

COMPUTER MODELING AND HIGH-PERFORMANCE COMPUTING



Centre for Natural Sciences and Technologies

J. E. Purkyně University in Ústí n. L. Faculty of Science Pasteurova 3632/15 400 96 Ústí nad Labem

doc. RNDr. Filip Moučka, Ph.D. E-mail: filip.moucka@ujep.cz Tel.: +420 475 286 636 Room: 2.02

doc. RNDr. Marek Malý, Ph.D. E-mail: marek.maly@ujep.cz Tel.: +420 475 286 651, +420 603 395 987 Room: 2.25

> UNIVERZITA J. E. PURKYNĚ V ÚSTÍ NAD LABEM Přírodovědecká fakulta

RESEARCH/TECHNOLOGY INTRODUCTION

Computer modeling poses a modern tool, suitable for **predicting or clarifying the behavior of systems and phenomena** in them, which is based on the relevant theoretical models and their software implementation. This field also includes **signal processing, including image processing, statistical evaluation of data and solution of various optimization problems**, which can be found in various areas of science, technology, management, planning and economics.

POTENTIAL USERS

We offer cooperation and services to scientific research institutions, companies and to any other organizations.

ADVANCEMENT OF TECHNOLOGY AND MARKET APPLICATION

Computer modeling is especially suitable in the following cases: 1. It replaces costly, dangerous, time-consuming, or unrealizable real **experiments**.

2. It allows **detailed insight into the investigated systems**, which is otherwise often unavailable.

 It allows to examine simplified or otherwise modified models, which facilitates the understanding of the investigated systems.
It enables optimization and automation of processes, especially by replacing and streamlining of manual, semi-manual or obsolete algorithmic procedures in the field of data processing or decision making processes, by sophisticated algorithms (typically based on artificial neural networks), without which, would be especially deeper analysis and interpretation of high volume data almost unthinkable.

High-performance computing, i.e. **computing, using highperformance hardware**, enable an order of magnitude acceleration of calculations in comparison with their realization on ordinary computers.

Our theoretical knowledge of mathematics, physics and computer methods create preconditions for a good understanding of the researched problems, formulation of their mathematical models and finding their optimal solutions.

ADDITIONAL INFORMATION

Our workplace can offer a complex service, which includes the following steps:

- 1. Theoretical analysis of a given problem, using advanced methods of mathematics and physics.
- 2. Formulation of suitable computer models of investigated systems and processes.
- 3. Implementation of models and necessary computational methods using effective computational programs.
- 4. Realization of calculations using powerful hardware.
- 5. Analysis, discussion and presentation of results.

Our workplace has experts in computer methods, especially in the following areas:

- 1. Particle-based modeling (molecular simulation Monte Carlo, Molecular dynamics).
- 2. Continuous modeling of heat and mass transfer (hydrodynamics, computational fluid dynamics).
- 3. **Optimization** (deterministic and stochastic methods with emphasis on evolutionary algorithms).

4. Complex data processing - classification, reconstruction, approximation, extrapolation, transformation related to the realization of autonomous decision functions, etc.

5. **Signal and image processing** (filtration, frequency analysis, object detection and subsequent higher level analysis).

- 6. Simulation and analysis of complex dynamical systems.
- 7. Parallel programming and efficient use of powerful hybrid (CPU / GPU) computing clusters.

Our workplace is equipped with powerful modern computing cluster (supercomputer), which includes hundreds of Intel Xeon Gold 6240 CPUs and dozens of NVidia RTX2080 Ti GPUs.





Computing cluster of Faculty of Science UJEP - photograph from server room