 additions oriented towards AI/Machine Learning & BD work



University of Luxembourg HPC cluster **Iris**

Math, Statistics & Optimization

- MATLAB
- Mathematica
- STATA
- CPLEX
- Gurobi Optimizer

Physics & Chemistry

- GROMACS
- ESPResSo
- Yambo
- QuantumESPRESSO
- Meep
- ABINIT
- NAMD
- CP2K
- NWChem
- VASP
- CRYSTAL

CAD, CAE & CFD

- ANSYS
- ABAQUS
- OpenFOAM

Development & Performance

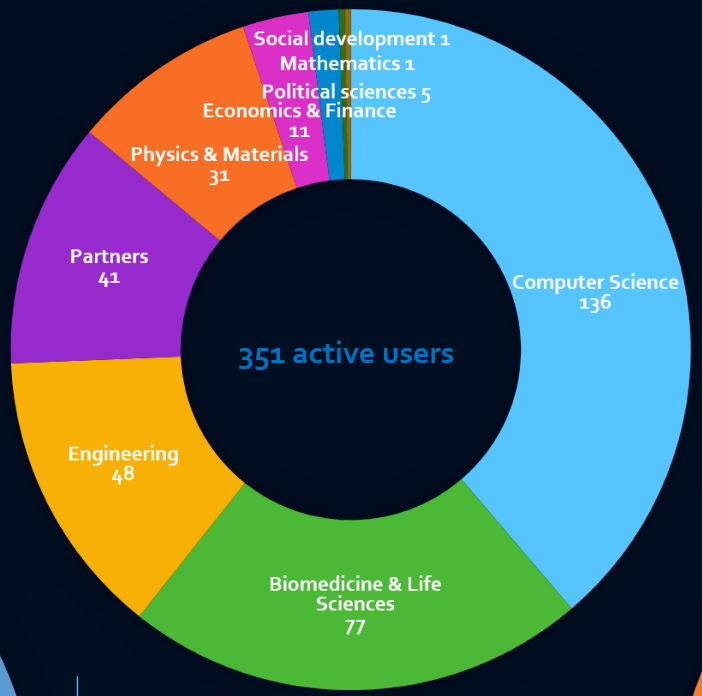
- Intel, GCC, PGI compiler suites
- Python, R & Perl
- Go & Rust
- Intel Advisor, Inspector, Trace Analyzer and Collector, VTune Amplifier
- ARM Forge & Performance Reports
- Scalasca & Score-P
- PAPI
- Singularity containers

Machine & Deep Learning

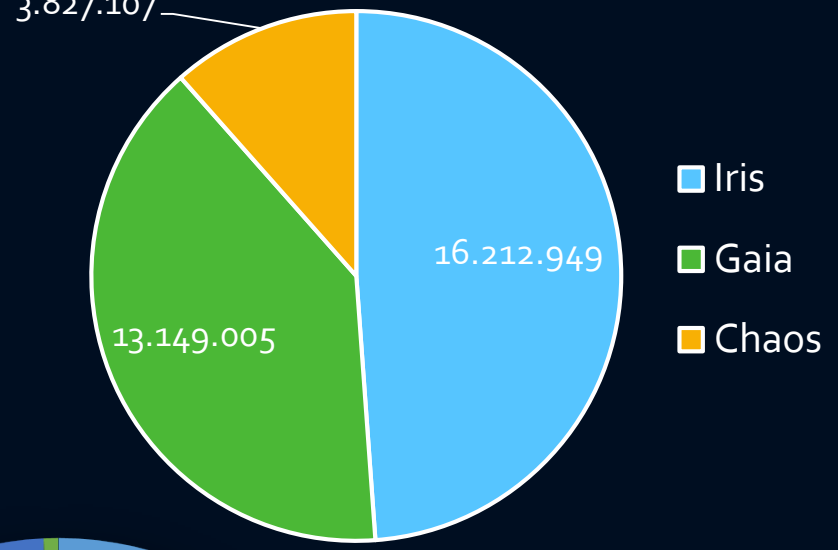
- Keras
- Tensorflow
- PyTorch
- MXNet
- Apache Spark

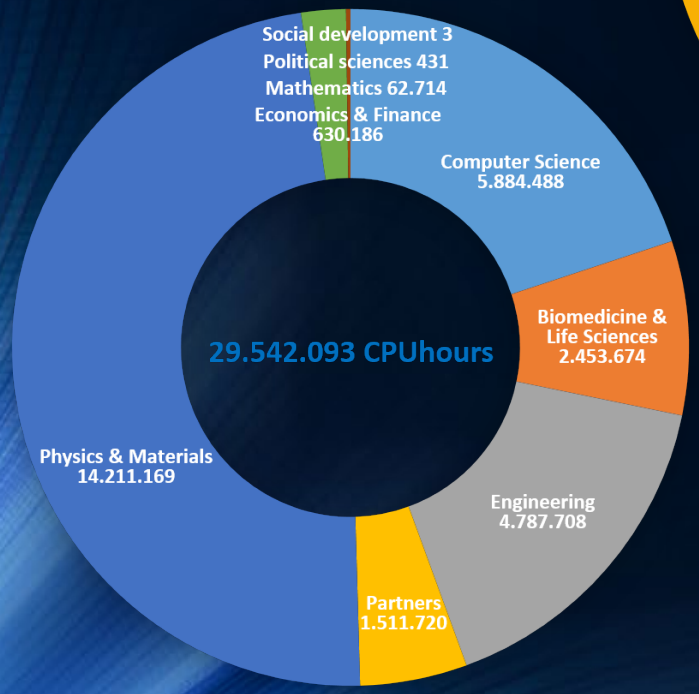
Rich software environment delivered to Uni.lu researchers and partners in 2018

Some figures



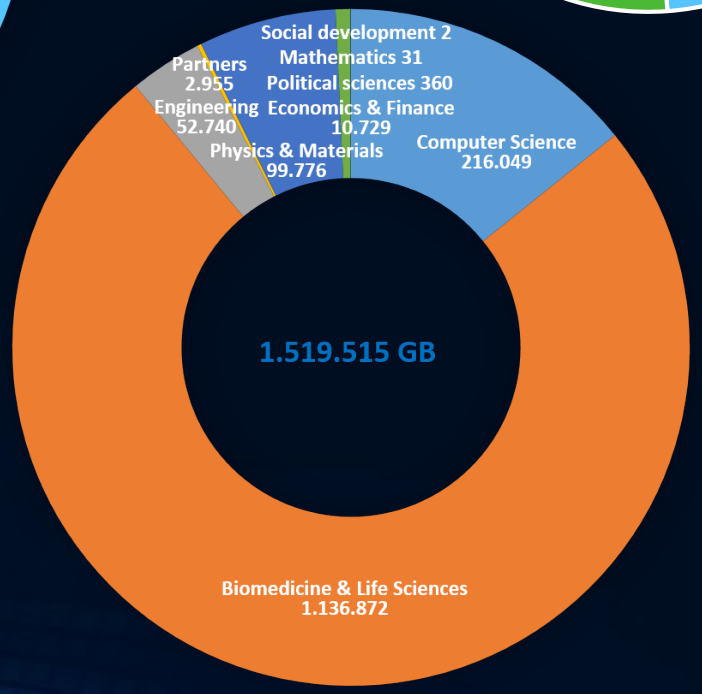
33M coreHours delivered for R&I
Nov 2017 – Nov 2018





June 2017

June 2018



Enabling outstanding science

At the ninth edition of the FNR Awards, several researchers of the University of Luxembourg won prizes in two categories for their work on a model of the human intestine and socially assistive robots, respectively.

Outstanding Scientific Publications category

Pranjul Shah and Paul Wilmes from the Luxembourg Centre for Systems Biomedicine (LCSB) of the University of Luxembourg won one of the two prizes that were awarded in the category "Outstanding Scientific Publications". They were honoured for their paper "A microfluidics-based in vitro model of the gastrointestinal human-microbe interface" that was published in the scientific journal "Nature Communications". In their research, they developed a technology to mimic the conditions in the human intestine.

FNR AWARDS 2017

"Grand Prix 2018 en sciences biologiques" awarded to Paul Wilmes

Share this article:

Published on Monday, 19 November 2018

The Grand Prix 2018 in biological sciences of the Institut Grand-Ducal, sponsored by the company Cactus, has been awarded to Associate Professor Paul Wilmes by an international jury consisting of professors and experts in biology.

He has received the prize on 17 November 2018 at the Chamber of Commerce of Luxembourg, on the occasion of an academic session.

Paul Wilmes is an Associate Professor of Systems Ecology at the Luxembourg Centre for Systems Biomedicine (LCSB) of the University of Luxembourg. He obtained his PhD in 2006 from the School of Environmental Sciences at the University of East Anglia in Norwich (UK), a part of his doctoral research having been conducted at the Max Planck Institute for Marine Microbiology in Bremen (Germany). After three years of postdoctoral research at the University of California, Berkeley (USA), he returned to his native Luxembourg in early 2010 through an ATTRACT Fellowship of the Luxembourg National Research Fund (FNR). He initially established his research group at the Centre de Recherche Public – Gabriel Lippmann (now Luxembourg Institute of Science and Technology, LIST) but later joined the LCSB where he is the Head of the Eco-Systems Biology research group.

Luxembourg'. Bioinformatics analyses presented in this paper were carried out in part using the HPC facilities of the University of Luxembourg (http://hpc.uni.lu).

ETP4HPC: The European Technology Platform for High Performance Computing

- Member and Uni.lu central contact point for the ETP4HPC Work Groups, I participate in 7 WG:
  HPC System Architecture & Components, Systems Software & Management, Programming Environment, Energy & Resilience, Balance Compute I/O & Storage Performance, Big Data & HPC Use Models, Extreme-scale demonstrators

- Worked on proposals for the European Commission's HPC Work Programme 2018-20.

- Worked on the **3rd Strategic Research Agenda** (SRA3): outline roadmap for the achievement of exascale capabilities by the European HPC ecosystem. Milestones used to define the contents of the HPC Technology R&D Work Programmes managed by the European Commission.

ISO/IEC JTC 1/SC 39: Sustainability for and by Information Technology

- ILNAS: Registered expert as national ICT standardization delegate.

- Participation to the standardization process on multi-year drafting process.

ISO/IEC JTC 1/SC 42: Artificial Intelligence (AI)

- Exploring work being done for AI standardization, in particular use-cases at international level

http://www.etp4hpc.eu/sra
https://www.iso.org/committee/654019.html

Teaching activities

Workshop on "High-Performance Computing and Cloud Computing Platform"

4 - 8 September 2017 at NECTEC, Thailand

Master in Information and Computer Sciences

UL MiCS3 - Parallel and Grid Computing course

Yearly, Winter Semester

UL HPC School

Advanced Track Sessions

Yearly (June 12-13 & November 23 in 2018)

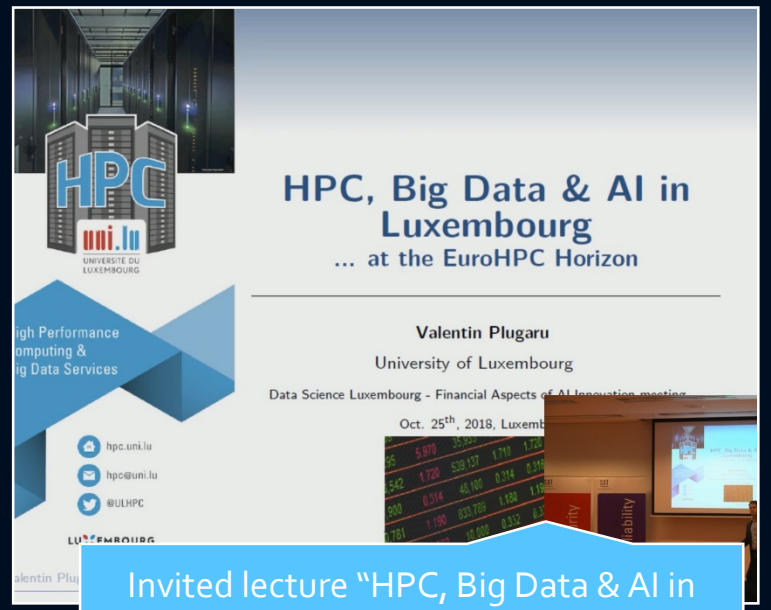
Knowledge transfer activities

Workshop on "High Performance Computing facility management"

with NSTDA-NECTEC (Thailand)
11 - 15 June 2018 (Luxembourg)

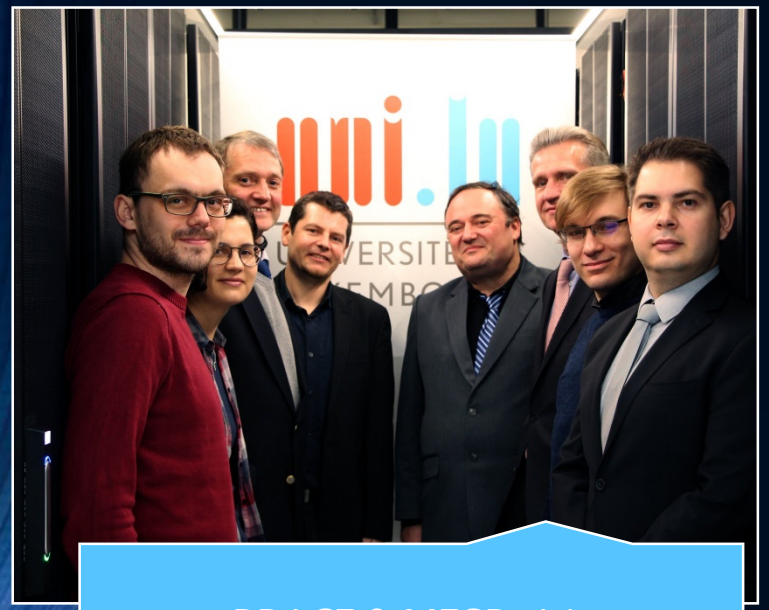
Workshop on "High Performance Computing facility management"

with TU Delft – DHPC (Netherlands)
6 September 2018 (Luxembourg)



Invited lecture "HPC, Big Data & AI in Luxembourg"
Data Science Luxembourg – *Financial aspects of AI Innovation*, 25 October 2018

Delegations & visits



PRACE & MESR visit
12 February 2018

EC – DC DIGIT, DC CNECT, DC HR & MECO visit

22 June 2018

HPC User Forum visit

HLRS / U. Stuttgart

1-2 October 2018

What comes next

National competence centre

… built with world's best technologies we've explored in the past years
… using HPC expertise in the software needed to run large-scale projects

for science and industry

LUXEMBOURG
LET'S MAKE IT HAPPEN

Valentin Plugaru
Parallel Computing and Optimization Group
High Performance Computing Team
University of Luxembourg