First winter school on chemometrics

WSC-1 took place Feb. 11–15, 2002 in Kostroma, Russia, a regional city situated some 350 km NE of Moscow. Kostroma has 350,000 inhabitants and boasts two universities. WSC-1 was a success with 42 attendees, some of which had come from far away, even from former Soviet republics. Attendees were lodged in a small sanatorium "Kostromskoi" in the inner suburb of the town. Kostromskoi is a health spa in old Russian style, with guest rooms of a modest-to-reasonable standard, health and exercise facilities and a movie theatre. The food is made locally under dietetic supervision. Such a rather secluded environment caters for much social interaction and improves concentration. Skis were also provided for cross-country trips along the banks of the Volga river in typical Eisenstein scenarios. The movie hall turned out to be excellent for plenary lectures and the local pedagogic university provided computer exercise rooms of a high standard.

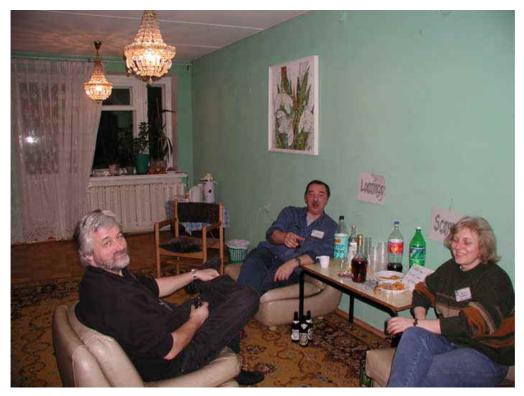The ideas behind WSC-1 are threefold:

–   Contributing to starting up chemometrics in Russia.

–   Establishing a framework for international chemometrics interaction.

–   Enabling both foreign and Russian scientist to participate on an equal economic footing.

Thus foreign attendees gets the whole shebang for a very modest $250, included all lodging, meals and local transportation, while Russian attendees are helped in every which possible way to a rather reduced fee. The international fees also contribute to this goal.

The organizing committee of WSC-1 had worked in a period of 18 months in order to get everything ready to start to promote chemometrics in Russia. While the need for chemometrics in Russia is immense, the practical and economic capabilities are severely constrained. WSC-1 is thus very grateful for sponsoring and financial support, which included ACRG (Porsgrunn, Norway), ACACSRG (Esbjerg, Denmark) Russian Foundation for Basic Research (RAS-grant No: 02-03-42001).

WSC-1 was associated with the State University in Kostroma, while the town's polytechnic university had never heard of chemometrics — and apparently did not want to discontinue this state of affairs, perhaps paradoxically. Nevertheless the interest from the State University's economics department was very clear.

The organizers were *Alexey Pomerantsev* and *Oxana Rodionova*, from the Semenov Institute of Chemical Physics of the Russian Academy of Sciences (RAS) and international committee member *Kim H. Esbensen*, Denmark. Also substantial contribution from the Vernadsky Institute of Geo- and Analytical Chemistry (prof. *Lev Gribov*, science secretary *Elena Korobova*) was critical in the long preparative phase of WSC-1. This indicates the growing interest for Chemometrics in Russia, not only among single enthusiasts but also scientific laboratories and institutes.

The organizing committee at the "Kostromskoi" sanatorium leisure area — after everything had finally gotten off to a good start. The WSC-1 help-yourself bar was, very appropriately, called "Scores and Loadings".

The committee had put together a broad program for introducing important basic concepts of chemometrics, Kim Esbensen: "*Introduction to the chemometric approach*" and Paul Geladi: "*Introduction to multivariate calibration*" — while more experienced participants were treated feature lectures "*Multivariate Image Analysis*" (Geladi) and "*Multivariate statistical process control, MSPC*" (Esbensen). Both these international invited speakers also conducted full-scale hands-on workshop during two days, on the practical aspects of doing chemometrics using both MATLAB and Unscrambler.

Language problems were solved efficiently by experienced translators, namely the in-house two Russian organisation committee members, Oxana and Alexey — who did an outstanding job not confined to the three scientific working days, but perhaps equally important, during the almost as long social/leisure periods. Indeed one of the foremost objectives of WSC-1, which was achieved above all expectations, owe its success to this very hard behind-the-scene work by Oxana and Alexey — who literally slept only some 4-5 hours every day of the gathering (not to mention their excellent organisation of the necessary two 6 hours' bus drive Moscow—Kostroma to/from, where several very Russian ice-breaker traditions were presented, with precisely the intended effects).

There was one whole day of purely Russian contributions (which were also fully translated however). Oxana Rodionova lectured on: "*Simple Interval Calculation (SIC) — a new bi-linear modelling method*", which is a non-regression prediction approach providing results directly on interval form. Alexey Pomerantsev focused on: "Non-linear regression analysis with "Fitter" ap-

plications". This technique provides opportunities to forecast (extrapolate) complex systems in settings far from the observed training data realms. These presentations helped to overcome the complicated mathematics, which is otherwise needed for these methods. These lectures were also followed by related hands-on workshops for the rest of the day. Several poster presentations from Russian scientists were discussed at the last day of the conference. It is intended that such homeland contributions are to increase gradually in proportion to the foreign counterparts as the WSC-series develops (see below). Future WSC's will thus be concerned with e.g. QSAR-investigations and Molecular Modelling (Chemical Department of the Lomonosov University and Vernadsky Institute of Geo and Analytical Chemistry), application of "grey models" for kinetic constants evaluation (Semenov Institute of Chemical Physics), while several groups of Russian scientists have been working in the field of design of experiment for many years.

Being the first endeavour of the Russian Chemometrics Society (RCS) at establishing a regular curriculum activity, and with a natural emphasis of introducing chemometrics to Russian newcomers to our field, WSC-1 never the less also succeeded in attracting a minor, but significant number of participants from abroad. Besides Geladi/Esbensen there was an additional international attendance geographically distributed as three from Armenia and one from the United States (established researchers all) and two Ph.D. students from Denmark. This complement of six, out of a total of 42 attendees can be considered as a reasonable start of the international objectives for the WSC-series of winter schools; it is the intention to continue for the next five years with lecturers, workshops and attendees in much the same format as WSC-1 though at widely different localisation within Russia (Altai, Siberia; St. Petersburg; Sochi (Black Sea) …..). This geographical spread will naturally both serve a national/regional need (Russia is a big country) as well as being meant to be a real enticement for future international participants — here really is a chance to explore Russia!

The entire WSC-1 attendee line-up — in front of the Kostroma State University main entrance

The participants turned out to be very enthusiastic learners, eager to ask questions and to apply the newly acquired knowledge to their own work.

Chris Marks, University of Virginia:

"I was excited to learn about and ultimately attend WSC-1 due to longtime interests in both Russia and Chemometrics. The experience far exceeded all my expectations, and I am already looking forward to attending next year. My prior chemometrics knowledge came solely from books, and I befitted greatly from the introductory lectures. The practical workshops allowed firsthand experience manipulating data, and the more advanced lectures revealed many possibilities of using chemometrics in my work.

However, by far the most useful aspect of WSC-1 was the availability of the lecturers to answer questions as they occurred. From breakfast at 8 AM until the informal discussions over beer or vodka late at night, one did not have to look far to find an answer. While the accommodations were of a distinctly different-from-American standards, the people from Kostroma Sanatorium and Kostroma State University worked quickly and enthusiastically to correct the few minor problems that occurred. My heartfelt thanks are extended both to them and to the organizing committee for putting on an excellent program."

Grigor S. Frangulyan, Heuristic Physics Laboratories, Armenia

"An earlier workshop on "Introduction to Multivariate Data Analysis", which was held last year in Moscow (also organized by Esbensen, Rodionova and Pomerantsev), was so informative about multivariate data analysis methods that I made the decision to have my second chemometrics conference participation in Kostroma this year. My decision was also conditioned by WSC-1's new additional focus: "Multivariate Image Analysis", "Multivariate statistical process control, MSPC", "Simple Interval Calculation, SIC", "Non-linear Regression" and the practical experience offered by the Matlab WORKBOOK 1 and 2 in the Geladi workshop. All my expectations were fulfilled. We worked hard and we became wiser in the chemometric realm. I also want to emphasize Kim's skills to make us all focus especially on the most important concepts ("Test is best"), Paul's brief but complete explanations, excellent simultaneous two-way translations by Oxana and Alexey and finally the friendship encountered by all attendees.

The problems discussed during 1WSC were many and comprehensive. However at the same time some other important problems, like the Data Mining, Design of Experiments, had to be left out, purely on capacity grounds. I also believe that the success of WSC-1 depends critically on of how much the participants are aware of the mathematical basis for the presented data analysis methods, which could perhaps be further strengthened at later occasions. I wish you good luck and all the best for the continued WSC-series."

Paul Geladi lectures on: "Multivariate Image Analysis" — a visit to a far-way place in Russia from the forefront of chemometrics — a perfect image of the aspirations and objectives of the Drushbametrics series.

David Muradian, Group leader, HPLA LLC, Armenia

"The conference was addressing many research workers interested in multivariate data analysis but with a very different background. Perhaps this was one of reasons why there was relatively little mathematics, but many explanations on applications during the lectures. I think however the main reason was the fact (clearly brought about by 1WSC) that it is much more difficult to understand real data than study matrix equations. As a mathematician, I was in need of the background equations because I have only very limited experience with e.g. PLS. However, as an applied mathematician having many years experience (joint works with geneticists, biologists, physicians, IC manufacturing engineers etc.) I was entirely satisfied. Both Kim Esbensen and Paul Geladi made very interesting overviews and did explain the kernel of multivariate analysis (especially PLS), while simultaneously also succeeding in indicating the (many) typical pitfalls for data analyst beginners - exclusively on real-world data. Besides, and this is very uncommon in the Russian academic tradition, we had ample possibility to state questions anytime during the lectures (and of course also during the workshops), even as late after 10 PM in the Kostroma Sanatorium - in the typical free chemometrics' environment (coffee, beer, vodka, cognac). Many thanks to them!

I would like to emphasize the great work of the conference organizers Oxana Rodionova and Alexey Pomerantsev. As a former citizen of USSR, I definitely can imagine the amount of very hardheaded practical problems that they were forced to solve organizing this winter school. They made the conference interesting, intense and with high morals. I was very interested in their scientific lectures; besides neat statistical solutions to difficult problems, they also realized some exciting aspects on data visualization. Many thanks to them!

Really, everything was excellent. I hope to meet all, or most, participants again next time (I made new friends with many). I plan to come to the next school non-empty-handed (maybe with some solutions on multivariate data visualization of my own)".

Key Russian reactions to the winter school include:

Vladimir Palyulin, Moscow State University

"It was a pleasure for me to attend the Chemometrics School at Kostroma -thank you for interesting and stimulating lectures and discussions."

Andrey Bogomolov, Advanced Chemistry Development Inc. Moscow

"I have learned that Chemometrics is not only a science. It is equally the art of having fun of solving "unsolvable" data analytical problems. It is great! Thank you!

Elena Korobova, Science Secretary of the Vernadsky Institute, Moscow:

"Two Ph.D. students and two senior scientists from GEOKHI actively participated in the WSC-1 conference and training.

The winter school held in Kostroma university presented itself as a good combination of intelligible presentations and well-prepared autonomous workshops, which provoked sharp interest in the audience and roused intentions to learn and apply the new knowledge in different fields of scientific research and technology. The overview lectures demonstrated that multivariate data analysis, which historically developed as chemometrics within chemistry, now embraces much wider areas. Therefore, datametrics seems to me perhaps as a more adequate term for the technique.

I consider this school to be a promising beginning for introductory chemometric course activities for students and specialists concerned with multivariate data processing. As a researcher in the field of environmental and landscape geochemistry I am particularly interested in reliable and adequate sampling and look forward to the next meeting which is planned to be devoted to this problem as well."

Discussing the expectation and results of WSC-1 at the final evaluation meeting, the participants and organizers emphasized the clear desirability to continue this series of winter schools in Russia, with the aim not only to attract the attention of scientists and laboratories to the wide range of data analytical problems that may be solved with the help of chemometric approach, but also to enhance specific chemometric issues, which were suggested as topics for the next Drushbametrics' events. It is hoped — strongly — that a gradually increasing international complement will find its way too…. Welcome!