NEW MEMBERS
PRESENTATIONS BY OUR NEW MEMBERS

Evangelos Floros - GRNET
Dr Alain Refloch - ONERA
Dr Giovanni Bracco - ENEA
Dr Sebastien Varrette – University of Luxembourg
Dr Mike Dewar – NAG Ltd
Sabri Pllana PhD - Individual member
Carlo Cavazzoni PhD on behalf of Quantum Expresso Foundation
Dr Johannes Langguth - Simula Research Laboratory
Dr Martin Palkovic - IT4Innovations National Supercomputing Center
Prof Jesus Carretera – University Carlos III Madrid
Vincent Hindriksen - StreamComputing
GREEK RESEARCH AND TECHNOLOGY NETWORK
SUPERCOMPUTING SERVICES

EVANGELOS FLOROS
Greek Research and Technology Network
Supercomputing Services

Vangelis Floros
ETP4HPC General Assembly
Munich, 21/3/2017
GRNET at a glance

Government owned company
• Operating under the auspices of Ministry of Education and the General Secretariat of Research and Technology

Academic & Research Network Provider
• Greek NREN. Connectivity to GEANT
• 87 PoPs
• 8410 km optical fibre network

Computing Services
• 4 Data Centers (Athens, Crete, Epirus)
• Grid Computing
• Cloud Computing
• High Performance Computing
ARIS (Advanced Research Information System)

Most powerful system in Greece for Scientific Computing
- 444 TFlop/s peak aggregate performance; 11,520 x86 cores
- Mixed architecture: Thin nodes, Fat nodes, NVidia GPUs (Tesla K40), Intel Xeon Phi (7120P)
- 2PB GPFS Storage, 2PB Tape Library
- Infiniband FDR 1:1 Interconnect
- Top500 #468 (June 2015)

System Usage
- Free access to Greek scientific community
- Access policy based on production and preparatory periodic calls
- So far: 3 production calls; 205 projects; 134M core-hours allocated
- PRACE Tier-1, DECI
Competence Areas

Areas and domains of interest and expertise include:
• e-Infrastructure provisioning and coordination activities
• Scientific community support
• Leading role in Greece & South-Eastern Europe HPC activities

Organizations - Memberships
• PRACE AISBL
• ETP4HPC
• EGI.eu
• EUDAT
• EPIC
• GEANT

HPC Projects
• PRACE-IPs
• ViSEEM (coordinators)
• HPC-Europa
• SESAME-Net
thank you

Useful Links
GRNET main web site: [http://www.grnet.gr](http://www.grnet.gr)
HPC Service web site: [http://hpc.grnet.gr](http://hpc.grnet.gr)

Generic Information: hpc-info@lists.grnet.gr
Access information: hpc-access@lists.grnet.gr
Tech support: support@hpc.grnet.gr
ONERA

Dr Alain Refloch
ONERA: The French Aerospace Lab

Innovation, expertise and long-term vision for industry, French government and Europe

A balanced business portfolio:
• 1/3 civil
• 1/3 defense
• 1/3 dual-use

• A public entity created in 1946
• Reporting to the Ministry of Defense
• 2,000 employees
• 247 doctoral students and post-docs
• 230 million euro budget
• 45% contract-based business
• Largest fleet of wind tunnels in Europe
ONERA & HPC : 1984 - 2017

- Cray supercomputer: 1 s (1984), 2 (in CCVR), XMP, YMP, C90
- Intel Paragon (1997): excellence center for DGA
- NEC super computer: SX4 (1998), SX5, SX6, SX8
- Superscalar BULL (2005): 528 cores Itanium

Spring 2017: 17360 cores BDW - 566 Tflops Linpack
End 2018: option for Skylake cores -> 1 Pflops

IPCC Intel with the FAST project
**elsA Multi-purpose CFD simulation platform**

- Internal and external aerodynamics, From low subsonic to high supersonic, for Compressible 3-D Navier-Stokes equations, with Moving deformable bodies, for Aircraft, helicopters, turbomachinery, CROR, missiles, launchers...
- Python/C++/Fortran 1.7 M lines of code

**Onera and research partners**

- Onera departments, Cerfacs, Dynfluid, LMFA, Cenaero, Von Karman Institute, …

**Industry users & clients**

- Airbus, Safran (*Snecma, Turbomeca, Techspace Aero*), Eurocopter, …

**CEDRE**: Simulation tools for propulsion and energetics, using **generalized unstructured grids** for **Multiphysics** simulations, with Internal Solvers:
  - Navier-Stokes multiple-species, turbulent, reactive, Dispersed phases (Eulerian), Dispersed phases (Lagrangian), Convection-Diffusion, …
Dr Giovanni Bracco
A 3 slides presentation about ENEA, the Italian National Agency for New Technologies, Energy and Sustainable Economic Development, now a member of ETP4HPC

ETP4HPC General Assembly, Munich 21/3/2017

G. Bracco, S. Migliori, A. Quintilian
ENEA Energy Technologies Department, DTE-ICT
giovanni.bracco@enea.it, silvio.migliori@enea.it, andrea.quintilian@enea.it
Research and development activities in the field of energy, environment and new technologies; dissemination and transfer of knowledge and innovation to industry, institution and civil society at large.

9 Research Centres, 5 Research laboratories
11 territorial offices, Brussels Liaison Office, Rome Headquarters
~2500 permanent staff

3 Departments:
- Fusion & Nuclear Safety
- Sustainability of territorial systems
- Energy Technologies:
  - Photovoltaics & Smart Networks
  - Thermal and Thermodynamic Solar Division
  - Bioenergy, Biorefinery and Green Chemistry
  - Efficient production, Conversion and Use of Energy
  - Smart Energy
  - Information and Communication Technology (HPC & Services, ~80 staff)
HPC ~20 permanent staff
**ENEAGRID/CRESO Clusters**

ENEA HPC resources are integrated into **ENEAGRID** (AFS file system HOMES, GPFS (1.3 PB) as PFS, LSF job management). 6 Research Centres connected by GARR, the Italian NREN. The main computing facilities are **CRESO clusters** (~165 Tflops), main site is **Portici** (Naples).

<table>
<thead>
<tr>
<th>Cluster name (Linux x86_64)</th>
<th>Network</th>
<th>Cores/Tflops</th>
<th>Research area 2015</th>
<th>Usage (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CRESCO3 AMD</td>
<td>IB DDR</td>
<td>2016/~17</td>
<td>Material science</td>
<td>55.7</td>
</tr>
<tr>
<td>CRESCO4 INTEL</td>
<td>IB QDR</td>
<td>4864/~100</td>
<td>Combustion</td>
<td>16.7</td>
</tr>
<tr>
<td>CRESCO5 INTELv3</td>
<td>IB QDR</td>
<td>672/~25</td>
<td>Nuclear energy</td>
<td>8.4</td>
</tr>
<tr>
<td>CRESCO6F AMD</td>
<td>IB QDR</td>
<td>456/~4</td>
<td>Climate</td>
<td>7.7</td>
</tr>
<tr>
<td>CRESCOC AMD</td>
<td>IB DDR</td>
<td>192/~1.5</td>
<td>Complex systems</td>
<td>1.1</td>
</tr>
<tr>
<td>K40 PHI/Large RAM</td>
<td>IB QDR</td>
<td>300/~17</td>
<td>Biotec</td>
<td>0.4</td>
</tr>
<tr>
<td><strong>Total in production</strong></td>
<td>~8500/~165</td>
<td></td>
<td>Aerospace</td>
<td>0.3</td>
</tr>
<tr>
<td><strong>Q3’17 CRESCO6</strong></td>
<td>SKL OPA</td>
<td>~10000/~700</td>
<td>Minor activities</td>
<td>9.7</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Type of users 2015</th>
<th>Number of users</th>
</tr>
</thead>
<tbody>
<tr>
<td>ENEA</td>
<td>67 (48.6 %)</td>
</tr>
<tr>
<td>ENEA contract</td>
<td>32 (23.2 %)</td>
</tr>
<tr>
<td>Italian Univ./Inst.</td>
<td>30 (21.7 %)</td>
</tr>
<tr>
<td>Foreign Univ./Inst.</td>
<td>5 (3.6 %)</td>
</tr>
<tr>
<td>Enterprises</td>
<td>4 (2.9 %)</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>138</td>
</tr>
</tbody>
</table>

In the context of the Italian HPC ecosystem, an agreement has been signed between ENEA and CINECA to promote joint activities. In this framework ENEA/CINECA has provided to EUROFUSION the **MARCONI-FUSION** system 1-5 Pflops, in operation since 2016/Q3.
ENEAG participation in National/European HPC/ICT projects

**Topics of interest and opportunities:**

- HPC infrastructures & technologies, applications (material science), distributed data management, I/O performances, collaboration and remote access tools...
- Many different systems for testing and benchmarking

**Main previous projects:**

- European: Dc4Cities 2013-2015 [An environmentally sustainable data center for Smart Cities]

**Running projects:**

  Energy oriented Centre of Excellence for computing application (Transversal basis, Meteorology, Materials, Water, Nuclear Fusion)
  - WP1/Task3 Efficient I/O (Juelich, PSNC, ENEA, CEA)
  - WP3 Materials (WP leader M.Celino, ENEA DTE-ICT)
- The Division participates with ICT support tasks to several H2020 projects: SEADATA CLOUD, NEXTOWER, M4F, INSPYRE, GEMMA... and to EERA-JPNM (Joint Programme on Nuclear Materials)
University of Luxembourg

Dr Sebastien Varrette
Research Excellence & HPC in Luxembourg

Prof. Pascal Bouvry, Dr. Sebastien Varrette
and the UL HPC Team

March 21\textsuperscript{th}, 2017

University of Luxembourg (\textit{UL}), Luxembourg

ETP4HPC General Assembly, Munich, Germany
Among Top 200 Universities Worldwide

- Multilingual European research university
  - founded in 2003
- \( \simeq \) 6300 students (incl. \( \sim \) 570 PhD)
  - 110 different student nationalities
  - 11 Bachelor & 32 Master Degrees, 7 Doctoral Schools
- \( \sim \) 1500 employees (researchers + staff)
  - 1098 scientific publications in 2014
    - 566 in refereed journals
  - 78 exchange agreements/research coop.
- 177.5 million euros total budget in 2014
Key numbers

- 401 users
- 98 servers
- 494 nodes
- 5428 cores
- 90.659 TFlops
- 50 accelerators
  + 76 TFlops
- 5354.4 TB
- 4 sysadmins
- 2 sites
  - Kirchberg
  - Belval

http://hpc.uni.lu
UL HPC User Base (up to Jan. 2017)

- Active HPC Users

Evolution of registered users within UL internal clusters

- LCSB (Bio-Medicine)
- URPM (Physics and Material Sciences)
- FDEF (Law, Economics and Finance)
- RUES (Engineering Science)
- SnT (Security and Trust)
- CSC (Computer Science and Communications)
- LSRU (Life Sciences)
- Bachelor and Master students
- Other UL users (small groups aggregated)
- External partners

Number of users

--- | --- | --- | --- | --- | --- | --- | --- | --- | ---
0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0

Prof. Pascal Bouvry (University of Luxembourg)
New iris cluster

- +2800 cores ($R_{\text{max}} \geq 94.08$ TFlops) Xeon E5-2680v4
- Infiniband Mellanox EDR 100Gb/s
- GPFS/SpectrumScale Storage: +1.44 PB (raw), > 10Gb/s RW

New UL HPC Data Center (operational end 2017)

- 2 server rooms for UL HPC DLC equipment \( \simeq 2 \times 1050\text{kW} \)
- 3 server rooms for Data storage equipment \( \simeq 3 \times 300\text{kW} \)
- Stepwise implementation starting Q4 2017
UL HPC: Incoming Milestones

- **New iris cluster**
  - +2800 cores ($R_{max} += 94.08$ TFlops)
  - Infiniband Mellanox EDR 100Gb/s
  - GPFS/SpectrumScale Storage: +1.44 PB (raw), > 10Gb/s RW

- **New UL HPC Data Center (operational end 2017)**
  - 2 server rooms for UL HPC DLC equipment ≃ 2x1050kW
  - 3 server rooms for Data storage equipment ≃ 3x300kW

  **Stepwise implementation starting Q4 2017**
Thank you for your attention...

Questions?

Prof. Pascal Bouvry
Dr. Sebastien Varrette
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2, avenue de l’Université
L-4365 Esch-sur-Alzette
mail: hpc@uni.lu

http://hpc.uni.lu
The Numerical Algorithms Group Ltd (NAG)

- Global software and services company with headquarters in Oxford, UK
  - Subsidiaries in USA and Japan, staff in France, Germany, Egypt.
  - Around 70 staff worldwide

- Specialists in:
  - Numerical Algorithms
  - High Performance Computing Applications and Technology Advice
  - Software Engineering for Science and Technology

- Not-for-profit Company
  - Founded as inter-University project in 1970
  - Became independent Company in 1976
  - Collaborates with leading mathematicians and computer scientists
Markets & Customers

- Over 3000 customer sites
- Broad range of industries and academic areas
- Key markets:
  - Financial Services (investment banking)
  - Energy (oil & gas)
- Work with major vendors (AMD, ARM, Intel, ...)
- Involved in many EU projects over the years:
  - EXA2CT
  - Fortissimo Experiments
  - POP
NAG & ETP4HPC

- NAG is part of European HPC community
  - ... so joining ETP4HPC is a natural step!

- Continuing EU support for HPC is crucial
  - Would like to see more focus on software and algorithms
  - Centres of Excellence are a great step forward

- Important that SMEs’ interests are served
  - Would like more flexibility and agility in projects
  - Perhaps more projects like Fortissimo
Individual member

Sabri Pllana PhD
Modeling and Optimization of Parallel Computing Systems: A Personal View

Sabri Pllana, PhD

Associate Professor
Department of Computer Science
Linnaeus University, Växjö, Sweden
http://homepage.lnu.se/staff/saplaa/
About Me

- **Associate Professor**
  - Department of Computer Science, LNU, Växjö (SE), since 2013

- **Before joining LNU**
  - worked 12 years at the Vienna University (Est. in 1365) in Austria
  - Ph.D. in Computer Science (with distinction), January 2007
  - coordinated PEPPHER (EU FP7)

- **Selected memberships**
  - CHIPSET
  - HiPEAC
  - IEEE Senior Member

PEPPHER presentation at HiPEAC’12 conference
Selected Research Results in Performance Modeling, Prediction, Optimization

- **Extension of UML** for performance modeling of parallel and distributed programs. *<<UML 2002>>*
- **Extension of UML** for Grid workflow applications. *AxGrids 2004*
- **High-level Specification of QoS-aware Grid Workflows.** *Scientific Programming Journal, 2006*
- **Platform Description Language for heterogeneous computing systems.** *Parallel Computing Journal, 2012*
- **Potential of the Intel Xeon Phi for Supervised Deep Learning and DNA Sequence Analysis.** *HPCC 2015, ISPA 2015*

**Timeline:**
- **2002**: Extension of UML for performance modeling of parallel and distributed programs.
- **2004**: Extension of UML for Grid workflow applications. AxGrids 2004

**Images:**
- Gescher Cluster (80 processors), a subcluster of single CPU nodes, a subcluster of 4xCPU SMP nodes
- Grid Computing Systems Picture: courtesy of the DataGrid Project
- Luna Multi-core Cluster, Dual-Core AMD Opterons, (288 processor cores)
- Cora, two quad-core CPUs and three GPUs (2x C2050 and 1x C1060)
- Emil, two 12-core CPUs and one Intel® Xeon Phi™ co-processor (61 cores)
Recent Work at LNU

- Parallelization for accelerated computing systems
  - DNA sequence analysis
  - Deep learning

REFERENCE
Thank you for your attention!

- **Buzzfeed**
  - Users View: 159,380

- **Snapchat**
  - Users Watch: 6,944,444

- **Netflix**
  - Subscribers Stream: 86,805

- **Google**
  - Translates: 69,500,000

- **YouTube**
  - Users Share: 100 Hours of New Video

- **Facebook Messenger**
  - Users Share: 216,302 Photos

- **Amazon**
  - Makes: $222,283 in Sales

- **Giphy**
  - Servs: 3,567,850 Text Messages Are Sent in the U.S.

- **Twitter**
  - Users Send: 569,217 Gifs

- **Tinder**
  - Users Swipe: 972,222 Times

- **Dropbox**
  - Receives: 13,888,889 Forecast Requests

- **The Weather Channel**
  - Receives: 833,333 New Files

[Credit: www.domo.com, 2016]
Carlo Cavazzoni PhD
on behalf of

Quantum Expresso Foundation
Objects coordinate and support research, education, and outreach within the QUANTUM ESPRESSO community.

own the trademarks and protect the open-source character of QUANTUM ESPRESSO.

raise funds to foster the QUANTUM ESPRESSO project.
the Company

- London-based non profit company limited by guarantee
- public company articles
Members

- Scuola Internazionale Superiore di Studi Avanzati, Trieste
- Ecole Polytechnique Fédérale de Lausanne
- International Centre for Theoretical Physics, Trieste
- Consiglio Nazionale delle Ricerche, Italy
- CINECA supercomputing center, Bologna
- University of North Texas

the Foundation is open to new groups / institutions wishing to join
the Business Model

where will the foundation’s money go

- dissemination (web sites, web-based community-oriented users’ assistance)
- training
- funding (micro-) prizes and super-computing grants
- code development and community-oriented code gluing

where will the foundation’s money come from

- membership fees
- (micro-) donations
- academic and corporate training
- brokering of custom-tailored code development / porting / optimization / benchmarking
Simula Research Laboratory

Dr Johannes Langguth
Simula Research Laboratory

Established: 2001
Number of employees: 140
Owner: The Norwegian government via the Ministry of Education and Research
Organisation: Limited company, strong connection with University of Oslo

Financing:
- Basic funding from the Norwegian Government
- Grants from the Norwegian Research Council and EU
- Private money from Statoil and other mostly oil (related) companies

Purpose:
- Fundamental ICT-research with applicable goals.
- Education
- Innovation

Simula welcomes more European collaborators
HPC research at Simula

Large Scale Biomedical Simulations
- Scientific computing (numerical methods, PDE software, large-scale simulations)
- Programming paradigms
- Use of heterogeneous supercomputers
- In-house expertise on modelling, methods, and HPC.

Media Performance Optimization
- Heterogeneous architectures for scalable media performance
- PCIe as an ultra-low latency interconnection network (*device lending*)

Expanding HPC activities into Data Science
HPC research at Simula

Networks and Cloud Computing

- Routing, fault tolerance, congestion management in HPC interconnection networks
- Utilisation of HPC interconnects to facilitate Big Data in the cloud (ERAC)
- Large shard-memory machines from off-the-shelf components (NumaMultiConnect)

Fabriscale spinoff (to become an ETP4HPC member)

- Goal: Commercialization of network and management research
- Products: Fabric manager (IB), SDN controller, monitoring system
- Financing: SME Horizon2020, external investors
IT4Innovations national supercomputing center

Martin Palkovič
IT4I is the national supercomputing center of the Czech Republic.
IT4I operates the most powerful supercomputers in the Czech Republic

State-of-the-art datacentre (April 2015):
• 500 m², 2x2.5MVA DUPS
• 5 independent hot and cold water loops (2+3)
• Heat recuperation

Supercomputer Anselm (June 2013):
• Performance **94 TFLOPS** Rpeak (3k cores)
• ~30 mil corehours/year

Supercomputer Salomon (June 2015):
• Performance **2 PFLOPS** Rpeak (24k+53k cores)
• ~200 mil corehours/year
• 863 Intel(r) Xeon Phi(tm) coprocessors
80+ researchers (FTE) in 5 labs active in EU and national projects related to HPC

- 5 FP7 projects (PRACE IP, EXA2CT, ...)
- 8 H2020 projects (see logos below, ...)
- 3 other international projects (IPCC, ESA TEP, ...)
- 3 applied research national projects
- 3 basic research national projects
- 2 large national projects (>10 mil EUR for 4+ years)
  - operation of large research infrastructure
  - support excellent research
University Carlos III of Madrid

- Created in 1989.
  - 25,000 students
  - 33 in ranking QS Top 50 Under 50
- Polytechnic Engineering School.
  - Computer Science & Engineering Department
  - Among top 200 in ARWU 2015 in Computer Science
- Research group: Computer Architecture and Systems (ARCOS)
- HPC research and application
  - **Goal:** Applied research on large-scale parallel and distributed systems (parallelization, runtimes and I/O).
  - **Research:** High-Performance I/O and programming models
  - **Applications:** bioinformatics, engineering process simulation, data and signal analytics, aeronautics, finance, ...
- **Cooperation:** Argonne Labs, Northwestern, CINVESTAV, DKRZ, INRIA, CNRI, CIBERSAM, IBM Research, CERN, ...
High-performance I/O Research

- Middleware for I/O coordination and control
- Decouple policy, control and data management
- Cross-layer abstractions and run-time
  - Facilitate the flow of control and data across the I/O stack
- In-memory data-locality aware storage
- Malleability in MPI

- Research opportunities
  - Dynamic I/O load balancing (S.R.A. 5.3.2)
  - Locality exploitation (S.R.A. 5.2.4, 5.3.1)
  - I/O elasticity (S.R.A. 5.2.4)
  - Adaptive buffering in parallel applications workflows (S.R.A. 5.5, 5.6.2)
  - Novel resilience protocols (S.R.A. 5.4.4, 5.5)
  - Data-aware parallel I/O scheduling (S.R.A. 5.2.4, 5.3.1)
  - Cross-layer optimizations (S.R.A. 5.3.6)

CLARISSE

- Policies
- Control plane
- Data plane

Hercules
- Integrated with Swift/T scheduler
Programming Models and Application Improvement

- Research activities:
  - Parallel patterns extraction from sequential legacy code (S.R.A. 5.3.3, 5.6.4).
  - Runtime support for parallel patterns/skeletons with special attention to Parallel Heterogeneous Architectures (S.R.A. 5.3.4, 5.3.6).
  - Refactoring from DSLs (e.g. MATLAB or R) into highly pattern/skeleton based parallel C++ (S.R.A. 5.3.5).
  - Contracts based programming to improve program correctness (S.R.A. 5.3.8).
- C++ language design and evolution: C++11, C++14, C++17, ...
- Recent Projects: REPARA (FP7), RePhrase (H2020)
Applications

- Novel Cone-Beam X-Ray Simulation framework (FUX-Sim)
- CPU/GPU-accelerated spherical deconvolution of diffusion MRI data (pHARDI)
- Epigraph. Flu simulator including social data
- Railway power consumption simulation
- Hydrogelogy modelling based on real-time data
StreamComputing

Vincent Hindriksen
**STREAM COMPUTING**

Performance Engineers

- Builds **fast** and **scalable** software on CPU, GPU and FPGA
- Focuses on Structured Big Data, Large-scale scientific experiments, Image/Video processing and AI
- Are OpenCL and CUDA experts
- Founded in 2010
- Distributed team in Europe
- Well-known in the GPU-world
- Clients in Europe, N-America and East-Asia
OpenCL on Networked FPGAs

What is it?

- Low latency < 5 µs
- 4 times faster development time (!)
- New version can be tested and deployed in one day.
- 80 to 90% of VHDL/Verilog-performance
- Focus on more complex and variable code

Why us?

- All IP under own control
- 3 years experience on OpenCL-on-FPGAs
OpenCL/CUDA on GPUs

What is it?

- NVIDIA Tesla and AMD Instinct
- 2 to 8 times speedup
- 20+ TFLOPS in 2017

Why us?

- Handling full projects
- Extensive algorithmic knowledge
- 7 years of experience: TATA, Stanford,
General info
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+31 854865760

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Questions?
THANK YOU FOR YOUR ATTENTION!

For more information:
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HPC strategy, work programmes and HPC related news:
ec.europa.eu/horizon2020-hpc