

## **Referaty zaakceptowane na KU KDM'10 / kolejność alfabetyczna wg tytułów/**

### **An Improvement to Glowworm Swarm Optimization Algorithm**

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### **Applications with Rich User Interface Powered by the GridSpace Virtual Laboratory**

*Maciej Malawski (1, 2), Tomasz Gubała (2), Tomasz Jadczyk (2), Katarzyna Prymula (3, 4), Irena Roterman  
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### **ATLAS experiment production system in WLCG Grid computing network**

*Andrzej Olszewski*

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### **Benefits of Provenance of Virtual Experiments**

*Bartosz Baliś and Marian Bubak*

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### **Calculations of the Chelatoaromatic Stabilization Energy in Metalcomplexes of Hydroxypyrones**

*Krzysztof K. Zborowski, Leonard M. Proniewicz*

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### **Component Approach to Distributed Multiscale Simulations**

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### **Convergence of Nuclear Shieldings Calculated with Basis Sets Designed for NMR Calculations**

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### **DGEMM Performance Tests of AMD Radeon HD 4870**

*Dawid Kuna (1), Ernest Jamro (1, 2), Paweł Russek (1, 2), Kazimierz Wiatr (1, 2)*

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### **Efficient Electrostatic Properties Calculations at the MP2 Theory Level**

*Grzegorz Mazur, Marcin Makowski, Jakub Sumera, Krzysztof Kowalczyk*

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### **Electronegativity Equalization Method in Force Field Atoms Resolution**

*Anna Stachowicz and Jacek Korchowiec*

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### **Electronic Structure Calculations of Alkaline Earth Metal Hydrides**

*Yuriy Natanzon and Zbigniew Łodziana*

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## **Estimation of Nuclear Shieldings in the Complete Basis Set Limit**

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## **Flexible Organization of Repositories for Provisioning Cloud Infrastructures**

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## **GridSpace Based Virtual Laboratory for PL-Grid Users**

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## **Implementation of Montgomery Exponentiation in FPGA for Cryptographic Applications**

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## **Improvements in the global a-posteriori error estimation of the FEM and MFDM solutions**

*Sławomir Milewski, Janusz Orkisz*

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## **Large Scale Calculations for Creating Polish Language Semantic and Syntactic Models**

*Bartosz Ziółko, Dawid Skurzok, Jan Wicjowski*

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## **Large Scale Computing to Search for Pharmacologically Active Proteins**

*Prymula K. (1,2), Piwowar M. (1), Kochanczyk M. (1,3), Flis L. (1,3), Maławski M. (4,5), Szepieniec T. (5), Evangelista G. (6), Minervini G. (6), Polticelli F. (6), Wiśniowski Z. (1), Sałapa K. (1), Matczyńska E. (1), Roterman I. (1)*

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## **MCdevelop - the Universal Framework for Stochastic Simulations**

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## **New Neural-Genetic Hybrid Algorithm: Optimization of Molecular Structure**

*Anna Styrcz and Janusz Mrozek*

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## **Pattern Discovery in Gene Expression Data with Multiobjective Estimation of Distribution Algorithm**

*Wiktor Mlynarski, Katarzyna Grzesiak-Kopec*

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## Pipeline Implementation of Peer Group Filtering in FPGA

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## Prototype of Automated Framework for Insertion of HLL Languages to HPC Applications

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## Seasonal Changes in Somatic Cell Content in Milk of Polish Holstein-Friesian Cows

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## Secure Access to Shibboleth Protected Clusters

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## Solvent Effect on the Absorption Spectra of Ketocyanine Dye Complexes - TDDFT Calculations with Explicit Solvent Modeling

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## Support for the Full e-Experimentation Cycle in the Virtual Laboratory Infrastructure

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## Tests of Fundamental Symmetries with Free Neutrons

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## Theoretical Studies on Convergence of Harmonic and Anharmonic Frequencies in the Gas Phase and Solution

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## Theoretical Studies on cytosine and 5-fluorocytosine. Prediction of Harmonic and Anharmonic Frequencies in the Gas Phase and Solution

Teobald Kupka (1), Aneta Buczek (1), Małgorzata Broda (1), Marzena Nieradka (1), Mariana Spulber (2),

Mariana Pinteala (2) and Adrian Fifere (2)

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## Theoretical Study of Phenoxyimine-based Catalysts in Olefin Polymerization

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## Torsionally Controlled Electronic Coupling in Mixed-Valence Oxodimolybdenum Nitrosyl Scorpionates - a DFT Study

Klemens Noga, Piotr P. Romańczyk, Andrzej J. Włodarczyk,  
Wojciech Nitek, and Ewa Broclawik

## Towards Autonomic Semantic-based Management of Distributed Applications

Włodzimierz Funika, Paweł Koperek, Mateusz Kupisz

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## **Validation of Polarization Approximation in Calculations of Interaction Energy Components**

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## **Virtual Laboratory for in-silico experiments in Computational Chemistry**

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