

ESF Strategic Workshop on

**UNCERTAINTY MANAGEMENT
IN SIMULATION-OPTIMIZATION
OF COMPLEX SYSTEMS:
ALGORITHMS AND APPLICATIONS**

Rome (Italy), 9-12 May 2012

Convened by:
Gabriella Dellino and Carlo Meloni

SCIENTIFIC REPORT

1. EXECUTIVE SUMMARY

Several optimization problems arise in production, transportation and logistics, energy management, finance, engineering and applied sciences; in all these contexts, managers carry on a decision making process, which is usually affected by uncertainties, so the final outcome can be noisy. There are applications in virtually any area of business, government, science and engineering, so methodologies to support decisions in uncertain environments are urgently needed.

The exploratory workshop aimed at investigating strategies to account for uncertainty in complex systems described by computer simulations. When optimizing the performances of these systems, accounting or neglecting uncertainty may lead to completely different results; therefore, uncertainty management is a major issues in simulation-optimization. Because of its wide field of applications, simulation-optimization issues have been addressed by different communities with different methods, and from slightly different perspectives. Alternative approaches have been developed, also depending on the application context, without any well-established method clearly outperforming the others.

Overall, 15 researchers from 9 European countries attended this exploratory workshop, coming from different—though interrelated—areas; namely, statistical methods, experimental design, stochastic programming, global optimization, metamodeling, and design and analysis of computer simulation experiments. The resulting multidisciplinary environment definitely provided an added value to the workshop, in attaining a much better mutual understanding of the commonalities and differences of the various approaches to simulation-based optimization, especially in uncertain environments.

The event received the appreciated moral support of four non-financial sponsors; namely, Fondazione C.D. Tardini – NPO; Italian Operational Research Society (AIRO); Conference of the University Colleges (CCU); European University College Association (EUCA).

The workshop was held in Rome, from Wednesday 9 May to Saturday 12 May, at the “Villa Nazareth” University College of Fondazione C. D. Tardini – NPO. All participants stayed at the Waldorf Hotel, which was within walking distance of both the meeting venue and the bus/subway station. This made the chosen location within easy reach of both the main railway station and the airport, whose convenience should not be underestimated.

We welcomed participants organizing a reception party in the hotel lounge, to accommodate for different arrival times of the participants and make them easier to get there. This preliminary meeting gave the participants the opportunity to know each other, and start interacting in a very friendly and informal environment. Other informal occasions for interaction were provided by the coffee breaks that were arranged in the back of the conference room, with direct access to the garden surrounding the main buildings of the University College hosting the event. Lunches and dinners took place at a restaurant close to both the hotel and the meeting venue, while the workshop social dinner was held downtown, in a typical local restaurant.

General atmosphere at the workshop was very proactive during the scientific events, with stimulating discussions among motivated researchers who were all highly willing to

cooperate and build up a thematic network on the workshop research topic. Such a friendly environment emerged during the informal meetings as well.

The workshop offered many opportunities for cooperation. To maximize its potential results we decided to organize in detail the event with the active contribution of all the invited participants.

Throughout the workshop preparation phase, internet-based research communications and meetings have been promoted by also using suitable web-based tools chosen by the participants. Internet-based tools have also been used for the preparation of manuscripts and presentations before the workshop and will support the editorial projects following the event.

An official website of the workshop has been set up (www.simopt.net). The dissemination among participants will continue through constantly updated news about the progress of the activities on related scientific and technological themes, and on financial opportunities for new research projects.

We believe we successfully achieved the main result to start a panel discussion on the topic, taking an important step towards an advancement of the state-of-the-art in this research area, also accounting for potential real-world applications to improve also the state-of-the-practice. Several follow-up actions and initiatives have been included in the agenda concluding the workshop, among them:

- publication of a book devoted to the workshop contents;
- special issue on a relevant scientific journal of the field (open to the scientific community);
- several research networking actions;
- application for the next COST Action, whose deadline is September 2012.

2. SCIENTIFIC CONTENT OF THE EVENT

The scientific activity of the workshop officially started on Thursday morning, with the welcome presentation by the convenors, who briefly introduce the European Science Foundation (further details have been provided by the ESF representative, Professor Julius Zilinskas, who joined the workshop in the late afternoon); then, they illustrated the aim of the workshop and introduced the participants composition, the institution hosting the event and the (non-financial) sponsors. Finally they sketched the workshop organization over the three days, and provided some notes on the workshop venue and the social events.

The Workshop was organized in different sessions as reported in Section 4. Overall, the participation in the sessions was very satisfactory. All participants attended mostly all sessions—apart from a few late arrivals/early departures, and there were some interesting conversations in the coffee breaks.

We had fruitful discussions for each presentation. Overall, each discussant had several questions and each presentation fostered a lively debate among the attendees. The convenors—acting as chairpersons in all the sessions—did not need to raise questions to start a discussion. Each talk also included an introduction of the speaker's research group and its activities, on-going projects and active collaborations.

The first session was devoted to advanced tutorials in simulation-optimization and consisted of three technical presentations.

The first talk was given by Prof. Jan Fransoo, having the title “Simulation Modeling and Optimization for Operations Management”.

The presentation gave a survey of opportunities for simulation optimization techniques to contribute to research in operations management and stimulated an interesting discussion among the participants. Different points of view were considered and various promising research topics were addressed. In the discussion, the role played by the publication sites for the simulation-optimization researches has been also analyzed.

The following talk, given by Dr. Dirk Deschrijver, was entitled “Optimization of computationally expensive black-box systems”.

This talk widely discussed the approaches that make use of simulation surrogate models for optimization purposes and its application to several examples. The presentation also referred to software tools developed by the author’s research group. The participants found several intersections with their own research works indicating also different possible cooperations. The topic addressed in this talk plays a central role in the scientific environment of the workshop and its early schedule in the program enabled the scientific discussion helping to clarify the research interests of each participant.

The latest talk of this session was given by Prof. Henri Pierreval on “On the use of several environmental conditions in an evolutionary simulation optimization search”.

The talk addressed the use of metaheuristic in simulation-optimization when robustness issues are taken into account. Authors proposed the use of a multimodal evolutionary simulation-optimization methodology. The discussion started from the optimization point of view and explored the robustness issues in simulation-optimization. The latter theme has been reported by several participants as one of growing research interest and indicated as a field of possible joint research activities requiring an interdisciplinary approach.

After the lunch break, the first afternoon session focussed on approaches for optimization and uncertainty management.

Dr. Veronica Piccialli gave a talk on “Partition based global optimization methods”.

This talk presented a class of algorithms for global optimization of interest in the field of simulation-optimization and black-box optimization. The participants appreciated the talk which gave several ideas to improve optimization procedures in use in simulation studies. In the discussion several ways to start joint research works arose.

The second presentation, entitled “Stochastic nonlinear programming by Monte-Carlo estimators”, was given by Prof. Leonidas Sakalauskas.

The talk first gave to participants a wide and useful survey on stochastic nonlinear programming methods, and then Monte-Carlo methods were presented in details. The presentation of methodologies was rigorous but the applications were also addressed. The participants appreciated the presentation and found several intersections with their current research works. The wide and articulated discussion fruitfully pointed out the relationships between the simulation-optimization research area and the Stochastic Programming area.

Prof. Thomas Bartz-Beielstein closed the session, giving a talk on “Uncertainty management using sequential parameter optimization”.

The talk discussed methods which are implemented in the Sequential Parameter Optimization (SPO) framework, a software environment developed by the research group led by the author. The presentation gave an outline of the software package and analyzed different real-world applications. The participants appreciated the presentation which gave them the possibility to consider the use of a powerful software tool starting collaboration with a research group particularly active in the field. The wide and articulated discussion dealt with both theoretical and practical aspects of SPO and its role in the simulation-optimization of complex systems.

The second afternoon session dealt with metamodeling techniques and bootstrapping approaches.

The first presentation was given by Prof. Russell Cheng and was entitled “Accounting for statistical uncertainty using regression metamodels with bootstrapping”.

This talk showed how statistical metamodels provide a flexible framework for understanding the structure and behaviour of complex stochastic systems. The talk focused on model building and showed how bootstrapping enables effective models to be fitted and validated even in cases difficult to solve through classical statistical methods. The presentation included different examples drawn from actual studies, with demonstrations of their solution. The participants appreciated the methodological tutorial given by the author. The discussion allowed to add details on the applicability of the presented methods and to address several technical aspects. A number of possible research directions and/or new applications has been discussed among participants.

The second presentation, given by Dr. Gabriella Dellino and co-authored by Prof. Meloni, investigated the “Variability of metamodels in simulation-optimization”.

The presentation gave an insight into the sources of uncertainty yielding the so-called metamodel variability. To quantify this variability, the authors combined validation and bootstrapping techniques. The method has the advantage to be general and can be used with different kinds of metamodels and validation techniques. The resulting methodology was illustrated through some examples using different metamodels. This contribution stimulated to discuss the sources of uncertainties in modeling and metamodeling activities and how to account for them in simulation-optimization studies. As the arguments were related, the participants had the possibility to extend and elaborate the discussion started at the end of the previous talk. This helped to identify several research issues deserving to be explored.

The last talk of the session was given by Prof. Wim Van Beers on “Kriging and bootstrapping: some applications”.

This presentation gave another contribute to the relevant topic of metamodels and bootstrapping techniques. In this talk the author discussed two applications of bootstrapping in expensive simulation. A sequential design that accounts for the specific I/O behavior was first presented and then a monotonicity-preserving Kriging method was considered. The participants were interested in the results showing that bootstrapping in expensive simulation can improve the Kriging metamodels. A wide discussion among participants enabled to create several links between different presentations dealing with metamodels and bootstrapping methods. A number of research issues have been considered for future possible joint research.

The first morning session on Day 2 has been devoted to simulation-optimization methods; however, it consisted in one presentation only, due to last-minute cancellation. The talk was given by Prof. Bertrand Iooss, and had the title “Uncertainty problems in simulation-based energy management: dealing with stochastic computer models”.

The presentation dealt with some recent works about uncertainty management using time consuming stochastic computer methods. Sensitivity analysis and Kriging metamodeling tools from deterministic computer codes have been extended to stochastic code cases. Connections with optimization problems and design issues have been discussed. Some industrial examples illustrated the proposed methodology. The participants appreciated the work presented by Prof. Iooss, and several links to the previous presentations have been considered in the discussion. The real-world applications presented in the talk stimulated several questions and comments helping to show the different possible approaches to follow.

After this presentation, Prof. Zilinskas—as ESF representative in the workshop—presented ESF and its funding initiatives to support research networking activities. In particular, encouraged by the high interest from all participants and their request for details and clarifications, Prof. Zilinskas extensively discussed the COST action initiative, including how to apply for proposing an action, how to join a funded action, and describing the whole process step-by-step.

Based on the useful presentation by Prof. Zilinskas, we moved to the first round table of the workshop, whose aim was to discuss the tools and initiatives to promote joint research works. First of all, applying for a COST action would be the most natural follow-up of this exploratory workshop in the area. Most participants welcomed the initiative, and were willing to cooperate in formulating a common proposal. Another initiative of potential interest was the ESF Research Conference, as mentioned by Prof. Zilinskas in his presentation; however, this received less interest, because it implied a higher effort in the organization of the event, with a higher number of participants and a potential risk of reducing the interaction among participants. The workshop environment, instead, was highly appreciated, because it remained more focused, with several occasions of direct interaction among participants.

We also proposed to collect the workshop proceedings in a book to be published by Springer, in the Operations Research/Computer Science Interfaces Series.

Finally, we discussed a number of networking actions to be followed: first of all, the website that was open before the workshop may remain active to support any follow-up activity, either directly related to the workshop (e.g., for presentations upload) or to share news and relevant contributions on the topic. Besides, we propose to form a EURO working group on Simulation-Optimization; being subject to approval by EURO, the initiative aroused great enthusiasm among many participants, especially because there are no other chapters/sections/working groups within EURO covering this area.

Other proposals directly came from the other participants, who suggested looking for Marie Curie Actions for research exchange programmes, and initiatives by the German Academic Exchange Service DAAD (Deutscher Akademischer Austausch Dienst) to support strategic partnerships and thematic networks.

The first afternoon session was devoted to simulation and optimization applications.

The first talk was given by Dr. Ebru Angün, entitled “Risk adjusted stochastic dual dynamic solution to a disaster preparedness and relief distribution”.

She discussed a multi-stage framework to solve a disaster management problem with risk adjustments, specifically aiming at determining the quantities of emergency supplies to distribute to disaster victims and the location of intermediate transfer centers, in order to meet the (uncertain) demand while dealing with random road capacities. Interesting results have been discussed based on a hypothetical earthquake scenario in Istanbul, Turkey. This application-based presentation allowed participants to consider several realistic issues on the use of simulation-optimization methods. The discussion analyzed the multi-stage characteristic of the problem addressed and the similarities with other applications. The emerging need to introduce suitable indicators and measures for the risk was another main topic of discussion among participants.

Dr. Annalisa Cesaro gave a talk on “Optimal stock allocation in the airport maintenance supply chain”. She tackled the problem of spare part allocation for protecting operations in airports against disruptions, focusing on a single echelon inventory system with complete pooling characterized by expensive spares, long repairing time and a strict service constraint. She proposed a non-convex integer programming formulation to solve the problem of minimizing the total costs for inventory holding, lateral transshipments and emergency shipments. The design of an efficient branch and bound procedure enabled to solve many practical instances to optimality, as shown through a set of computational experiments relying on realistic data. This talk gave the opportunity to discuss several aspects of realistic supply chains with severe service level requirements. The participants found several research issues deserving further investigation for possible joint research projects. In particular, simulation-optimization cases with rare events and high computational cost are considered enough challenging and relevant problems to justify a research work.

Finally, Dr. Kostanca Katragjini presented a work entitled “Applications of simulation and optimization research in logistics”. In particular, she discussed a real problem she had to solve with her research group on waste management in a municipality. The aim was to design a decision support system to identify when and how to collect the waste containers over a weekly planning horizon, in order to minimize the associated costs while preventing container overflows. A mixed integer linear programming model was proposed, and successfully tested on a number of instances. An interesting direction for future research was outlined in adopting simulation and evolutionary optimization methods to account for data uncertainty in the waste management system. This encouraged discussion among participants on the challenging aspects related to uncertainty management in real problems even when the deterministic version of the problem seems tractable. The discussion was centered on the behavior of the decision makers about the choice of investments in more researches or more suitable decision support tools. Almost all the participants illustrated their experience on this theme which affects the development of applications and the dissemination of new methods.

The second afternoon session was organized as a round table aimed at focussing on the many application areas of potential interest for simulation-optimization methodologies managing uncertainty. The different background and complementary expertise of the participants would provide substantial benefits to joint research projects on real/realistic applications. Therefore, participants agreed on sharing algorithmic frameworks and software tools currently in use by each research group for design of experiments, optimization, simulation, input/output analysis, etc. Moreover, it would be highly desirable to identify (and share) a number of test problems to jointly tackle with possibly different perspectives.

The final aim would be to enlarge the research network not only from the methodological point of view, but also from the applications point of view, thus contributing to survey and advancing the state-of-the-practice.

Another occasion to progress in the application area would be to contribute to a Special Issue on “Simulation-Optimization of Complex Systems: Methods and Applications” for the Elsevier Journal of Simulation Modelling Practice and Theory, which has been actively supported by Prof. Pierreval, who will co-editing this special issue together with the workshop convenors. This special issue, not being restricted to workshop participants only, has the clear purpose of expanding the network of simulation-optimization researchers, collective relevant contributions to the topic worldwide.

The last session on Day 3 was a round table entirely devoted to summarize and discuss workshop achievements, including key decisions on the follow-ups.

Participants agreed on taking advantage from the website to share information and keep colleagues updated on any new initiatives of potential interest. Some participants suggest adding links to software tools to be shared within the group, and to announce conferences and/or scientific events related to the activities of the group through the website. We also agreed on uploading not only the workshop presentations but also tutorials on relevant topics. Moreover, we will add a private section (for registered users only, namely the workshop participants) to share their chapter work contributing to the Springer book. In fact, this would help to provide coherence and unity to the whole volume, as wished by many participants. The convenors, as editors of the volume, will coordinate the activities and pay special attention to organize clusters on a thematic base, in order to publish a comprehensive work intended to become a reference work in the area. To this aim, we will evaluate the opportunity to include external invited contributions on specific topics.

All the participants agreed on applying to the coming COST call for action proposals, involving also invited speakers who were not able to attend the workshop anymore. Besides that, the participants suggest to keep organizing scientific events like this exploratory workshop on a regular basis, as well as proposing special tracks, working group meetings and/or satellite events in well-established conferences.

3. ASSESSMENT OF THE RESULTS, CONTRIBUTION TO THE FUTURE DIRECTION OF THE FIELD, OUTCOME

The workshop allowed to point out as several optimization problems arise in different domains and how in all them the decision making process is usually affected by uncertainties, so the final result can be noisy. Such a process might be based on a computer simulation model, a Monte Carlo evaluation of a complex function, or even a physical experiment. The presentations and the discussions in the workshop contribute to consider and classify the topic with respect to different points of view, such as the specific field, the methodology, and the publication sites.

The workshop presentations confirm the pervasive character of the topic under study. In fact, so the development of methodologies to support the decision process in quite diverse environments is a topic of growing interest involving both applied and fundamental research.

This exploratory workshop primarily focused on problems where quantitative evaluations are expensive (e.g., some computer models can take a day or even more to generate a single

data entry); therefore, only a limited number of samples can eventually be processed and often surrogates or metamodels are used in both analysis and optimization activities.

A common goal addressed in the workshop's presentations is optimizing the performances of a system, identifying one or more key performance indicators. When the goal is to efficiently identify an optimal (or at least reasonably good) solution, the search for good solutions and the collection of information to guide the search are tightly coupled. Then the experience shows that it is necessary to solve a trade-off between exploration (i.e., global search) and exploitation (i.e., local search). Besides that, uncertainties can affect the overall decision process and some form of robustness is required, to guarantee practicable solutions. This specific topic is under development and it seems to require further research efforts.

Because of its wide field of applications, simulation-optimization has been addressed by different communities with different methods, and from slightly different perspectives. Currently, communities are largely tied to problem categories (e.g., finite vs. infinite number of alternatives; discrete vs. continuous decision variables, etc.). Uncertainty management has been frequently identified as a major issue, causing unstable performance whenever it is neglected. So far, some research has been set up to tackle this aspect; however, there are no well-established methodologies in this area. This exploratory workshop bringing together researchers from different—though interrelated—areas (e.g., statistical methods, experimental design and response-surface modeling, stochastic programming, global optimization, metamodeling, and design and analysis of computer experiments) is setting up a group able to guide the research on the topic and to promote significant actions towards the advancement of the state-of-the-art and the improvement of the current practice on the field.

The main goal of the workshop proposal, to take advantage of a multidisciplinary discussion and co-operation, to attain a much better mutual understanding of the commonalities and differences of different approaches to simulation-based optimization has been successfully achieved. Overall, the workshop offered many possibilities for cooperation. The achievement of these positive results was favored by the workshop's organization conducted with the active contribution of the invited participants.

For the entire duration of the workshop preparation, internet-based research communications and meetings were promoted by using suitable web-based tools chosen by the participants. Internet-based tools has been used also for the preparation of contributes and presentations before the workshop and for the editorial projects that follow the event. This approach enabled the co-operation and the fast collection of opinions among the participants. The same tools allow us to fruitfully keep in touch with all invited participants including those that cancelled their participation to the event.

An official website (www.simopt.net) of the workshop has been set up. The idea is to use this website also after the workshop in order to disseminate information among participants (and other interested people) through constantly updated news about the progress of the activities on related scientific and technological themes, on relevant publications, and on financial opportunities for new research projects.

The discussion and results of the workshop will be collected in an edited book to reach people that did not take part in the research project but who could be equally interested in up-coming activities (e.g., research groups and networks to promote new research projects or share new research experiences and challenges). At this aim an editorial project has been proposed to the well-known publisher Springer Science+Business Media (New York). The

project has been approved and the book will be published in the Operations Research/Computer Science Interfaces Series with the title “Uncertainty Management in Simulation-Optimization of Complex Systems — Algorithms and Applications”, edited by Gabriella Dellino and Carlo Meloni.

Besides the Springer volume devoted to the workshop contents, the participants to the Exploratory Workshop promote the organization of a journal special issue on the wider theme of Simulation-Optimization. The aim is to “explore” the scientific community and create a new occasion to share experiences and enlarge the network of researchers active in the field. The special issue is entitled “Simulation-Optimization of Complex Systems: Methods and Applications” and will appear on the journal *Simulation Modelling Practice and Theory* published by Elsevier. The guest editors of the special issue are G. Dellino, C. Meloni, and H. Pierreval.

As pointed out in the Workshop, there has been a great deal of work on simulation-optimization in the research literature, and optimization routines have been recently incorporated into several commercial simulation software tools. Techniques for simulation-optimization vary greatly depending on the problem setting and how the possible uncertainties are considered. There also appears to be a significant gap between those methods that have been extensively studied in the research literature and those that are commonly used in practice. Indeed, this difference is widely recognized, and this Special Issue aims to help bridging this gap.

In conclusion, the event was rather successful, because the research area was established, different leaders in the field have been involved and a strong network has been created.

In order to promote the research area, the discussions among the participants suggest that the research area of Simulation and Optimization of Complex Systems should be defined in such a way to contain (but not limited to):

- Black-box modelling based optimisation;
- Surrogate modelling;
- Simulation and modelling;
- Robust optimisation;
- Sensitivity based modelling and optimisation;
- Response surface analysis based optimisation;
- Kriging;
- Bootstrapping;

that are not covered by classical mathematical programming, stochastic programming, combinatorial optimisation and metaheuristics.

The applications in this area can cover problems arising in strategic planning, environmental planning, risk and safety analysis, military applications, complex business systems, etc.

The participants agreed that a status of EURO Working Group (i.e. an official Working Group of The Association of European Operational Research Societies) could be a useful tool for promotion of research in the area and for networking purposes. For these reasons this initiative is included in the agenda of follow-up actions.

The main initiative planned during the Workshop is the development of a proposal for a COST Action. The target is to apply for the call for proposals ending in September 2012. The convenors of the Workshop have been charged to coordinate the activities in order to formulate and apply the proposal. On this point the Workshop received a valuable contribution by the ESF's representative which gave useful information to the participants, clarifying all aspects of the ESF initiatives and the COST Action.

The agenda of future actions and initiatives that will be activated by the participants includes: Marie Curie Programme, DAAD programme, and the cooperation in PhD programs and doctoral schools.

4. FINAL PROGRAMME

Wednesday, 9 May 2012

Afternoon	<i>Arrival</i>
19.30-21.00	<i>Welcome party</i>

Thursday, 10 May 2012

09.50-10.10	<i>Registration</i>
10.10-10.30	Welcome by Convenors Gabriella Dellino (IMT Institute for Advanced Studies, Lucca, IT) Carlo Meloni (Politecnico di Bari, Bari, IT)
10.30-11.00	<i>Coffee / Tea Break</i>
11.00-12.30	Morning Session: Advanced tutorials in simulation-optimization
11.00-11.30	"Simulation modeling and optimization for operations management" Jan Fransoo (Eindhoven University of Technology, Eindhoven, NL)
11.30-12.00	"Optimization of computationally expensive black-box systems" Dirk Deschrijver (Ghent University, Ghent, BE)
12.00-12.30	"On the use of several environmental conditions in an evolutionary simulation optimization search" Henri Pierreval (Institut Français de Mécanique Avancée, Aubière, FR)
12.30-14.30	<i>Lunch</i>
14.30-16.00	Afternoon Session I: Optimization and uncertainty management approaches
14.30-15.00	"Partition based global optimization methods" Veronica Piccialli (Università di Roma Tor Vergata, Rome, IT)
15.00-15.30	"Stochastic nonlinear programming by Monte-Carlo estimators" Leonidas Sakalauskas (Vilnius University, Vilnius, LT)
15.30-16.00	"Uncertainty management using sequential parameter optimization" Thomas Bartz-Beielstein (Cologne University of Applied Sciences, Cologne, DE)
16.00-16.30	<i>Coffee / Tea break</i>
16.30-18.00	Afternoon Session II: Metamodeling and bootstrapping

16.30-17.00	"Accounting for statistical uncertainty using regression metamodels with bootstrapping" Russell Cheng (University of Southampton, Southampton, UK)
17.00-17.30	"Variability of metamodels in simulation-optimization" Gabriella Dellino (IMT Institute for Advanced Studies, Lucca, IT)
17.30-18.00	"Kriging and bootstrapping: some applications" Wim Van Beers (University of Amsterdam, Amsterdam, NL)
19.30	<i>Dinner</i>

Friday, 11 May 2012

Morning session I has been shortened, due to a last-minute cancellation by Prof. Van Nieuwenhuysse, whose talk was originally scheduled from 9 to 9.30. Therefore, we decide to postpone the session starting time, and to devote the emptied slot providing administrative assistance to participants, managing their reimbursement inquiries.

09.00-09.30	<i>Management of reimbursement inquiries</i>
09.30-10.00	Morning Session I: Simulation-optimization methods
09.30-10.00	"Uncertainty problems in simulation-based energy management: dealing with stochastic computer models" Bertrand Iooss (Université Mathématiques de Toulouse, Toulouse, FF)
10.00-11.00	Presentation of the European Science Foundation (ESF) Julius Zilinskas (ESF Standing Committee for Physical and Engineering Sciences - PESG)
11.00-11.30	<i>Coffee / Tea Break</i>
11.30-12.45	Morning Session II: Methodology – Issues and Challenges
11.30-11.45	Introduction to the topic
11.45-12.15	Panel discussion
12.15-12.45	Actions
12.45-14.45	<i>Lunch</i>
14.45-16.15	Afternoon Session I: Simulation and optimization applications
14.45-15.15	"Risk adjusted stochastic dual dynamic solution to a disaster preparedness and relief distribution" Ebru Angün (Galatasaray University, Istanbul, TR)
15.15-15.45	"Optimal stock allocation in the airport maintenance supply chain" Annalisa Cesaro (ISTAT Istituto Nazionale di Statistica, Rome, IT)
15.45-16.15	"Applications of simulation and optimization research in logistics" Kostanca Katragjini (Universidad Politécnica de Valencia, Valencia, S)
16.15-16.45	<i>Coffee / Tea break</i>
16.45-18.00	Afternoon Session II: Applications – Old and new opportunities
16.45-17.00	Introduction to the topic
17.00-17.30	Panel discussion
17.30-18.00	Actions

19.30 *Social dinner*

Saturday, 12 May 2012

09.00-11.00	Morning Session: Forward-looking discussion
09.00-10.00	Proposals of joint research programmes
10.00-11.00	Discussion on follow-up activities and plans for future cooperation Round table
11.00-13.00	<i>End of Workshop and departure</i>

5. FINAL LIST OF PARTICIPANTS

A number of modifications affected the participants list, due to conflicting schedules and last-minute cancellations. In particular, the following early changes were communicated and approved by the ESF Committee: Professor Tom Dhaene was replaced by Dr. Dirk Deschrijver, a post-doctoral fellow working with Prof. Dhaene in his research group, and co-author of the work presented in the workshop. Dr. Korina Katsaliaki has cancelled her attendance, and was not able to provide a direct replacement from her research group; therefore, we invited Dr. Kostanca Katragjini, who is also an active researcher in industrial applications of simulation and optimization.

We also had some attendance cancelled on short notice or last-minute cancellations: Professor Jack Kleijnen, Dr. Matthew Reindorp, and Professor Inneke Van Nieuwenhuyse had to cancel; one of them has been replaced by Dr. Jesus Adria Sanchez, from a “back-up” list maintained by the convenors.

Convenors:

1. **Carlo MELONI**
Polytechnic of Bari, Bari, Italy
2. **Gabriella DELLINO**
IMT Institute for Advanced Studies, Lucca, Italy

ESF Representative:

3. **Julius ZILINSKAS**
Vilnius University, Vilnius, Lithuania

Participants:

4. **Jesús Vicente ADRIÁ SÁNCHEZ**
Universidad Politécnica de Valencia, Valencia, Spain
5. **Ebru ANGÜN**
Galatasaray University, Ortaköy, Istanbul, Turkey
6. **Thomas BARTZ-BEIELSTEIN**
Cologne University of Applied Sciences, Gummersbach, Köln, Germany

7. **Annalisa CESARO**
ISTAT – Istituto Nazionale di Statistica, Rome, Italy
8. **Russell C.H. CHENG**
University of Southampton, Southampton, United Kingdom
9. **Dirk DESCHRIJVER**
Ghent University, Ghent, Belgium
10. **Jan C. FRANSOO**
Eindhoven University of Technology, Eindhoven, The Netherlands
11. **Kostanca KATRAGJINI**
Universidad Politécnica de Valencia, Valencia, Spain
12. **Bertrand IOOSS**
Université Paul Sabatier, Toulouse, France
13. **Veronica PICCIALLI**
Università di Roma Tor Vergata, Rome, Italy
14. **Henri PIERREVAL**
Institut Français de Mécanique Avancée, Campus de Clermont-Ferrand, Aubiere, France
15. **Leonidas SAKALAUŠKAS**
Institute of Mathematics and Informatics, Vilnius University, Vilnius, Lithuania
16. **Wim C.M. VAN BEERS**
University of Amsterdam, Amsterdam, The Netherlands

6. STATISTICAL INFORMATION ON PARTICIPANTS

Total number of participants (including ESF representative) 16

Gender	# participants
Female	5
Male	11

Country	# participants
Belgium	1
France	2
Germany	1
Italy	4
Lithuania	2
Spain	2
The Netherlands	2
Turkey	1
United Kingdom	1

	# participants
Junior	7
Senior	9

7. LOCAL ORGANIZING COMMITTEE

Administrative Chair:

Carlo MELONI
Polytechnic of Bari

Organizational Chair:

Gabriella DELLINO
IMT Institute for Advanced Studies

Members:

Marco Di Nonno, Matteo Mancini, Biagina Marrocco
Fondazione C.D. Tardini – NPO

8. NON-FINANCIAL SPONSORS



Fondazione C.D.
Tardini - NPO



Italian Operational
Research Society



Conference of the
University Colleges



European University
College Association

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**UNCERTAINTY MANAGEMENT
IN SIMULATION-OPTIMIZATION
OF COMPLEX SYSTEMS:
ALGORITHMS AND APPLICATIONS**

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Convened by:
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SCIENTIFIC REPORT APPENDIX

Abstracts

Risk-adjusted stochastic dual dynamic solution to a disaster preparedness and relief distribution problem

Ebru Angün

We consider a multi-stage disaster management problem with risk adjustments. The first-stage determines the quantities of emergency supplies to be pre-positioned at the known suppliers and the locations of transfer centers. These first-stage decisions are made before observing the random demands of the disaster victims for these supplies and the random road capacities. We assume that both demands and road capacities have joint and continuous distributions with known distribution functions. After the occurrence of a disaster and observing the realizations of the random data, the second-stage determines the quantities of supplies to be transported from the suppliers to the disaster victims through the transfer centers located at the first-stage.

We formulate this problem as a multi-stage stochastic programming problem, with Conditional Value-at-Risk (CV@R) constraints. We solve the reformulated multi-stage problem through the so-called *Stochastic Dual Dynamic Programming* (SDDP) algorithm combined with the *Sample Average Approximation* (SAA) method. Finally, we present the numerical results of a large-scale example, which considers an earthquake scenario in Istanbul.

Uncertainty Management Using Sequential Parameter Optimization

Thomas Bartz-Beielstein

I will discuss methods which are implemented in the Sequential Parameter Optimization (SPO) framework. SPO implements a sequential approach for constructing a meta-model based on noisy data. Simple strategies such as resampling will be compared with enhanced techniques such as Optimal Computational Budget Allocation.

Optimal stock allocation in the airport maintenance supply chain

Annalisa Cesaro and Dario Pacciarelli

We study a single echelon inventory system with complete pooling characterized by expensive spares, long repairing time and a strict service constraint. Specifically we face the problem of spare part allocation for protecting operations in airports against disruptions. The latter happen randomly, therefore explicitly representing uncertainty in inventory models is a safe way for modeling realistically such system dynamics. We model uncertainty through a stochastic inventory model and specifically we formulate the spares allocation problem as a non convex integer program. The objective is the minimization of the total costs for inventory holding, lateral transshipments and emergency shipments. The special structure of the problem allows designing an efficient branch and bound procedure. Computational experiments, carried on practical data, show that this method solves at optimality many practical instances.

Variability of metamodels in simulation-optimization

Gabriella Dellino and Carlo Meloni

Metamodels are often used in simulation-optimization for the design and management of complex systems enabling the integration of discipline-dependent analysis into the overall decision process. These metamodels yield insight into the relationship between responses and decision variables, providing fast analysis tools in place of the more expensive computer simulations. The combined use of stochastic simulation experiments and metamodels introduces a source of uncertainty in the decision process that we refer to as metamodel variability. To quantify this variability, we combine validation and bootstrapping techniques. The rationale behind the method relies on the fact that, after the validation process, the relative validation errors are small indicating that the metamodels give an adequate

approximation and bootstrapping these errors allows quantifying the metamodels' variability in an acceptable way. The method has the advantage to be general and can be used with different kind of metamodels and validation techniques. The resulting methodology is illustrated through some examples using regression and Kriging metamodels.

Accounting for Statistical Uncertainty using Regression Metamodels with Bootstrapping

Russell Cheng

This talk is based on several workshops conducted by the author on 'understanding statistical uncertainty' for Defence Science and Technology Laboratories. We consider how statistical metamodels provide a flexible framework for understanding the structure and behaviour of complex stochastic systems. The talk will focus on model building and show how bootstrapping enables effective models to be fitted and validated even in cases that are considered difficult using classical statistical methods. Examples drawn from actual studies, with demonstrations of their solution, will be presented.

Optimization of computationally expensive black-box systems

Dirk Deschrijver, Ivo Couckuyt, Tom Dhaene

For many problems in science and engineering it is impractical to perform experiments on the physical world directly. Instead, complex, physics-based simulation codes are used to run experiments on computer hardware. While allowing scientists more flexibility to study phenomena under controlled conditions, such experiments require a substantial investment of computation time. This places a serious computational burden on associated optimization problems. Surrogate-based optimization becomes standard practice in analyzing such expensive black-box problems. This talk discusses some approaches that make use of surrogate models for optimization and its application to several examples.

Simulation modeling and optimization for operations management

Jan Fransoo

Simulation modeling has been used for several decades now to model and study operational processes, such as in warehousing, logistics, manufacturing, and services. Over the past decades, the orientation of these studies has become more and more applied, and consequently, the research contributions to the operations management field have decreased. Recently, new advances in the field of simulation, generally captured under the concept of simulation optimization, are finding their way through in application in operations. The current research paradigm is however not yet receptive to these new methodologies. In this talk, I will outline the opportunities for simulation optimization techniques to contribute to research in operations.

Applications of simulation and optimization methods in logistics: municipal waste collection by means of assignment problems

Kostanca Katragjini, Federico Perea, Rubén Ruiz

In this talk we will show the results obtained when working on a problem proposed by a municipality regarding their waste management. More specifically, the municipality wants a support system able to decide when and how to collect their waste containers so that the associated costs are minimized. In problem settings, there are two types of waste that are collected simultaneously, typically cardboard and general waste, as these two types of waste are the most frequent and abundant. In order to do so, a special truck with two compartments is employed. Balance in the amount of collected waste per day is also a concern of the company. We propose a mixed integer linear programming (MILP) model that decides which locations should be collected on each service day, so that no container overflows, the amount of waste collected per service day is relatively constant, and the locations visited on each service day are as close to each other as possible, over a weekly

planning horizon. A computational experience over a number of instances shows the applicability of our methods. However, uncertain components inherent within waste management systems may render many deterministic optimization techniques unsuitable. The major sources of uncertainty in waste management are due to the considerable dynamic and seasonal fluctuations in the quantities, types, and composition of the collected wastes. Evolutionary simulation and optimization techniques can be adapted to incorporate data uncertainty directly into optimal solution creation.

Uncertainty problems in simulation-based energy management: dealing with stochastic computer models

Bertrand Iooss and Fanny Douard

In this talk, we will present some recent works about the uncertainty management using cpu-expensive stochastic computer codes. Sensitivity analysis and kriging metamodeling tools from deterministic computer codes have been extended to stochastic code cases. Connections will be done with optimization problems and design issues will be discussed. Moreover, a few industrial examples will illustrate our purpose.

A first example deals with oil production forecasts based on numerical simulation models. In this case, the stochastic characterization of the geological layer induces the randomness of the computer code. A second example concerns the optimization of the whole life cost of EDF nuclear fleet using exceptional maintenance tasks strategies. Such tasks may be preventive or corrective toward a wearing mechanism that may lead to a failure with a low probability and high potential consequences. To help the decision maker to choose the best strategy, EDF has developed a dedicated tool based on Monte-Carlo simulation to compute many technical economic indicators among which the density function of the Net Present Value (NPV) is the most relevant.

Partition based global optimization methods

Gianpaolo Liuzzi, Stefano Lucidi, Veronica Piccialli

This talk considers partition-based deterministic algorithms for global optimization of Lipschitz-continuous functions without requiring knowledge of the Lipschitz constant. After describing a general partition-based algorithm scheme, we focus on DIRECT (Dividing RECTangles), a successful and efficient algorithm belonging to this class. It is well known however, that this algorithm may have some problems when the dimension of the considered problem increases and it has difficulties to exploit information on the problem. Starting from the DIRECT algorithm we introduce some modifications that made possible to tackle difficult real world problems. In particular, we focus on three problems with different difficulties:

- (i) the minimization of Morse potential of molecular clusters,
- (ii) the box-constrained global optimization problem arising in the detection of gravitational waves emitted by coalescing binary systems of compact objects,
- (iii) an optimal design problem arising from multidisciplinary design optimization : three coupled disciplines (structure, aerodynamics, and propulsion) are used to represent a simplified aircraft model, with 10 variables.

The first class problems are difficult due to the large dimension, while the second problem has an objective function involving a small number of variables, but highly nonlinear and expensive to evaluate, and presents a huge number of local extrema and unavailable derivatives. As for the third one, it is a pure black-box function and highly constrained.

For all these test problems, we were able to get competitive results by using our algorithms.

On the use of several environmental conditions in an evolutionary simulation optimization search

Henri Pierreval, Ahlem Baccouche

The use of metaheuristic in simulation optimization has been widely reported in the literature. On the one hand, one major benefit of these optimization approaches is that they are generally less sensitive to local optima than other types of approaches. Unfortunately, on the other hand, metaheuristics are known to be computationally expensive methods. This is an important shortcoming since running the simulation model can also be time consuming (especially if long runs or replications are needed). When the analyst is also concerned with the robustness of the simulation optimization results, then several environments may also be contemplated to evaluate a given solution (e.g., using Taguchian principles). Unfortunately, evaluating using simulation every solution under several environmental conditions can be extremely long and therefore not suited for many concrete applications. To cope with such a difficulty, we will propose the use of multimodal evolutionary simulation optimization. We will explain how the results can be studied using several environments, so as to build a table of results from which we can derive non dominating solutions. We also show how these results can be exploited to get a better insight than a single robustness measure.

Stochastic Nonlinear Programming by Monte-Carlo estimators

Leonidas Sakalauskas

Optimal decisions in business and finance are provided often by solving a nonlinear stochastic programming problems with linear constraints:

$$F(x) \equiv Ef(x, \xi) \rightarrow \max_{x \in X}, \quad (1)$$

where the objective function is an expectation of certain random function $f: \mathfrak{R}^n \times \Omega \rightarrow \mathfrak{R}$

and where the feasible set $x \in X \subset \mathfrak{R}^n$ is a bounded and convex linear set in

general: $X = \{x | Ax = b, x \geq 0\}$, $b \in R^m$, A is the $n \times m$ -matrix, $X \neq \emptyset$.

The methods of stochastic approximation are proposed first to solve stochastic programming problems, ensuring the convergence by varying certain step-length multipliers in a scheme of stochastic gradient search (see Robins-Monro, 1951, Kiefer-Wolfowitz, 1952, Ermoliev, 1976, Michalevitch et al, 1987, Kushner, 1997, etc.). However, the rate of convergence of stochastic approximation slow down up for constrained problems (Vazan, 1969, Ermoliev, 1976, Uriasyev 1990), besides, the gradient type projection method, usually applied here, can no converge when constraints are linear due to "zigzagging" or "jamming" (Bertsekas, 1982, Polyak, 1987).

The Monte-Carlo method is a flexible tool applied in solving problems of stochastic optimization appearing here, particularly, in that of stochastic linear programming (Prekopa (2005), Ermoliev et al, 2003). Application of this method to stochastic optimization rely on replacing of the objective function, being an mathematical expectation, by averaged means, provided during Monte-Carlo simulation (see, e.g., Shapiro (1989), L.Sakalauskas (2002), EJOR). Note, sampled Monte-Carlo estimators usually have the Gaussian distribution in asymptotics (see V.Bentkus and F.Gotze (1999)) that offers a way of applying the standard theory of normal statistics to a simple computation of confidence intervals of estimators and testing of optimality hypotheses, etc.

The properties mentioned have been used in the development of the approach for unconstrained and constrained stochastic optimization by Monte-Carlo estimators (Sakalauskas, 2004, 2006), where the optimality is tested in a statistical manner and the rule for Monte-Carlo sample size adjustment has been introduced in order to decrease the total amount of Monte-Carlo trials and, at the same time, to guarantee the solution of an optimization task with an admissible accuracy. We extend this approach to stochastic problems with linear constraints using the method ε -flexible estimators. Financial applications with counterexamples are considered, too.

Kriging and bootstrapping: two examples

Wim van Beers

Kriging (or Gaussian process) metamodels approximate the input/output (I/O) functions implied by the underlying simulation models. These metamodels may serve both sensitivity analysis and optimization, because Kriging models can adequately approximate complicated I/O functions over large (global) experimental areas. Simulation optimization requires an adequate metamodel. In expensive random simulation, distribution-free bootstrapping may improve these metamodels. Assuming that each simulated input combination is replicated several times through non-overlapping pseudo-random number streams, the bootstrap simply resamples—with replacement—these replicated simulation outputs. This enables the estimation of the variances of predictions for inputs not yet simulated. Whereas simulation may take much computer time, bootstrapping takes virtually no computer time. In this talk we discuss two applications of bootstrapping in expensive simulation: 1) a sequential design that accounts for the specific I/O behavior and 2) monotonicity-preserving Kriging metamodels. Empirical results show that bootstrapping in expensive simulation improves the Kriging metamodels.