Mid-term Evaluation of ÅAU Center of Excellence: Optimization and Systems Engineering

1) Presentation of the evaluator

Lorenz T. Biegler is currently the Bayer University Professor of Chemical Engineering at Carnegie Mellon University, which he joined after receiving his PhD from the University of Wisconsin in 1981. His research interests lie in computer aided process engineering (CAPE) and include flowsheet optimization, optimization of systems of differential and algebraic equations and algorithms for constrained, nonlinear process control. Prof. Biegler has been an institute fellow at the National Energy Technology Lab, a scientist-in-residence at Argonne and Sandia National Labs, a Chang Jiang scholar at Zhejiang University, a Gambrinus Fellow at the University of Dortmund, a Fulbright Fellow at the University of Heidelberg, a Distinguished Jubilee Lecturer at IIT-Bombay and a Hougen Visiting Professor at the University of Wisconsin. He has authored over 300 archival publications and two books, edited 11 books and research volumes, and given hundreds of presentations at scientific conferences. The evaluator has known the CoE Principal Investigator, Prof. T. Westerlund, for over twenty years and participated in the PhD Examination of his student (Dr. S. Karlsson) in 2001. Prof. Grossmann, the evaluator's colleague at Carnegie Mellon, is on the CoE's International Scientific Panel. Aside from following the work of Prof. Westerlund through conference interactions, technical publications and presentations, the evaluator has had no additional research collaborations with CoE investigators.

2) The research plan, realization and the future

The CoE focuses on four intertwined themes of optimization, mathematical statistics, systems theory and systems engineering. The structure of the center is arranged around a two-way interaction between theoretical development of the themes coupled with applications in engineering, physics and bioinformatics. The research is organized through seven work packages; the first four are devoted to theory and methods while the last three are devoted to applications that arise from the first four areas. The CoE includes a highly qualified team of 13 senior researchers and 3 postdoctoral researchers along with an international research panel and adjunct faculty from industry. At 2.5 years into the program, the CoE has produced considerable research output and made significant breakthrough contributions in its thematic areas. In particular, 3 completed doctoral theses and 9 master's theses have been funded by this CoE. The CoE currently supports the research of 8 doctoral candidates. Specific areas of progress are noted within the individual work packages.

WP1: Optimization

The optimization work package is devoted to furthering the development of theory and algorithms for the global solution of mixed integer nonlinear programming (MINLP) problems. Within this area, the research team has focused on the following breakthrough topics with recent journal publications. The first deals with algorithms for convex MINLPs with nonsmooth elements, where the investigators have shown that this problem cannot be easily generalized for existing MINLP methods. Nevertheless, for the class of nonsmooth problems, where the subdifferential is a convex combination of a finite number of subgradients, a modified outer approximation algorithm could be applied that converges to the global optimum. Second, global optimization algorithms are developed for mixed-integer signomial programming problems. For this topic, a novel algorithm was developed that avoids the classical spatial branch and bound strategy. Instead, successively refined piecewise linear approximations allow fast mixed integer searches to be applied, thus leading to an easily implementable algorithm. Finally, the classical αBB type underestimator was extended to a more general framework that allows tighter under-approximations through the use of off-diagonal quadratic terms, thus leading to better performance for global optimization. Four PhD students are affiliated with this work package and algorithmic development, refinement and validation is strong, with good future directions based on the above topics. Moreover, WP1 has very strong synergies with application areas WP5, WP6 and WP7.

WP2: Systems engineering

This work package deals with robust system identification for linear and nonlinear systems. Current activities in this work package include support vector regression and sparse optimization in order to perform system identification in the presence of unknown outliers, offsets and trends. In addition, current work is focused on state-space Fourier-series representations, which allows for computation of optimal time-invariant Kalman-filter-type state estimators for time-periodic systems, as well as other related areas. One PhD student is affiliated with this work package and journal papers are in preparation based on results given in conference presentations.

WP3: Systems theory

This work package deals with the abstract representation and analysis of state/signal systems, which replace the classical view of state/input/output systems. Main developments for the CoE include a general realization theory for state/signal systems. This detailed analysis also includes new results of the state/signal theory for an older class of well-posed input/state/output systems, including canonical passive systems, along with conservative state/signal shift realizations of arbitrary passive continuous time behaviors. One PhD thesis was completed for this CoE; another is also funded by the CoE for this work package. Around 10 recent publications relate to these new results. Because of the fundamental and abstract setting of this work it is hard to gauge its immediate links to the other WPs or direct applications, although they do lead to important longer term implications for state/signal system.

WP4: Mathematical statistics

This work package deals with stochastic computational modeling strategies for the analysis of complex data sets. This approach is grounded on recent advances in Bayesian predictive modeling and adaptive stochastic Monte Carlo computation. A number of breakthrough activities have occurred within this WP, including asymptotic and small-sample properties of various predictive classification models, theory for learning genetic population structures and generalized context-specific undirected graphical models and context-specific Bayesian networks. These have been described in numerous publications and have widespread applications including clustering models for bacterial metagenomics, large-scale bacterial genome data analysis, medical statistics and thermodynamics databases. WP4 is somewhat complementary to WP1, as both are theory-based and have seen significant recent activity with direct influence on applications. For WP4 this can be seen in WP6, Task 3. Two PhDs are funded through this work package.

WP5: Physics and material science

This work package seems to be focused on a specific application domain, the creation of mathematical models for minimizing the energy of electron configurations in disordered materials. Here Coulomb glasses are considered, where the conduction electrons are localized to impurity sites; these include lightly doped semiconductors at low temperatures. The energy minimization models can be formulated as 0-1 variable quadratic assignment problems (QAPs), which fall into the class of MINLP problems considered in WP1. In a recent paper, these have been addressed through semidefinite programming as well as linear and convex reformulation techniques. In addition, another recent work has explored an exact linear reformulation of QAPs, which allows fast solution with state-of-the-art MILP solvers. Future work will be devoted to greater application of specialized MINLP formulations to this problem class.

WP6: Biotechnology and medicine

This work package is divided into three tasks. Most of the advances were described for Task 1, which deals with peptide docking. The configuration of peptide docking can be modeled as a global optimization problem, where the total energy conformation of the peptide should be minimized. For instance, in the ECEPP/3 (empirical conformational energy program of peptides) potential model, the total conformation energy contributions include electrostatic, nonbounded, hydrogen bounded, torsional and loop-closing energies. The energy minimization problem leads to a smooth nonconvex problem, which has been addressed by recent advances of the αBB algorithm in WP1.

No recent progress has been described for Task 2, which deals with Systems Biology.

Task 3 is strongly linked to WP4 and deals with medical statistics. No recent progress is described here, but this area has benefited from stochastic computational modeling strategies for the analysis of complex data sets with applications that include clustering models for bacterial metagenomics, large-scale bacterial genome data analysis, medical statistics and thermodynamics databases, as described in recent CoE publications.

WP7: Engineering

This work package is divided into two tasks: *Large-Scale Industrial Scheduling* and *Time-periodic Systems*. CoE results for this work package have focused on the first task, where quadratic assignment problems have been studied. For industrial production networks, scheduling problems were considered for flexible multi-stage production, where numerous raw materials and products need to be scheduled over long horizons. This leads to mixed integer optimization problems with thousands of variables and constraints. Recent results reported in WP1 for the solution of QAPs has been very useful in improving solution strategies for these demanding problems. It is clear that the research results from WP1 will have major impact on this task.

No progress report was given for Task 2, which deals with time-periodic processes.

3) Scientific publications and other results

Since the beginning of the CoE, around 90 publications can be claimed. These include 70 peer-reviewed journal papers, a monograph on semigroups, four book chapters and 16 refereed articles in conference proceedings. From the included 10 representative publications, it is quite clear that the quality of these publications is very high. The 10 publications represent the strengths of the CoE and demonstrate the world-class nature of the CoE's research. In addition, the output of doctoral and MSc theses, the leveraging of additional research funding and the visibility of the research through popular channels demonstrates the productivity of the CoE and the high probability of successful research outcomes.

4) Scientific activities, especially international cooperation

The CoE has engaged in strong scientific activities that promote excellent research productivity. The senior researchers of the CoE are highly visible at an international level. They are active in conference participation and organization and perform exemplary editorial and advisory roles in the scientific community.

Moreover, there is an excellent plan to integrate CoE researchers with international collaborators. In particular, with an annual OSE seminar from an international panelist and research exchanges and extended visits of CoE researchers with the panelists, the CoE has ensured an exposure to leading international research and an essential cross-fertilization for the CoE's activities.

As a result of these activities, the CoE has made links to the strongest groups in MINLP and global optimization around the world. The CoE international scientific panel in this area is second to none. Moreover, the collaborations in WP3 with D. Arov in Ukraine and G. Weiss in Israel appear to be very productive and fruitful, although less organized. In WP2 and WP4 links to international groups are also less organized and more sparse, but they still appear strong.

5) The research group

The CoE's research group is characterized by high quality senior researchers. The steering committee consists of world-class investigators, who have made a strong impact in optimization and systems engineering. In addition, the team of post-doctoral researchers and doctoral candidates are working at a high research level and are generating impressive results, especially over the duration of the current CoE.

As a result, I believe the CoE and its activities in the work packages are proceeding well. Based the above remarks about the activities on the theory-related work packages, it is clear that WP1 is proceeding very well with innovative new results that continue to make a strong impact on the global solution of MINLPs. Similarly, WP4 activities are complementary to WP1 through stochastic computational modeling strategies built on Bayesian predictive modeling and adaptive stochastic Monte Carlo computation. These are especially useful in data analytics for the huge data sets that arise in a number of application domains. It is hoped that over time, there will be greater synergies between the methods and applications of WP1 and WP4. The system identification area in WP2 has seen some recent progress, and additional tasks in WP2, described in the original CoE proposal, could benefit from synergies with WP1. Finally, because of the fundamental and abstract nature of its topic, WP3 seems to be somewhat independent and separated from activities in the other work packages. Nevertheless, the fundamental results for state/signal systems in WP3 should lead to a long-term impact in a number of application areas.

With respect to the applications work packages, WP5 shows some interesting synergies with WP1 in Coulomb glasses, and this interaction is hoped to expand with further applications in materials design. WP6, with Tasks 1-3 on biomedical applications represent an innovative approach to look at important problems. Here WP1 and WP4 can find common ground and these activities will lead to breakthrough areas in systems biology and medical statistics. Finally, in WP7, Tasks 1 and 2, the manufacturing application projects have strong industrial connections, which should lead to considerable real-world impact.