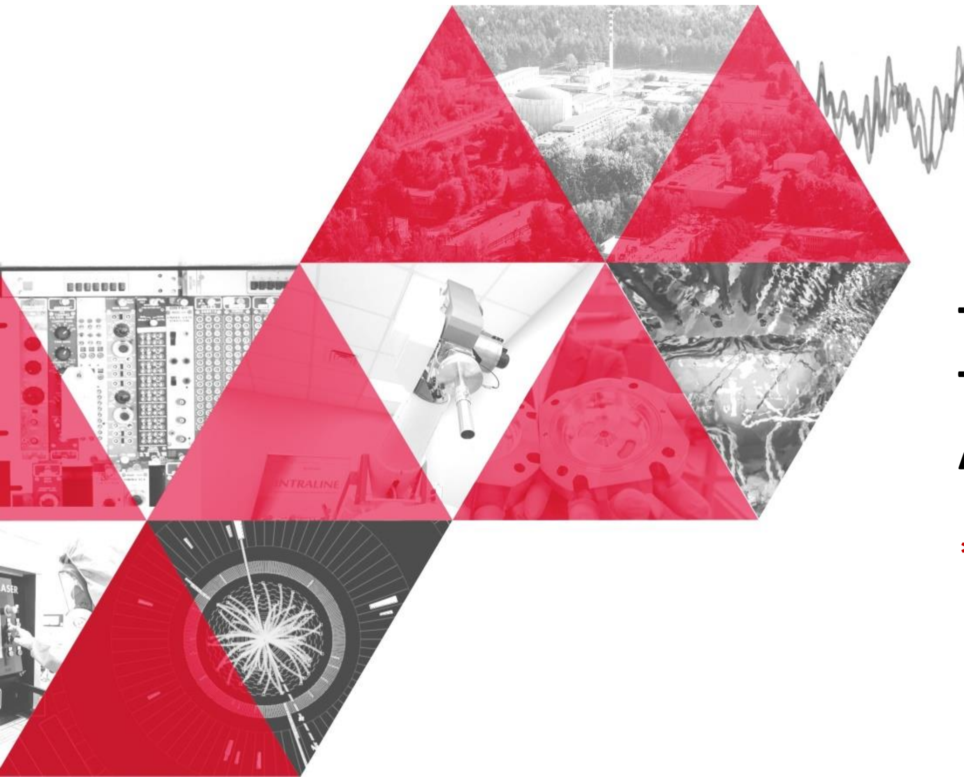
Assessment of High Performance Computing for nuclear reactor design and safety applications

NATIONAL CENTRE FOR NUCLEAR RESEARCH
ŚWIERK



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Motivation

Motivation

The more advanced the code and the research problem, the time needed to obtain final results is respectively longer. Therefore, it is important to consider not only computational capabilities but also an **efficient use of the available resources**.

The computational capabilities at Świerk Computing Centre (CIS) are assessed by performing scalability tests with the massive parallel code NEK5000.

The tests assessed the influence of:

- CPU architecture
- network configuration

Based in the execution time of a generic test case

Subsequently, selected applications are presented. These applications concern the Direct Numerical Simulations (DNS) of Pressurized Thermal Shock (PTS) and fluid flow in a bare rod bundle.

HPC infrastructure

High Performance Computing - HPC

- **High performance computing** (HPC), also known as supercomputing, involves thousands of processors working in parallel to analyse billions of pieces of data in real time, performing calculations thousands of times faster than a normal computer. In the digital era, it is at the core of major advances and innovation and a strategic resource for Europe's future.

by European Commission

Świerk Computing Centre (CIS)

- Located at:

National Centre for Nuclear Research (NCBJ), Poland

- Mission:

„The mission of the CIS is to achieve the status of the largest and best provider of cutting-edge computing services for state administration units and units investing in the development of the nuclear sector in Poland…"

Świerk Computing Centre – main building

- Installation period 2009-2015
- Budget: *25 mln €*
  (85% European Regional Development Fund)
- Build in accordance with certification requirements for EU and NATO classified data
- Support for nuclear power program

www.cis.gov.pl

Świerk Computing Centre (CIS)

- 1.16 PFLOPS in blade servers HP (AMD), SuperMicro (Intel), Bull (Inlet), Format (Intel), Asus (Nvidia)
- 19.5 PB disk storage (NetApp, HP, EMC, Seagate, TYAN)
- Cooling: 800 kW chilled water (SuperMicro, HP, Asus),
  600 kW hot water (Bull, Format)
- First large scale HPC installation in Poland with Direct Liquid Cooling technology
- Internal network: Infiniband QDR/FDR/EDR, Ethernet: 1/10/40 Gbps
- External network: 2 x 6.5 Gbps

Hardware Capabilities (general)

- CIS cluster:
  - 1454 servers
  - 2968 CPUs
  - 33080 physical cores
  - 64240 logical cores
  - 190.39 [TB] RAM
  - 611.80 [TB] HDD
  - 1164 [TFLOPS] computing power

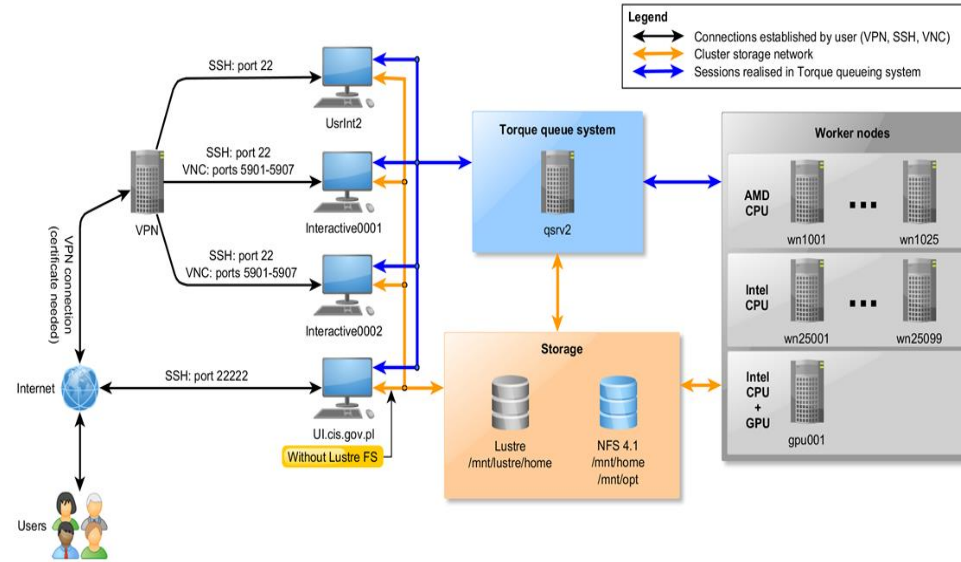
- The system processes approximately 100 000 jobs per month, and the job size varies from 1 to 10 000 cores.

Safety and Security of the Cluster

- Redundant WAN connection, fibres physically separated
- Physically separated sub-networks: Ethernet (user network) and admins/management network
- Three different 110 kV power lines at NCBJ from different power plant, Computing Center supplied by two independent underground 15 kV lines + UPS + 1250 kVA generator
- Access control, CCTV, VESDA + gas extinguishing system, 24h monitoring
- Dedicated IT security team
- Physical security provided by NCBJ

Accessing CIS cluster resources

- Secure access services using Virtual Personal Network (VPN) and public key infrastructure
- Torque + MAUI cluster:
  - Torque – version 5.1.2 as a resource manager;
  - MAUI – version 3.3.1 as a job scheduler;
  - queues: 12 hrs, 24 hrs, 1 day, 3 days, 7 days, 14 days and dedicated with personalized maximum execution time
  - 736 nodes in total + 20 dedicated GPU's
- Slurm cluster:
  - Slurm – version 19.05 – scheduler + resource manager;
  - MariaDB – version 5.5 – accounting + configuration database
  - 132 nodes in total



Simplified access scheme to the resources of the CIŚ computing cluster

NEK5000 dedicated subcluster

- Dedicated cluster is a blade system consisting of **208 servers** with **Intel Xeon E5-2680v3** processing units

- Each nodes is equipped with:
  - 2 processors
  - 128 GB of RAM and
  - a SSD 400 GB hard drive

- There are 4992 physical CPU cores and 9984 logical cores when using Intel Hyper Threading technology
- The worker nodes are interconnected with a high speed Ethernet and InfiniBand networks
- The system is using Direct Liquid Cooling

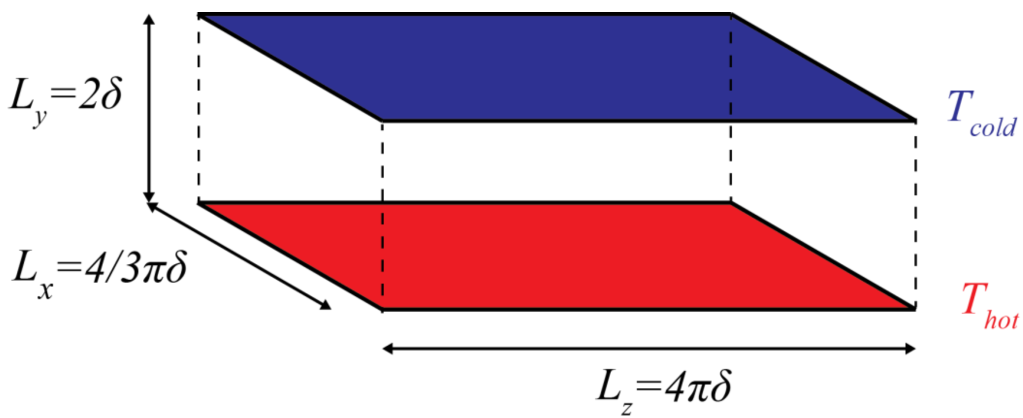
Scalability tests

Scaling of NEK5000

- NEK5000 – a fast and scalable high-order solver for computational fluid dynamics (spectral element code)

Scaling of NEK5000

- Test case: Channel flow @ $Re_\tau = 180$
- Spectral elements: 132 000
- N = 5
- Grid points: $1.66\ x\ 10^7$

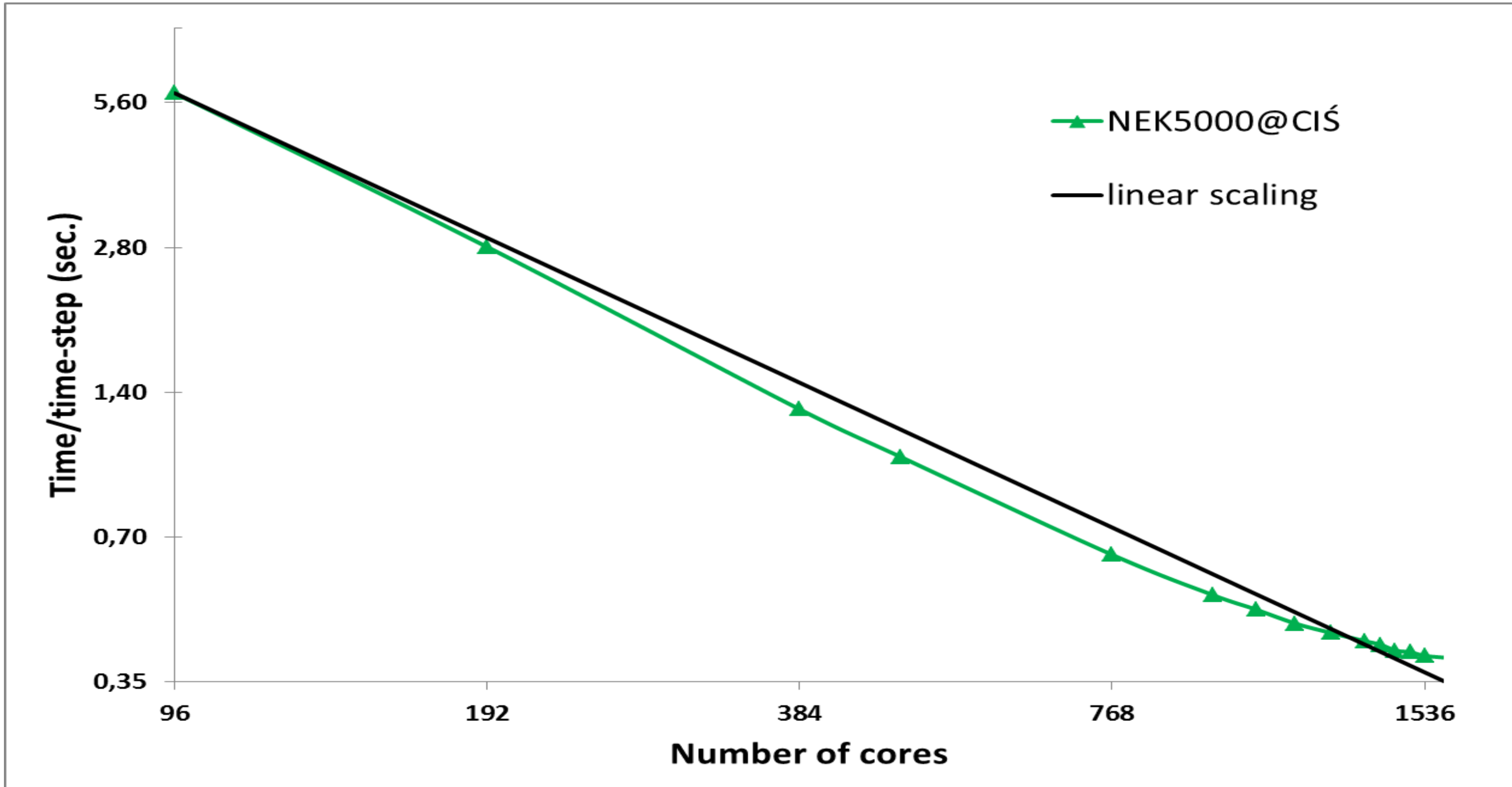


Sketch of the three-dimensional computational domain for a turbulent planar channel flow with differentially heated walls

Scaling of NEK5000

number of cores

- The wall time per time step for NEK5000 as a function of the **number of cores**.



Scaling of NEK5000

CPU architecture

	Intel Xeon E5-2680 v2	Intel Xeon E5-2680 v3
AVX	8 operation per cycle	16 operations per cycle
Architecture	Intel Ivy Bridge	Intel Haswell
Number of CPU/server	2	2
Physical cores/CPU	10	12
Total number of cores/server	20	24
Total number of threads/server	40	48
Frequency	2.8 GHz	2.5 GHz
RAM	128GB	128 GB

Scaling of NEK5000

CPU architecture

- The tests has been performed in several time length variants:
  - variant 1 (v1): 1 000 time steps
  - variant 2 (v2): 5 000 time steps (after 2 500 time steps a check point was saved)
  - variant 3 (v3): 5 000 time steps (without saving a checkpoints)
  - variant 4 (v4): 10 000 time steps

- Every variant was run at least ten times in order to get more reliable statistics of results – by means of execution time.

- Efficiency of utilization of AVX by NEK5000

Test number	Average total solver time – T [min]		Standard deviation – σ [min]		E5-2680 v3/ E5-2680 v2
	Intel Xeon E5-2680v2	Intel Xeon E5-2650v3	Intel Xeon E5-2680v2	Intel Xeon E5-2650v3	
t1	14.77	6.62	0.71	0.12	0.45
t2	58.72	26.47	5.22	0.70	0.45
t3	56.59	26.04	5.69	0.52	0.46
t4	107.31	50.17	6.81	1.44	0.47

network configuration

	Intel Xeon E5-2680 v2	Intel Xeon E5-2680 v3
Interconnect	1 x Ethernet (1 Gbit/sec per port) 1 x Infiniband QDR (40 Gbit/sec per port)	1 x Ethernet (10 Gbit/sec per port) 1 x Infiniband FDR (56 Gbit/sec per port)

Scaling of NEK5000

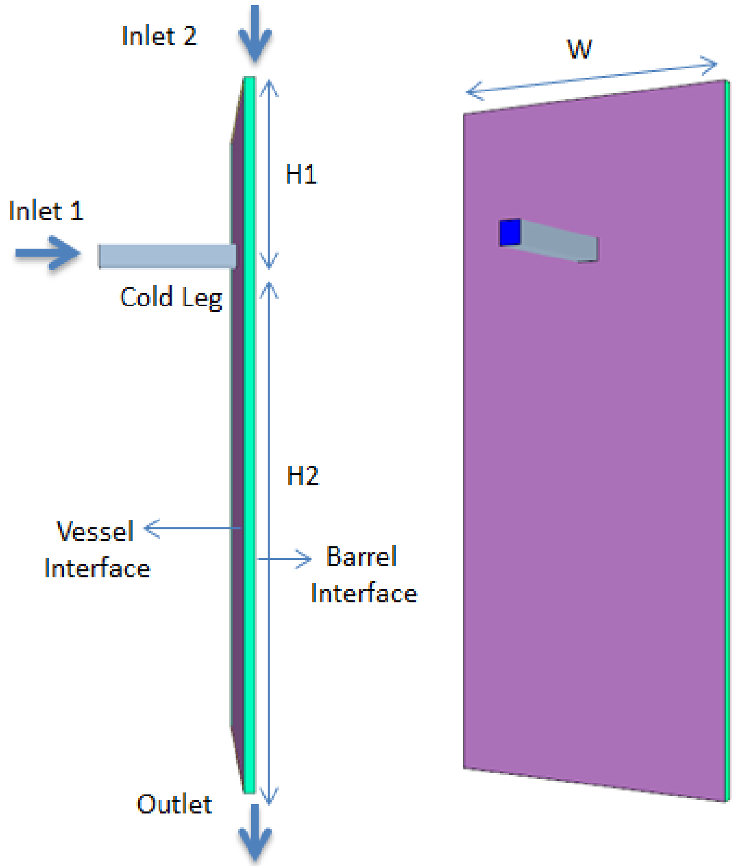
network configuration

Machine	Average total solver time – T [min]		Standard deviation – σ [min]		Slowdown
Intel Xeon E5-2680v2	**40 Gbit/s**	**2.5 Gbit/s**	**40 Gbit/s**	**2.5 Gbit/s**	**2.5/40 Gbit/s**
	30.43	48.77	1.6	0.48	1.60

Machine	Average total solver time – T [min]		Standard deviation – σ [min]		Slowdown
Intel Xeon E5-2650v3	**56 Gbit/s**	**10 Gbit/s**	**56 Gbit/s**	**10 Gbit/s**	**10/56 Gbit/s**
t1	6.68	8.71	0.07	0.32	1.30
t4	47.38	63.49	1.53	0.84	1.34

Applications

Pressurized Thermal Shock (PTS)



Code – NEK5000

- Spectral Element Code

Mesh:

- 0.75 Million Elements
- 162 Million Degrees of Freedom

Computational Power:

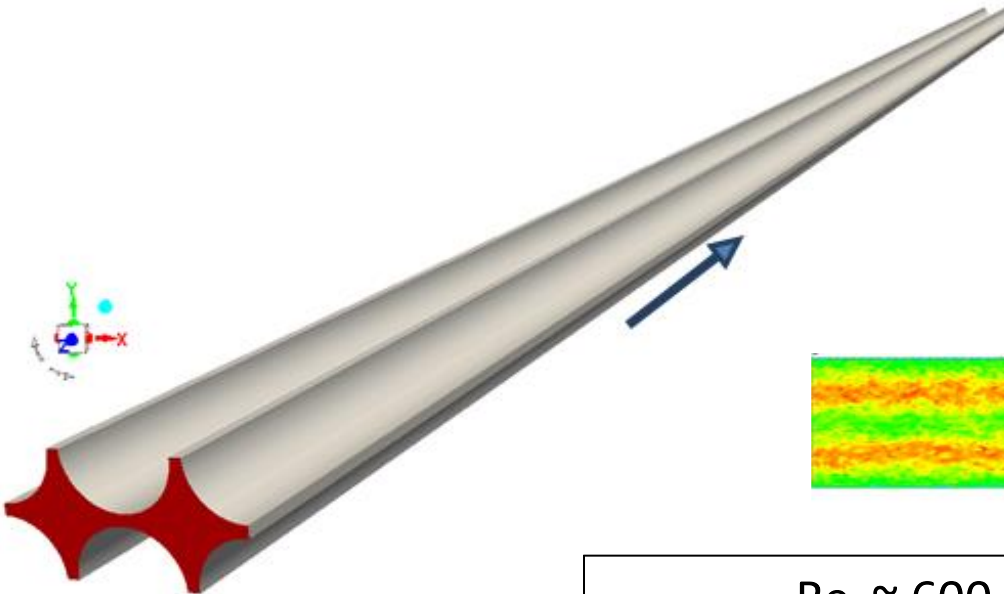
- 40 Million core hours

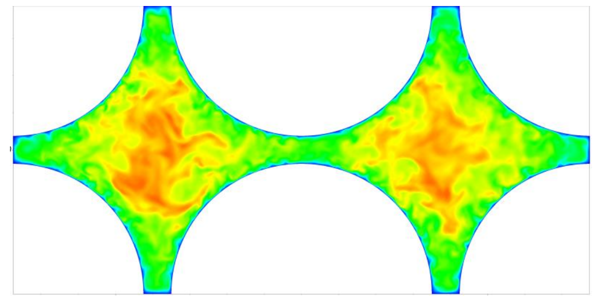
A. Shams, D. De Santis, D. Rosa, T. Kwiatkowski, E.J.M. Komen,
Direct numerical simulation of flow and heat transfer in a simplified pressurized thermal shock scenario,
International Journal of Heat and Mass Transfer, Volume 135, 2019, Pages 517-540

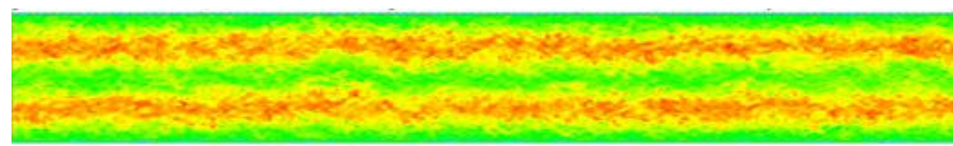
Ack: NEK5000 Development Team
P. Fischer, E. Merzari, A. Obabko

Bare rod bundle

> 110 million core hrs







A. Shams et.al.,
High-Performance Computing for Nuclear Reactor Design and Safety Applications,
Nuclear Technology, 2019

Re_{τ} ~ 600

i) iso-flux ii) iso-thermal

Pr = 7, 2, 1 & 0.025

Code – NEK5000
- Spectral Element Code

Mesh:
- 1 Million Elements
- 660 Million Degrees of Freedom

- **2018: ATH18** – Advances in Thermal Hydraulics, Orlando, FL, USA

HIGH PERFORMANCE COMPUTING FOR NUCLEAR REACTOR DESIGN AND SAFETY APPLICATIONS

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ABSTRACT

This paper presents technical aspects of large-scale direct numerical simulation (DNS) using high performance computing (HPC) cluster. It is divided in two parts. The first part contains a detailed description of HPC infrastructure used for the task, located in Świerk Computing Centre (CIŚ), Poland. The description includes hardware configuration, software used for on-demand deployment of dedicated

Achievements

- **2019: NURETH18** – 18th International Topical Meeting on Nuclear Reactor Thermal Hydraulics, Portland, OR, USA

Oral presentation

ASSESMENT OF HIGH PERFORMANCE COMPUTING FOR NUCLEAR REACTOR THERMAL-HYDRAULICS APPLICATIONS

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ABSTRACT

Over the last decade High Performance Computing (HPC) has become an attractive tool in nuclear safety analysis due to the fast progress in building large computing clusters. In particular, Computational Fluid Dynamics (CFD) technique is recognized as a valuable research tool for the analysis of thermal-hydraulics phenomenon. However, the more advanced the code and the research

Achievements

- **2019/2020: Nuclear Technology - Selected papers from Advances in Thermal Hydraulics 2018**

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ANS

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High-Performance Computing for Nuclear Reactor Design and Safety Applications

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Abstract — *Large-scale computations play an important role in many engineering and scientific applications. In the nuclear field, in particular, the crucial need for accurate simulations and reliable reference data for validation purposes makes high-fidelity simulations an extremely important tool. Due to the too-large computational resources required, these simulations must be performed on dedicated computational facilities. This paper focuses on the description of the high-performance computing facility at the Świerk Computing Centre*

Achievements

- **2019/2020: Nuclear Technology - Selected papers from Advances in Thermal Hydraulics 2018**

- **To cite this article:**

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Summary

Summary

- The NCBJ-CIS cluster consists of several types of computing hardware from different vendors and offers its own HPC solutions
- One of such solution was applied for a sub-cluster consisting of 208 servers with Intel Xeon E5-2680 v3 processing units
- Accordingly, this sub-cluster is used to perform the DNS of important thermal-hydraulic applications
- Performed tests confirmed, that on the installed hardware NEK5000 is used efficiently
- NEK5000 relies heavily on AVX performance, so the CPUs and the machines should be optimized for this when configuring a cluster for this application
- The interconnection speed is an important factor, which also cannot be neglected
- Performance test can be extended in order to check the dependency on underlaying filesystem, various storage options and operating system

Acknowledgments

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Thank you for attention

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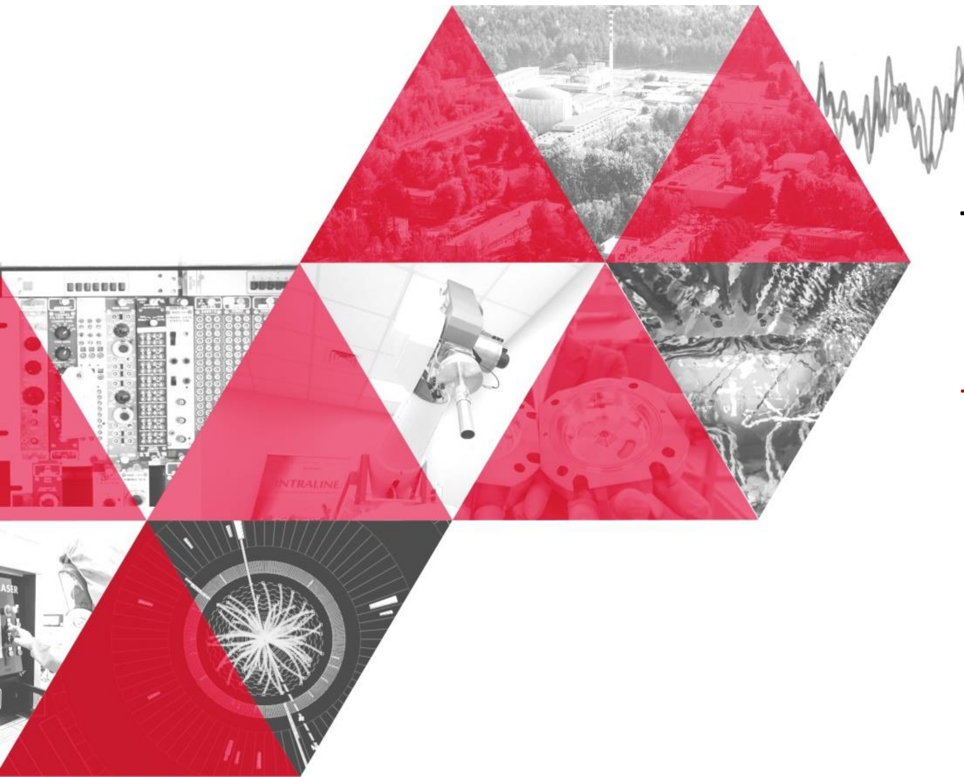

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