



AGENDA

Thursday, 6 th March	
Chair: Jacek Kitowski	
9 ³⁰	Opening – Kazimierz Wiatr
9 ⁴⁵	Kazimierz Wiatr – ACK CYFRONET AGH – Mission and Computing Resources
10 ¹⁵	Norbert Attig – IBM Blue Gene for Scientific Computations
11 ⁰⁰	<i>coffee</i>
Chair: Janusz Orkisz	
11 ³⁰	Irena Roterman – Large Scale Computing in Pharmacology
12 ⁰⁰	Paweł Wróblewski, Krzysztof Boryczko – Parallel Simulation of a Fluid Flow by Means of the SPH Method: OpenMP vs MPI Comparison
12 ¹⁵	Organizational announcements
12 ³⁰	Poster session
P1.	Dorota Pawlus – Critical Loads Calculations of Annular Three-Layered Plates with Soft Elastic or Viscoelastic Core
P2.	Piotr Zazakowny, Mariusz Sterzel, Marek T. Pawlikowski – The Absorption and Fluorescence Study of 1,4,5,8- Naphthalenetetracarboxylic Dianhydride (NTCDA)
P3.	Klemens Noga, Piotr P. Romańczyk, Andrzej J. Włodarczyk and Ewa Broclawik – Theoretical Modeling of Electrochemical Interactions in Bimetallic Molybdenum Nitrosyl Complexes Incorporating Saturated Bridges
P4.	Marcin Andrzejak – Theoretical Reproduction of Vibronic Structures for the $A_{1g} \leftarrow B_{1u}$ Transition in Oligothiophenes Containing 2-6 Thiophene Rings
P5.	Marcin Makowski, Grzegorz Mazur – Design of a Load Balancing Algorithm for Computational Chemistry Applications
P6.	Grzegorz Mazur, Marcin Makowski – Development and Optimization of Computational Chemistry Algorithms
P7.	Katarzyna Rycerz, Marian Bubak, Peter M.A. Sloop – HLA Component Model for Multiscale Simulations
P8.	Marian Bubak, Tomasz Gubala, Maciej Malawski, Bartosz Balis, Włodzimierz Funika, Tomasz Bartynski, Eryk Ciepela, Daniel Harezlak, Marek Kasztelnik, Joanna Kocot, Dariusz Krol, Piotr Nowakowski, Michal Pelczar, Jakub Wach, Matthias Assel – Virtual Laboratory for the Development and Execution of Collaborative Applications
P9.	Wielgosz Maciej, Jamro Ernest, Kazimierz Wiatr – Highly efficient Twin Module Structure of 64 Bit Exponential Function Implemented on SGI RASC Platform
P10.	Witold Byrski, Henryk Połcik, Bartłomiej Zawada, Mariusz Murawski – Modelowanie procesu krystalizacji wybranych stopów metali nieżelaznych przy pomocy programu FLUENT
P11.	S. Kluska-Nawarecka, A. Smolarek-Grzyb, A. Byrski, D. Wilk-Kołodziejczyk – Optimalisation of Simulation Model Parameters for Solidification of Metals with Use of Agent-Based Evolutionary Algorithm
13 ¹⁵	<i>lunch</i>
Chair:	
14 ¹⁵	Jacek Kitowski – Grid Initiatives in Poland: PL-Grid Case Study
14 ⁴⁵	Mariusz Sterzel – Grid as a Computation Platform for Chemistry
15 ⁰⁰	A.Olszewski – Eksperymenty Fizyki Wysokich Energii w Sieciach Komputerowych Grid
15 ³⁰	<i>coffee</i>
Chair: Irena Roterman	
16 ⁰⁰	Mariusz Radoń, Ewa Broclawik – Electronic Structure and Conformation of Cobalt(II) Acetylacetonate: CASPT2 and DFT Study
16 ¹⁵	Jacek Korchowicz and Jakub Lewandowski – Elongation Cutoff Technique for Linear SCF Scaling
16 ³⁰	Yuriy Natanzon and Zbigniew Łodziana – Elastic Properties of Doped Tetragonal Yttrium Stabilized Zirconium Dioxide
16 ⁴⁵	Małgorzata Rachwalska – The Simple – $KBrO_3$, H_2SO_4 Oscillator
19 ⁰⁰	<i>dinner</i>

Friday, 7th March

Chair: Marian Bubak	
9 ⁰⁰	Japp A. Kaandorp – Computational Modelling of Corals: from Genes to Colony
9 ⁴⁵	Paweł Russek – Computation Acceleration on SGI RASC: FPGA based Reconfigurable Computing Hardware
10 ¹⁵	J. Orkisz, S. Milewski – On Optimal Acceleration of Iterative Solution Methods of Simultaneous Algebraic Equations
10 ³⁰	Maciej Gierdziewicz – Analysis of Execution Time and its Components in Parallel Estimation of Additive Relationship Coefficients
10 ⁴⁵	<i>coffee</i>
Chair: Michał Turała	
11 ¹⁵	Maciej Twardy – System składowania danych w ACK CYFRONET AGH
11 ³⁰	M. Filipowicz, V.M. Bystritsky, J. Woźniak – Monte Carlo Fitting of Data from Muon Catalyzed Fusion Experiments in Solid Hydrogen
11 ⁴⁵	Stanisław Jadach – Theoretical Calculation in Form of the Monte Carlo for Particle Collider Experiments
12 ⁰⁰	T. Szymocha, A. Kaczmarek, P. Malecki, E. Richter-Wąs – The ATLAS Experiment Simulations as the Computing Challenge for the ACK Cyfronet AGH
12 ¹⁵	K. Korcyl, T. Szymocha, J. Pieczykolan, T. Kryza, K. Balos, W. Funika, K. Guzy, R. Słota, L. Dutka, K. Zieliński, J. Kitowski – The ATLAS Experiment on-line Monitoring and filtering as an Example of Real-time Application
12 ³⁰	Ł. Janyst, A. Kaczmarek, M. Wolter, A. Zemła – Multivariate Tools for Tau identification in the ATLAS Experiment
13 ⁰⁰	<i>lunch</i>
Chair: Jacek Niwicki	
14 ³⁰	Krzysztof Boryczko, Marcin Kurdziel – Parallel Clustering Algorithm for Noisy Data
14 ⁴⁵	Joanna Dulińska, Stefan Świąć – Evaluation of Dynamic Characteristics of Masonry Arch Bridges: Linking Full-Scale Experiment and FEM Modeling
15 ⁰⁰	Aleksander Siwek – Numerical Simulation of the Laser Welding
15 ¹⁵	Joanna Dulińska – Effect of Wave Propagation Velocity on the Dynamic Response of Multiple-Support Structures: FEM Analysis and <i>in situ</i> Investigation
15 ³⁰	Łukasz T. Stępień – Application of Waterloo MAPLE 9.5 and Wolfram MATHEMATICA 5.1 Software for Analytic Solving of Certain Nonlinear Partial Differential Equations of Physics
15 ⁴⁵	<i>coffee, discussion</i>

Invited lectures

Lectures from Cyfronet