Memorandum of Collaboration

Parties:

(1) Brno University of Technology, Faculty of Mechanical Engineering (Holder of leader host institution LRI RIME21)

Brno University of Technology
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(2) VSB – Technical University of Ostrava, University Department IT4Innovations National Supercomputing Center (part of the larger research e-infrastructure of the Czech Republic titled e-INFRA CZ).

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Preamble:

(3) This newly proposed large research infrastructure (LRI) is titled Research Infrastructure for 21st century Mechanical Engineering (Research Infrastructure for 21st century Mechanical Engineering (RIME21)). RIME21 is a distributed research infrastructure comprised of single point access (SPA) and individual NODES.

(4) The IT4Innovations National Supercomputing Center (hereinafter IT4I) is a leading research, development and innovation centre in the area of high-performance computing (HPC), data analysis (HPDA) and artificial intelligence (AI), operating the highest-performance supercomputing systems in the Czech Republic. IT4I, together with the institutions CESNET and CERIT-SC, make up the strategic research infrastructure of the Czech Republic, titled e-INFRA CZ. The IT4I also includes a parallel algorithm research laboratory, a research infrastructure laboratory, a nanotechnology modelling laboratory, a big data analysis laboratory and a laboratory for data-intensive analyses and simulations.

(5) Taking into account the capacities comprising LRI RIME21 (namely their professional output to date) and regarding the areas of research proposed as part of the LRI RIME21 consolidation, certain thematic areas have been identified for possible use of IT4I capacities. At the same time, these thematic areas currently represent the scientific basis for mutual collaboration in research, development and technological projects (collaborative research, co-authored output), both in relation to the development of technologies, as well as the expertise of both research infrastructures. These thematic areas are sketched out in Appendix 1 of this Memorandum.

Basis for Collaboration

(6) Approval of the Memorandum by all interested parties creates the conditions for close collaboration and coordination of common approaches and activities of all parties, aiming to prepare and execute collaborative research projects and/or project approaches to IT4I research infrastructure from RIME21, or its individual nodes.

(7) Collaboration is entered into on a voluntary basis. The autonomy of the individual parties when fulfilling their common goals is not affected by this Memorandum.

Goals of the Collaboration

(8) Formulation of collaborative projects, taking into account the focus of IT4I laboratories and the research areas of RIME21. Calibration of the possibilities and uses of IT4I professional and technological capacities in relation to research tasks, common integration projects of members of the RIME21 consortium and the needs of RIME21 users.

(9) Improving access to capacities, i.e. the research infrastructure of IT4I in the form of RIME21 access projects, or to individual RIME21 nodes supported from the central RIME21 budget, provided under the open-access rules of IT4I.

(10) Development of digitalisation and advanced technologies for industrial and primarily also engineering applications. Use of the open source tools of IT4I, dissemination and application of approaches for open source tool utilisation.

(11) System support (resources for networking, data management, analyses of big data, incorporation of AI, etc.) for the development of digital products, datasets, databases, digital twins, material models, protocols for additive technologies, models of mechanical contact and other resources for the purposes of providing users with remote access to technologies and processes.

Common and Final Provisions

(12) This Memorandum on mutual collaboration does not represent a regular contract or even a preliminary contract between the parties and is not legally binding. Pre-contractual liability according to Articles 1728 and 1729 of the Civil Code is therefore ruled out.

(13) The parties shall inform their members, associates and bodies of the acceptance of the Memorandum and the subject of collaboration in an appropriate manner.

(14) This Memorandum is concluded as a digitally signed document, and after signing, each of the parties will receive a copy.

(15) The Memorandum shall expire at the written agreement of the parties or on the delivery of a written notification by one party, informing the other they no longer wish to abide by the Memorandum.

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Appendix 1: Determination of Thematic Areas for Possible Collaboration

In the area of materials research, respectively material engineering, this mainly involves the development of methods for understanding and predicting the properties of materials based on computational models. Areas of collaboration:

i. Development of SPRKKR quantum-mechanical multiscale software for describing the electron, magnetic and spectroscopic properties of 2D and 3D materials for predicting the properties of functional materials for sensory application. SARPES in collaboration with Munich University LMU (Ludwig-Maximilians-Universität München).
ii. Solution of realistic computational models in the research of the properties of materials for classical and molecular electronics, mechatronic systems, optoelectronics, photonics and spintronics n the range containing hundreds and thousands of atoms (research of ferroelectric materials, magnetic alloys and steel).
iii. Utilisation of IT4I expertise for the parallelisation and optimisation of developed SW tools, and the incorporation of algorithms of artificial intelligence to materials research (using NVIDIA DGX-2) and collaboration in the IT4I "flagship" on research activity "Material Design – Towards Reality via Exascale Computing" (Dr. D. Legut). Collaboration with IT4I is already developing – e.g. by the preparation of publications for the journal PNAS (Kurleto, Legut et al. Effects of momentum dependent hybridization in CeCoIn5).
iv. Numerical simulations for complex virtual analysis of composite structures, particularly in micro, nano and atomistic scales; speeding up calculations for numerical hybrid analysis, e.g. connecting the simulation of hybrid molecular dynamics (MD) with finite element models (FEM, XFEM).
v. Advanced calculations and more detailed clarification of multiphase interfaces of polymer composites (fibre–matrix, fibre–nanoparticle–matrix); biodegradability of composite fibre structures.
vi. Utilisation of the possibilities of the DIGIMAT SW platform for modelling materials in order to perform detailed analyses of materials on a microscopic level and to derive mechanical material models.

In the area of mechanics, it mainly involves modelling the formation and development of material defects, fatigue damage, friction and behaviour of materials under thermal loads. A significant issue is the development of methods for modelling flow phenomena. Areas of collaboration:

i. Compilation of complex mathematical models describing the deformation resistance of metallic materials, or diagrams of the anisothermal decomposition of austenite depending on the chemical composition of steel and thermomechanical parameters effecting the initial microstructure.
ii. Interconnection of mechanical response and degradation models within numerical models based on MKP for research of phenomenological models, in particular of low-cycle fatigue and ductile interference.
iii. Multi-scale models of materials – modelling the material properties of new materials, modelling the formation and development of material defects, predicting the theoretical properties of materials.
iv. Use of computational capacity for complex structural finite element calculations (Ansys system).

v. Numerical models of the macro-behaviour of materials and components with defects. Study of the formation and development of defects in the brittle failure of materials, propagation of fatigue cracks or failures due to creep. Study of the behaviour of materials under thermal loads or thermo-mechanical fatigue.
vi. Use of computational capacity in the area of tribology for molecular dynamic simulation of lubrication, where the performance of the computer system is a limiting factor.
vii. Continuation in collaboration with IT4I on the development of new computational approaches to modelling flow phenomena using the Lattice Boltzmann method and also the development and implementation of this method. Collaboration with IT4I for high-performance computing and expertise when setting multifibre tasks.
viii. The complex non-stationary two-phase flow that is present in virtually all types of jets, requires extreme computing power and detailed knowledge of the researcher (rapid and accurate prototyping of jets without needing to produce them).
ix. Verification and adjustment of computational models of experimental measurements on real mechanisms and machines, in particular for obtaining boundary conditions, with the aim of simulating their behaviour more realistically.

In the area of production and systems, this involves models and simulations relating to additive manufacturing technologies, virtual prototyping, development of digital twins, and the implementation of CPS systems in production systems. The need for cyber security solution is increasing, with the development of IoT in 5G (6G) network environments. Areas of collaboration:

i. Complex tasks for additive technologies for computer simulations of component deposition to achieve the best possible shape accuracy and to minimise residual stresses and for verification of simplified models
ii. Simulation of heat transfer in 3D printing to predict thermal dilation and distortion of printed components (or in the creation of an algorithm that will predict these deformations).
iii. Shape and topological optimisation for additive technologies – determination of topological shape optimisation to utilise the greatest potential of additive technologies.
iv. Processing of point clouds obtained by 3D scanning– use of the computational power of supercomputers in the analysis and processing of point clouds obtained by a 3D scanner or a CMM machine.
v. Simulation of real operating conditions – computationally demanding simulations for the optimal solutions of structures without shape simplifications to replace laboratory measurements with a virtual model, which speeds up the component and unit design process and enables the impacts of individual changes on their functionality to be assessed without the need to create a physical prototype.
vi. Prediction of individual production processes through digital twins. Processing and analysis of empirical data from processes during research of technologies DMLS, WAAM and laser technologies including models visualising the thermal effects of various heat sources (electric arc, induction heating, plasma arc, lasers) on materials, simulation of thermal effects with gradual verification on equipment using structural, mechanical and optical data.
vii. Cyber security and IoT in a 5G local network environment.
viii. Collaboration in the incorporation of metamaterials into existing machine parts and for optimising processes in order to implement multidisciplinary approaches to the development of CPS systems, and in particular for the application of virtual twins and monitoring, or the diagnostics of critical applications (energy, aerospace engineering).
ix. Tasks for the analysis of the motion and interaction of a large number of particles in complicated geometries to predict the behaviour of a large number of particles for the structural design of equipment.