

Monitor section

## Meeting report: Fourth winter symposium on chemometrics—WSC4 “Multivariate Data Analysis”, 15–18 February, 2005, Institute of Problems of Chemical Physics, Chernogolovka

Sergei Kucheryavski<sup>a,\*</sup>, Christopher Marks<sup>b</sup>, Kurt Varmuza<sup>c</sup>

<sup>a</sup>*Altai State University, Barnaul, Russia*

<sup>b</sup>*University of Virginia, Charlottesville, USA*

<sup>c</sup>*Vienna Technical University, Vienna, Austria*

Available online 3 June 2005

The fourth regular event in the Drushbametrics (friendship-metrics) program, WSC-4, took place in Chernogolovka, a science city near Moscow, Russia, February 15–18, 2005. The conference was organized by the Russian Chemometrics Society, the Institute of Problems of Chemical Physics and the Institute of Chemical Physics. Beginning with this conference, these meetings have been renamed “Winter Symposium on Chemometrics” from “Winter School on Chemometrics”. The WSC is now primarily a place for presenting new ideas and having fruitful discussions in a friendly informal atmosphere. The educational part of the Drushbametrics mission was maintained by providing a school for beginners prior to the symposium. The main goal of Drushbametrics is to provide an opportunity for young scientists to make their first steps in chemometrics, as well as to meet leading scientist in this field.

Chernogolovka is a small town near Moscow that was founded in the 1960s by Nikolay Semenov, a Noble Prize winner and the head of the Institute for Chemical Physics (ICP). Initially established as a campus for a new branch of ICP, Chernogolovka grew into a real “science city” with over 20,000 inhabitants, consolidating a number of institutes for natural sciences, during the next two decades. The ICP subsidiary has become an independent institution, the Institute for Problems of Chemical Physics (IPCP), which hosted WSC-4.

More than 50 scientists from Austria, Belgium, Denmark, England, Spain, USA, and Russia participated in WSC-4. Each session consisted of one lecture and two or more contributed talks. Vladimir Razumov, deputy director of IPCP, gave the opening lecture, “Principal component analysis in photochemistry”. The invited lectures were devoted primarily to the theoretical problems of modeling and their applications in wide scientific and industrial areas. Roma Tauler raised some interesting questions concerning relations between hard and soft modeling and gave an introduction to using grey modeling for investigation of chemical processes. Agnar Hoskuldsson lectured on the Heisenberg principle of mathematical modeling. Alexey Pomerantsev illustrated the core principles of Simple Interval Calculation with simple and vivid examples. Kurt Varmuza presented very interesting results of using multivariate methods of exploration and classification from archaeometry and space science. John Kalivas spoke about defining model complexity in different modeling methods. Juan Fernandez Pierna gave an overview for estimating the uncertainty in multivariate calibration. Finally Oleg Karpukhin shared his philosophical reasoning about the past, present, and future of chemometrics and its role in science.

The Elsevier and Wiley publishing companies provided sample issues of “Journal of Chemometrics” and “Chemometrics and Intelligent Laboratory Systems” for participants, which were eagerly received by the younger attendees. Elsevier also provided a special prize for the best oral or poster presentation by a young Russian scientist at WSC-4. The 20th volume of Data Handling in Science and Technology series—“Handbook of Chemometrics and Quali-

\* Corresponding author. Tel.: +7 385 2 363571; fax: +7 385 2 364183.

E-mail addresses: [svk@asu.ru](mailto:svk@asu.ru) (S. Kucheryavski), [cam8h@virginia.edu](mailto:cam8h@virginia.edu) (C. Marks), [kvarmuza@email.tuwien.ac.at](mailto:kvarmuza@email.tuwien.ac.at) (K. Varmuza).



Fig. 1. Attendees of WSC-4 in the Star City near “Mir” space station simulator.

metrics, Part A”–was presented to Sergei Zhilin from the Altai State University, Barnaul, Russia for his talk “Simple Method for Outlier Detection In Fitting Experimental Data Under Interval Error”. Agnar Hoskuldsson who presented the prize to the winner expressed hopes that this opportunity will help Sergei to enrich new science horizons.

On Thursday, attendees had a chance to visit Gagarin’s Cosmonaut Training Center in the Star City. This excursion, which began at the Yuri Gagarin monument, the place where cosmonauts get together after returning from space, was very imposing. The unique centrifuge, “MIR” station simulator, and the neutral buoyancy simulator were the most popular areas shown to participants (Fig. 1).

“Introduction to multivariate data analysis methods”, the school for beginners, was also held at ICPC, 13–14

February. A total of 38 attendees, mainly from Russia and Ukraine, took part in the school. The program included lectures on PCA, PLS and multivariate classification. Attendees also had the opportunity to try out these methods with the UNSCRAMBLER software. Finally, Alexey Pomerantsev gave an overview of multivariate data analysis in different scientific and industrial areas. All attendees received Camo’s book “Multivariate Data Analysis in Practice”, written by Kim Esbensen in short translation edited by Oxana Ye. Rodionova.

The next Drushbametris event, WSC-5, will take place in Samara on the bank of Volga river during February 2006. As usual, the organizers plan a balanced formal and informal scientific program in addition to cultural and social activities.