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Project-Team DOLPHIN

Discrete multi-objective Optimization for Large scale Problems with Hybrid dIstributed techNiques

Lille - Nord Europe

THEME NUM

Activity Report

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Table of contents

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2. Overall Objectives

2.1. Presentation

The goal of the DOLPHIN[1] project is the modelization and resolution of large multi-criteria combinatorial problems using parallel and distributed hybrid techniques. We are interested in algorithms using Pareto approaches which generate the whole Pareto set of a given Multi-Objective Problem (MOP). For this purpose, the research actions can be resumed as follows:

- **Modeling and Analysis of MOPs:** Solving Multi-Objective Problems requires an important analysis phase to find the best suitable method to solve it. This analysis deals with the modeling of the problem and the analysis of its structure.

[1] Discrete multi-objective Optimization for Large scale Problems with Hybrid dIstributed techNiques.

To propose efficient models for a Multi-Objective Optimization problem, an important aspect is to integrate all the constraints of the problem. Therefore an interesting preliminary approach is to develop efficient models for the problem in its mono-objective forms in order to be able to develop methods that are taking into account characteristics of the studied problem. While studying the problem in its multi-objective form, the analysis of the structure is another interesting way.

The analysis of the structure of the Pareto front by means of different approaches (statistical indicators, meta-modeling, etc.) allows the design of efficient and robust hybrid optimization techniques. In general, the current theory does not allow the complete analysis of optimization algorithms. Several questions are unanswered: i) why a given method is efficient? ii) why certain instances are difficult to solve? Some work is needed to guide the user in the design of efficient methods.

The NFL (No Free Lunch) theorem shows that two optimization methods have the same global performance on the whole set of uniform optimization problems. Then, it is crucial to make some hypotheses on the studied problem. This may be done in two steps:

- analyzing the target problem to identify its landscape properties,
- including this knowledge in the proposed optimization method.

Our interest in this project is to answer these questions and remarks for the multi-objective case. Another point considered is the performance evaluation of multi-objective optimization methods. We are also working on approximation algorithms with performance guarantee and the convergence properties of stochastic algorithms.

- **Cooperation of optimization methods (metaheuristics and/or exact methods):**

  The hybridization of optimization methods allows the cooperation of complementary different methods. For instance, the cooperation between a metaheuristic and an exact method allows to take advantage of the intensification process of an exact method in finding the best(s) solution(s) in a sub-space, and the diversification process of the metaheuristic in reducing the search space to explore.

  In this context, different types of cooperation may be proposed. Those approaches are under study in the project and we are applying them to different generic MOPs (flow-shop scheduling problem, vehicle routing problem, covering tour problem, access network design, and the association rule problem in data mining).

- **Parallel optimization methods:** Parallel and distributed computing may be considered as a tool to speedup the search to solve large MOPs and/or to improve the robustness of a given method. Following this objective, we design and implement parallel metaheuristics (evolutionary algorithms, tabu search approach) and parallel exact methods (branch and bound algorithm, branch and cut algorithm) for solving different large MOPs. Moreover, the joint use of parallelism and cooperation allows the improvement of the quality of the obtained solutions.

- **Framework for parallel and distributed hybrid metaheuristics:** Our team contributes to the development of an open source framework for metaheuristics, named ParadisEO (PARAllel and DIStributed Evolving Objects). Our contribution in this project is the extension of the EO (Evolving Objects) framework [2], which consists in: i) the generalization of the framework to single solution metaheuristics such as local search, tabu search and simulated annealing; ii) the design of metaheuristics for multi-objective optimization; iii) the design of hybrid methods; iv) the development of parallel and distributed models.

  In this project, our goal is the efficient design and implementation of this framework on different types of parallel and distributed hardware platforms: cluster of workstations (COW), networks of workstations (NOW) and GRID computing platforms, using the different suited programming environments (MPI, Condor, Globus, PThreads). The coupling with well-known frameworks for

[2] This framework was initially developed by Geneura TEAM (Spain), INRIA (France), LIACS (Netherlands). http://paradiseo.gforge.inria.fr.

exact methods (such as COIN) will also be considered. The exact methods for MOPs developed in this project will be integrated in those software frameworks.

The experimentation of this framework by different users and applications outside the DOLPHIN project is considered. This is done in order to validate the design and the implementation issues of ParadisEO.

- **Validation:** the designed approaches are validated on generic and real-life MOPs, such as:
  - scheduling problems: Flow-shop scheduling problem;
  - routing problems: Vehicle routing problem (VRP), covering tour problem (CTP)...;
  - mobile telecommunications: Design of mobile telecommunications networks (contract with France Telecom R&D) and design of access networks (contract with Mobinets);
  - genomics: Association rule discovery (data mining task) for mining genomic data, protein identification, docking and conformational sampling of molecules.
  - engineering design problems: Design of polymers.

  Some benchmarks and their associated optimal Pareto fronts or the best known Pareto fronts have been defined and made available on the Web. We are also developing an open source software, named GUIMOO[3], which integrates different performance evaluation metrics and 2D/3D visualization tools of Pareto fronts.

2.2. Highlights of the year

Best Student Paper Award, **Jean-Charles Boisson**.
J-C. Boisson, L. Jourdan, E-G.Talbi and D. Horvath, Parallel multi-objective algorithms for the molecular docking problem IEEE 2008 Symposium on Computational Intelligence in Bioinformatics and Computational Biology (CIBCB), 2008.

Clarisse Dhaenens finalist of the Excellencia Prize (see http://www.excellencia.eu) - trophée de la Femme ingénieur High-Tech.

3. Scientific Foundations

3.1. Modeling and landscape analysis

The modeling of problems, the analysis of structures (landscapes) of MOPs and the performance assessment of resolution methods are significant topics in the design of optimization methods. The effectiveness of metaheuristics depends on the properties of the problem and its landscape (roughness, convexity, etc). The notion of landscape has been first described in [82] by the way of the study of species evolution. Then, this notion has been used to analyze combinatorial optimization problems.

3.1.1. Modeling of problems

Generally there are several ways of modeling a given problem. First, one has to find the most suitable model for the type of resolution he plans to use. The choice can be made after a theoretical analysis of the model, or after computational experiments. The choice of the model depends on the type of method used. For example, a major issue in the design of exact methods is to find tight relaxations for the problem considered.

Let us note that many combinatorial optimization problems of the literature have been studied in their mono-objective form even if a lot of them are naturally of a multi-objective nature.

[3] Graphical User Interface for Multi-Objective Optimization (http://guimoo.gforge.inria.fr).

Therefore, in the Dolphin project, we address the modeling of MOPs in two phases. The first one consists in studying the mono-objective version of the problem, where all objectives but one are considered as constraints. In the second phase, we propose methods to adapt the mono-objective models or to create hand-tailored models for the multi-objective case. The models used may come from the first phase, or from the literature.

3.1.2. Analysis of the structure of a problem

The landscape is defined by a neighborhood operator and can be represented by a graph $G = (V, E)$. The vertices represent the solutions of the problem and an edge (e_1, e_2) exists if the solution e_2 can be obtained by an application of the neighborhood operator on the solution e_1. Then, considering this graph as the ground floor, we elevate each solution to an altitude equals to its cost. We obtain a surface, or landscape, made of peaks, valleys, plateaus, cliffs, ...The problem lies in the difficulty to have a realistic view of this landscape.

As others, we believe that the main point of interest in the domain of combinatorial optimization is not the design of the best algorithm for a large number of problems but the search for the most adapted method to an instance or a set of instances of a given problem. Therefore, we are convinced that no ideal metaheuristic, designed as a black-box, may exist.

Indeed, the first studies realized in our research group on the analysis of landscapes of different mono-objective combinatorial optimization problems (traveling salesman problem, quadratic assignment problem) have shown that not only different problems correspond to different structures but also that different instances of the same problem correspond to different structures.

For instance, we have realized a statistical study of the landscapes of the quadratic assignment problem. Some indicators, that characterize the landscape of an instance have been proposed and a taxonomy of the instances including three classes has been deduced. Hence it is not enough to adapt the method to the problem under study but it is necessary to specialize it according to the type of treated instance.

So in its studies of mono-objective problems, the DOLPHIN research group has introduced into the resolution methods some information about the problem to be solved. The landscapes of some combinatorial problems have been studied in order to investigate the intrinsic natures of their instances. The resulting information have been inserted into an optimization strategy and allowed the design of efficient and robust hybrid methods. The extension of these studies to multi-objective problems is a part of the DOLPHIN project [80], [81], [79], [78].

3.1.3. Performance assessment

The DOLPHIN project is also interested in the performance assessment of multi-objective optimization methods. Nowadays, statistical techniques developed for mono-objective problems can be adapted to the multi-objective case. Nevertheless, specific tools are necessary in many cases: for example, the comparison of two different algorithms is relatively easy in the mono-objective case - we compare the quality of the best solution obtained in a fixed time, or the time needed to obtain a solution of a certain quality. The same idea cannot be immediately transposed to the case where the output of the algorithms is a set of solutions having several quality measures, and not a single solution.

Various indicators have been proposed in the literature for evaluating the performance of multi-objective optimization methods but no indicator seems to outperform the others [83]. The DOLPHIN research group has proposed two indicators: the *contribution* and the *entropy* [75]. The contribution evaluates the supply in term of Pareto-optimal solutions of a front compared to another one. The entropy gives an idea of the diversity of the solutions found. These two metrics are used to compare the different metaheuristics in the research group, for example in the resolution of the bi-objective flow-shop problem, and also to show the contribution of the various mechanisms introduced in these metaheuristics.

These metrics and others (generational distance, spacing, ...) are integrated in the open software GUIMOO developed within the framework of the DOLPHIN project. This software is dedicated to the visualization of landscapes (2D and 3D) for multi-objective optimization and the performance analysis by the use of special metrics.

3.1.4. Goals

One of the main issues in the DOLPHIN project is the study of the landscape of multi-objective problems and the performance assessment of multi-objective optimization methods to design efficient and robust resolution methods:

- *Landscape study:* The goal here is to extend the study of landscapes of the mono-objective combinatorial optimization problems to multi-objective problems in order to determine the structure of the Pareto frontier and to integrate this knowledge about the problem structure in the design of resolution methods.

  This study has been initiated for the bi-objective flow-shop problem. We have studied the convexity of the frontiers obtained in order to show the interest of our Pareto approach compared to an aggregation approach, which only allows to obtain the Pareto solutions situated on the convex hull of the Pareto front (supported solutions).

  Our preliminary study of the landscape of the bi-objective flow-shop problem shows that the supported solutions are very closed to each other. This remark leads us to improve an exact method initially proposed for bi-objective problems. Furthermore, a new exact method able to deal with any number of objectives has been designed.

- *Performance assessment:* The goal here is to extend GUIMOO in order to provide efficient visual and metric tools for evaluating the assessment of multi-objective resolution methods.

3.2. Hybrid multi-objective optimization methods

The success of metaheuristics is based on their ability to find efficient solutions in a reasonable time [74]. But with very large problems and/or multi-objective problems, efficiency of metaheuristics may be compromised. Hence, in this context it is necessary to integrate metaheuristics in more general schemes in order to develop even more efficient methods. For instance, this can be done by different strategies such as cooperation and parallelization.

The DOLPHIN project deals with *"a posteriori"* multi-objective optimization where the set of Pareto solutions (solutions of best compromise) have to be generated in order to give to the decision maker the opportunity to choose the solution that interests him/her.

Population-based methods, such as evolutionary algorithms, are well fitted for multi-objective problems, as they work with a set of solutions [73], [70]. To be convinced one may refer to the list of references on Evolutionary Multi-objective Optimization maintained by Carlos A. Coello Coello [4] which contains almost 3 000 references. One of the objectives of the project is to propose advanced search mechanisms for intensification and diversification. These mechanisms have been designed in an adaptive manner, since their effectiveness is related to the landscape of the MOP and to the instance solved.

In order to assess the performances of the proposed mechanisms, we always proceed in two steps: first, experiments are carried out on academic problems, for which some best known results exist; second, we use real industrial problems to cope with large and complex MOPs. The lack of references in terms of optimal or best know Pareto set is a major problem. Therefore, the obtained results in this project and the test data sets will be available at the URL http://www.lifl.fr/OPAC at Benchmarks.

3.2.1. Cooperation of metaheuristics

In order to cope with advantages of the different metaheuristics, an interesting idea is to combine them. Indeed, the hybridization of metaheuristics allows the cooperation of methods having complementary behaviors. The efficiency and the robustness of such methods depend on the balance between the exploration of the whole search space and the exploitation of interesting areas.

[4] http://www.lania.mx/~ccoello/EMOO/EMOObib.html

Hybrid metaheuristics have received considerable interest these last years in the field of combinatorial optimization. A wide variety of hybrid approaches have been proposed in the literature and give very good results on numerous single objective optimization problems, which are either academic (traveling salesman problem, quadratic assignment problem, scheduling problem, ...) or real-world problems. This efficiency is generally due to combinations of single-solution based methods (iterative local search, simulated annealing, tabu search...) with population-based methods (genetic algorithms, ants search, scatter search...). A taxonomy of hybridization mechanisms may be found in [77]. It proposes to decompose those mechanisms into 4 classes:

- *LRH class - Low-level Relay Hybrid*: This class groups algorithms in which a given metaheuristic is embedded into a single-solution metaheuristic. Few examples from the literature belong to this class.
- *LTH class - Low-level Teamwork Hybrid*: In this class, a metaheuristic is embedded into a population-based metaheuristic in order to exploit strengths of single-solution and population-based metaheuristics.
- *HRH class - High-level Relay Hybrid*: Here, self contained metaheuristics are executed in a sequence. For instance, a population-based metaheuristic is executed to locate interesting regions and then a local search is performed to exploit these regions.
- *HTH class - High-level Teamwork Hybrid*: This scheme involves several self-contained algorithms performing a search in parallel and cooperating. An example will be the island model, based on GAs, where the population is partitioned into small subpopulations and a GA is executed per subpopulation. Some individuals can migrate between subpopulations.

Let us notice, that if hybrid methods have been studied in the mono-criterion case, their application in the multi-objective context is not yet widely spread. The objective of the DOLPHIN project is to integrate specificities of multi-objective optimization into the definition of hybrid models.

3.2.2. Cooperation between metaheuristics and exact methods

Until now only few exact methods have been proposed to solve multi-objective problems. They are based either on a Branch-and-bound approach, on the algorithm A^* or on dynamic programming. However, those methods are limited to two objectives and are, most of the time, not able to be used on a complete large scale problem. Therefore, sub search spaces have to be defined in order to be able to use exact methods. Hence, in the same manner as hybridization of metaheuristics, the cooperation of metaheuristics and exact methods is also a main issue in this project. Indeed, it allows to use the exploration capacity of metaheuristics, as well as the intensification ability of exact methods, which are able to find optimal solutions in a restricted search space. Sub search spaces have to be defined along the search. Such strategies can be found in the literature, but they are only applied to mono-objective academic problems.

We have extended the previous taxonomy for hybrid metaheuristics to the cooperation between exact methods and metaheuristics. Using this taxonomy, we are investigating cooperative multi-objective methods. In this context, several types of cooperations may be considered, according to the way the metaheuristic and the exact method cooperate. For instance, a metaheuristic can use an exact method for intensification or an exact method can use a metaheuristic to reduce the search space.

Moreover, a part of the DOLPHIN project deals with studying exact methods in the multi-objective context in order: i) to be able to solve small size problems and to validate proposed heuristic approaches; ii) to have more efficient/dedicated exact methods that can be hybridized with metaheuristics. In this context, the use of parallelism will push back limits of exact methods, which will be able to explore larger size search spaces [71].

3.2.3. Goals

Based on the previous works on multi-objective optimization, it appears that to improve metaheuristics, it becomes essential to integrate knowledge about the problem structure. This knowledge can be gained during the search. This would allow to adapt operators which may be specific for multi-objective optimization or not.

The goal here is to design auto-adaptive methods that are able to react to the problem structure. Moreover, regarding the hybridization and the cooperation aspects, the objectives of the DOLPHIN project are to deepen those studies as follows:

- *Design of metaheuristics for the multi-objective optimization:* To improve metaheuristics, it becomes essential to integrate knowledge about the problem structure, that we may get during the execution. This would allow to adapt operators that may be specific for multi-objective optimization or not. The goal here is to design auto-adaptive methods that are able to react to the problem structure.
- *Design of cooperative metaheuristics:* Previous studies show the interest of hybridization for a global optimization and the importance of problem structure study for the design of efficient methods. It is now necessary to generalize hybridization of metaheuristics and to propose adaptive hybrid models that may evolve during the search while selecting the appropriate metaheuristic. Multi-objective aspects have to be introduced in order to cope with specificities of multi-objective optimization.
- *Design of cooperative schemes between exact methods and metaheuristics:* Once the study on possible cooperation schemes is achieved, we will have to test and compare them in the multi-objective context.
- *Design and conception of parallel metaheuristics:* Our previous works on parallel metaheuristics allow us to speed up the resolution of large scale problems. It could be also interesting to study the robustness of the different parallel models (in particular in the multi-objective case) and to propose rules that determine, given a specific problem, which kind of parallelism to use. Of course these goals are not disjoined and it will be interesting to simultaneously use hybrid metaheuristics and exact methods. Moreover, those advanced mechanisms may require the use of parallel and distributed computing in order to easily make evolve simultaneously cooperating methods and to speed up the resolution of large scale problems.
- *Validation:* In order to validate results obtained we always proceed in two phases: validation on academic problems, for which some best known results exist and use on real problems (industrial) to cope with problem size constraints.

  Moreover, those advanced mechanisms are to be used in order to integrate the distributed multi-objective aspects in the ParadisEO Platform (see the paragraph on software platform).

3.3. Parallel multi-objective optimization: models and software frameworks

Parallel and distributed computing may be considered as a tool to speedup the search to solve large MOPs and to improve the robustness of a given method. Moreover, the joint use of parallelism and cooperation allows improvements on the quality of the obtained Pareto sets. Following this objective, we will design and implement parallel models for metaheuristics (evolutionary algorithms, tabu search approach) and for exact methods (branch-and-bound algorithm, branch-and-cut algorithm) for solving different large MOPs.

One of the goal of the DOLPHIN project is to integrate the developed parallel models into software frameworks. Several frameworks for parallel distributed metaheuristics have been proposed in the literature. Most of them focus only either on evolutionary algorithms or on local search methods. Only few frameworks are dedicated to the design of both families of methods. On the other hand, existing optimization frameworks either do not provide parallelism at all or just supply at most one parallel model. In this project, a new framework for parallel hybrid metaheuristics is proposed, named *Parallel and Distributed Evolving Objects (ParadisEO)* based on EO. The framework provides in a transparent way the hybridization mechanisms presented in the previous section, and the parallel models described in the next section. Concerning the developed parallel exact methods for MOPs, we will integrate them into well-known frameworks such as COIN.

3.3.1. Parallel models

According to the family of addressed metaheuristics, we may distinguish two categories of parallel models: parallel models managing a single solution, and parallel models that handle a population of solutions. The major single solution-based parallel models are the following: the *parallel neighborhood exploration model* and the *multi-start model*.

- *The parallel neighborhood exploration model* is basically a "low level" model that splits the neighborhood into partitions that are explored and evaluated in parallel. This model is particularly interesting when the evaluation of each solution is costly and/or when the size of the neighborhood is large. It has been successfully applied to the mobile network design problem (see Application section).
- *The multi-start model* consists in executing in parallel several local searches (that may be heterogeneous), without any information exchange. This model raises particularly the following question: is it equivalent to execute k local searches during a time t than executing a single local search during $k \times t$? To answer this question we tested a multi-start Tabu search on the quadratic assignment problem. The experiments have shown that the answer is often landscape-dependent. For example, the multi-start model may be well-suited for landscapes with multiple basins.

Parallel models that handle a population of solutions are mainly: the *island model*, the *central model* and *the distributed evaluation of a single solution*. Let us notice that the last model may also be used with single-solution metaheuristics.

- In *the island model*, the population is split into several sub-populations distributed among different processors. Each processor is responsible of the evolution of one sub-population. It executes all the steps of the metaheuristic from the selection to the replacement. After a given number of generations (synchronous communication), or when a convergence threshold is reached (asynchronous communication), the migration process is activated. Then, exchanges of solutions between sub-populations are realized, and received solutions are integrated into the local sub-population.
- *The central (Master/Worker) model* allows to keep the sequentiality of the original algorithm. The master centralizes the population and manages the selection and the replacement steps. It sends sub-populations to the workers that execute the recombination and evaluation steps. The latter returns back newly evaluated solutions to the master. This approach is efficient when the generation and evaluation of new solutions is costly.
- *The distributed evaluation model* consists in a parallel evaluation of each solution. This model has to be used when, for example, the evaluation of a solution requires access to very large databases (data mining applications) that may be distributed over several processors. It may also be useful in a multi-objective context, where several objectives have to be computed simultaneously for a single solution.

As these models have now been identified, our objective is to study them in the multi-objective context in order to use them advisedly. Moreover, these models may be merged to combine different levels of parallelism and to obtain more efficient methods [72], [76].

3.3.2. Goals

Our objectives focus on these issues are the following:

- *Design of parallel models for metaheuristics and exact methods for MOPs*: We will develop parallel cooperative metaheuristics (evolutionary algorithms and local search such as Tabu search) for solving different large MOPs. Moreover, we are designing a new exact method, named PPM (Parallel Partition Method), based on branch and bound and branch and cut algorithms. Finally, some parallel cooperation schemes between metaheuristics and exact algorithms have to be used to solve MOPs in an efficient manner.
- *Integration of the parallel models into software frameworks*: The parallel models for metaheuristics will be integrated in the ParadisEO software framework. The proposed multi-objective exact methods must be first integrated into standard frameworks for exact methods such as COIN and BOB++. A *coupling* with ParadisEO is then needed to provide hybridization between metaheuristics and exact methods.

- *Efficient deployment of the parallel models on different parallel and distributed architecture including GRIDs*: The designed algorithms and frameworks will be efficiently deployed on non-dedicated networks of workstations, dedicated cluster of workstations and SMP (Symmetric Multi-processors) machines. For GRID computing platforms, peer to peer (P2P) middlewares (XtremWeb-Condor) will be used to implement our frameworks. For this purpose, the different optimization algorithms may be re-visited for their efficient deployment.

4. Application Domains

4.1. Academic generic problems

In this project, some well known optimization problems are re-visited in terms of multi-objective modelization and resolution:

- **Workshop optimization problems:**

  Workshop optimization problems deal with optimizing the production. In this project, two specific problems are under study.

  - **Flow-shop scheduling problem:** The flow-shop problem is one of the most well-known scheduling problems. However, most of the works of the literature use a mono-objective model. In general, the minimized objective is the total completion time (makespan). Many other criteria may be used to schedule tasks on different machines: maximum tardiness, total tardiness, mean job flowtime, number of delayed jobs, maximum job flowtime, etc. In the DOLPHIN project, a bi-criteria model, which consists in minimizing the makespan and the total tardiness, is studied. A tri-criteria flow-shop problem, minimizing in addition the maximum tardiness, is also studied. It will allow to develop and test multi-objective (and not only bi-objective) exact methods.
  - **Cutting problems:** Cutting problems occur when pieces of wire, steel, wood, or paper have to be cut from larger pieces. The objective is to minimize the quantity of lost material. Most of these problems derive from the classical one-dimensional cutting-stock problem, which have been studied by many researchers. The problem studied by the DOLPHIN project is a two-dimensional bi-objective problem, where rotating a rectangular piece has an impact on the visual quality of the cutting pattern. First we have to study the structure of the cutting-stock problem when rotation is allowed, then we will develop a method dedicated to the bi-objective version of the problem.

- **Logistics and transportation problems:**
  - **Packing problems:** In logistic and transportation fields, packing problems may be a major issue in the delivery process. They arise when one wants to minimize the size of a warehouse or a cargo, the number of boxes, or the number of vehicles used to deliver a batch of items. These problems have been the subjects of many papers, but only few of them study multi-objective cases, and to our knowledge, never from an exact point of view. Such a case occurs for example when some pairs of items cannot be packed in the same bin. The DOLPHIN project is currently studying the problem in its one-dimensional version. We plan to generalize our approach to two and three dimensional problems, and to more other conflict constraints, with the notion of *distance* between items.
  - **Routing problems:** The vehicle routing problem (VRP) is a well-known problem and it has been studied since the end of the 50's. It has a lot of practical applications in many industrial areas (ex. transportation, logistics, ...). Existing studies of the VRP are almost all concerned with the minimization of the total distance only. The model studied in the DOLPHIN project introduces a second objective, whose purpose is to balance the length of the tours. This new criterion is expressed as the minimization of the difference between the length of the longest tour and the length of the shortest tour. As far as we know, this model is one of the pioneer work of the literature.

The second routing problem is a generalization of the covering tour problem (CTP). In the DOLPHIN project, this problem is solved as a bi-objective problem where a set of constraints are modeled as an objective. The two objectives are: i) minimization of the length of the tour; ii) minimization of the largest distance between a node to be covered and a visited node. As far as we know, this study is among the first works that tackle a classic mono-objective routing problem by relaxing constraints and building a more general MOP.

The third studied routing problem is the Ring Star Problem (RSP). This problem consists in locating a simple cycle through a subset of nodes of a graph while optimizing two kinds of costs. The first objective is to minimize a ring cost that is related to the length of the cycle. The second one is to minimize an assignment cost from non-visited nodes to visited ones. In spite of its natural bi-criteria formulation, this problem has always been studied in a single-objective form where either both objectives are combined or one objective is treated as a constraint.

Recently, within a cooperation with SOGEP, the logistic and delivery subsidiary company of REDCATS (PINAULT PRINTEMPS REDOUTE), a new routing problem is under study. Indeed, the COLIVAD project consists in solving a logistic and transportation problem that has been reduced to a vehicle routing problem with additional constraints. First we are designing a method to solve exactly a bi-objective version of the problem in order to evaluate the interest of modifying the current process of delivery. We are also working on the resolution of a single-objective version of this problem to design an operational tool dedicated to the SOGEP problem.

For all studied problems, standard benchmarks have been extended to the multi-objective case. The benchmarks and the obtained results (optimal Pareto front, best known Pareto front) are available on the Web pages associated to the project and from the MCDM (International Society on Multiple Criteria Decision Making) web site. This is an important issue to encourage comparison experiments in the research community.

4.2. Application to mobile telecommunication networks

With the extraordinary success of mobile telecommunication systems, service providers have been affording huge investments for network infrastructures. Mobile network design appears of outmost importance and then is a major issue in mobile telecommunication systems. The design of large cellular networks is a complex task with a great impact on the quality of service and the cost of the network. With the continuous and rapid growth of communication traffic, large scale planning becomes more and more difficult. Automatic or interactive optimization algorithms and tools would be very useful and helpful. Advances in this area will certainly lead to important improvements concerning the service quality and the deployment cost.

In this project, the solution of planification problems, in terms of modelization and resolution, are developed in a multi-criteria context associating financial criteria (cost of the network), technical criteria (coverage, availability), and marketing criteria (quality of service). Two complementary design problems are considered:

- Radio mobile network design: This work is realized in collaboration with France Telecom R&D. Engineering of radio mobile telecommunication networks involves two major problems: the design of the radio network, and the frequency assignment. The design consists in positioning base stations (BS) on potential sites, in order to fulfill some objectives and constraints. The frequency planning sets up frequencies used by BS with criteria of reusing. In this project, we address the first problem. Network design is a NP-hard combinatorial optimization problem. The BS problem deals with finding a set of sites for antennas from a set of pre-defined candidate sites, determining the type and the number of antennas, and setting up the configuration of different parameters of the antennas (tilt, azimuth, power, ...). A new formulation of the problem as a multi-objective constrained combinatorial optimization problem is considered. The model deals with specific objectives and constraints due to the engineering of cellular radio network. Reducing costs without sacrificing the quality of service are issues of concern. Most of the proposed models in the literature optimize a single objective (cover, cost, linear aggregation of objectives, etc.).

- Access network design: This work is realized in collaboration with Mobinets. The problem consists in minimizing the cost of the access network and maximizing its availability. Operators can only be competitive and economical if they have an optimized access network. Since the transmission costs are becoming high compared to the equipment costs, and the traffic demands are increasing with the introduction of new services, it is vital for operators to find cost-optimized transmission network solutions at higher bit rates. Many constraints dealing with technologies and service providers have to be satisfied. All deployed important technologies (ex. GSM, UMTS) will be considered.

4.3. Application to Bioinformatics

Bioinformatic research is a great challenge for our society and numerous research entities of different specialities (biology, medical or information technology) collaborating on specific thema.

4.3.1. Genomic and Post-Genomic studies

Previous studies of the DOLPHIN project mainly deal with genomic and postgenomic applications. These have been realized in collaboration with academic and industrial partners (IBL: Biology Institute of Lille; IPL: Pasteur Institute of Lille; IT-Omics firm).

First, genomic studies aim to analyze genetic factors which may explain multi-factorial diseases such as diabetes, obesity or cardiovascular diseases. The scientific goal was to formulate hypotheses describing associations that may have any influence on diseases under study.

Secondly, in the context of post-genomic, a very large amount of data are obtained thanks to advanced technologies and have to be analyzed. Hence, one of the goals of the project was to develop analysis methods in order to discover knowledge in data coming from biological experiments.

These two problems have been modeled as classical datamining tasks. First it as been modeled as an association-rule mining problem. As the combinatoric of such problems is very high and the quality criteria not unique, we proposed to model the association-rule mining problem as a multi-objective combinatorial optimization problem. An evolutionary approach has been adopted in order to cope with large scale problems. Then, in order to make more efficient such approaches, a complementary datamining task has been studied: the feature selection problem. This problem is of multi-objective nature and a multi-objective approach has been proposed.

4.3.2. Protein identification

Another application deals with Proteomics. Proteomics consists in the global analysis of proteins. In fact, proteomics is very important to understand the biological mechanisms in the living cells, but also how different factors can influence them. The main goal of the proteomic is to identify experimental proteins. In this domain, we collaborate with the team of C. Rollando (research Director at CNRS) head director of the proteomic platform of the genopole of Lille.

Our objective is to automatically discover proteins and new protein variants from experimental spectrum. The protein variants and new protein identification is a complex problem. In fact, it cannot be summarized as a simple scoring of an experimental protein against protein databases, it needs additional processes to explore the huge space of potential solutions. For the protein variant, there are many modifications: insertion, deletion or substitution of an amino acid and also post-traductional modifications on it. So it is not practically feasible to generate all the possibilities of combination of modifications for a given size of protein (exponential complexity). The new protein identification problem is close because we cannot generate all possible proteins (with also modifications) in order to find the experimental one. For both a method of optimization is necessary.

4.3.3. Docking and conformational sampling

In molecular modelling, conformational sampling and docking procedures allow to provide help for understanding the interaction mechanisms between (macro)molecules involved in physiological processes. The processes to be simulated are of a combinatorial complexity (molecule size, number of degrees of freedom) that represents an important challenge for the currently available computing power. Such challenge can be expressed by three major objectives: (1) the proposition of mathematical models of maximum simplicity that nevertheless provide a relevant description of molecular behavior, (2) the development of powerful distributed optimization algorithms (evolutionary algorithms, local search methods, hybrid algorithms) for sampling the molecular energy surface for stable, populated conformations, and (3) deploying those intrinsic distributed algorithms on computational Grids.

Within the framework of ANR DOCK and Decrypton projects, the focus is to propose with the collaboration of Institute of Biology at Lille (H. Dragos) multi-objective formulations of the conformational and docking problems. The goal is to take into account different criteria characteristics of the complex docking process. Furthermore, in order to deal with the multimodal nature of the problems it is important to define new hybrid mechanisms allowing to provide algorithms with both diversification and intensification properties. Finally, to deal with the exponential combinatory of these problems when large proteins are concerned parallel and grid computing is highly required. Using grid computing is not straightforward, so a "gridification" process is necessary. Such process allows to adapt the proposed algorithms to the characteristics of the grid. The gridification process must be exploited by the user in a transparent way. Therefore, coupling Paradiseo-Peo with a generic grid middleware such as Globus is important to provide robust and efficient algorithms to be exploited transparently.

5. Software

5.1. ParadisEO

Participants: Jean-Charles Boisson, Clive Canape, Jérémie Humeau, Laetitia Jourdan, Thomas Legrand, Arnaud Liefooghe, Nouredine Melab, El-Ghazali Talbi [correspondent], Alexandru Tantar.

ParadisEO (PARallel and DIStributed Evolving Objects) is a C++ white-box object-oriented framework dedicated to the flexible design of metaheuristics. See web pages http://paradiseo.gforge.inria.fr/. Based on EO, a template-based ANSI-C++ compliant evolutionary computation library, it is composed of four modules:

- Paradiseo-EO provides tools for the development of population-based metaheuristic (Genetic algorithm, Genetic programming, Particle Swarm Optimization (PSO)...)
- Paradiseo-MO provides tools for the development of single solution-based metaheuristics (Hill-Climbing, Tabu Search, Simulated annealing, Iterative Local Search (ILS), Incremental evaluation, partial neighborhood...)
- Paradiseo-MOEO provides tools for the design of Multi-objective metaheuristics (MO fitness assignment shemes, MO diversity assignment shemes, Elitism, Performance metrics, Easy-to-use standard evolutionary algorithms...)
- Paradiseo-PEO provides tools for the design of parallel and distributed metaheuristics (Parallel evaluation, Parallel evaluation function, Island model)

Furthermore, ParadisEO also introduces tools for the design of distributed, hybrid and cooperative models:

- High level hybrid metaheuristics: coevolutionary and relay model
- Low level hybrid metaheuristics: coevolutionary and relay model

The ParadisEO framework has been especially designed to best suit to the following objectives:

- Maximum design and code reuse: ParadisEO is based on a clear conceptual separation of the solution methods from the problems they are intended to solve. This separation confers to the user a maximum code and design reuse.
- Flexibility and adaptability: the fine-grained nature of the classes provided by the framework allow a higher flexibility compared to other frameworks.
- Utility: ParadisEO allow the user to cover a broad range of metaheuristics, problems, parallel distributed models, hybridization mechanisms, etc.
- Transparent and easy access to performance and robustness: As the optimization applications are often time-consuming the performance issue is crucial. Parallelism and distribution are two important ways to achieve high performance execution. ParadisEO is one of the rare frameworks that provide the most common parallel and distributed models. These models can be exploited in a transparent way, one has just to instantiate their associated provided classes.
- Portability: The implemented models are portable on distributed-memory machines as well as on shared-memory multiprocessors, as they use standard libraries such as MPI and PThreads.

Recently, many efforts have been made for ParadisEO to become a cross-platform easy-to-use software. All the documentation, source code, articles and resources have been gathered to build the "ParadisEO GForge project". The INRIA GForge (http://gforge.inria.fr/) provides a set of web-interfaced utilities that allow an advanced project management. The ParadisEO project is now composed of a website, several forums and mailing-lists, a subversion repository, many announce and task publishers... Moreover, as the components (EO, MO, MOEO, PEO) were initially downloaded and installed separately, a lot of problems came-up because of dependencies and it could be difficult for a non experimented user to compile and run the whole library. Therefore, a single archive, containing the four modules (including the sources, the framework documentation, new tutorials) has been built and an installation script has been proposed to the users. The install process is now performed automatically. Another important change has also been operated to allow the compilation on any platform having a standard C++ compiler. The build process is now managed by CMake and the classical autotools (Autoconf, Automake) have been forgotten. Thanks to this migration, ParadisEO can now be used under several environments (Windows, Unix-like systems, Mac).

5.1.1. ParadisEO-EO and Particle Swarm Optimization integration

ParadisEO-EO is a template-based, ANSI-C++ compliant evolutionary computation library. It contains classes for almost any kind of evolutionary computation. EO was started by the Geneura Team at the University of Granada but the development team has been many times reinforced. Recently, we joined the developer staff to start a new contribution with ParadisEO. The goal was to create new classes and components increasing the compatibility between the framework (ParadisEO-EO) and its extensions (ParadisEO-MO, ParadisEO-MOEO and ParadisEO-PEO). Several technical features have also been improved from both sides. Furthermore, a set of classes allowing the implementation of any Particle Swarm Optimization (PSO) algorithm has been proposed to the EO community. As it was successfully integrated and tested, an extension of the sequential PSO is actually in progress and will be finalized before the end of the year. Thus, ParadisEO will propose a full support for the PSO: sequential models (including many topologies, binary flight ...), parallel and distributed models (evaluation function, island scheme...).

5.1.2. Paradiseo-MOEO

Paradiseo-MOEO (Multi-Objective Evolving Objects) is the module dedicated to multi-objective optimization. It embeds some features and techniques for scalar, dominance- and indicator-based resolution. A genuine conceptual effort has been done to provide a set of classes allowing to ease and speed up the development of efficient programs in an incremental way while having a minimum programming effort. ParadisEO-MOEO provides a broad range of fine-grained components including fitness assignment strategies (the achievement functions, dominance rank, dominance count, dominance depth, indicator-based schemes and more), the most common diversity preservation mechanisms (sharing, nearest neighbour, crowding), some elitist-related features as well as statistical tools. Furthermore, some state-of-the-art evolutionary algorithms (such as NSGA-II or IBEA) have been implemented into the library in a user-friendly way, only by using the fine-grained components of ParadisEO. This year, a new set of classes and templates have been integrated in a modular way into the framework in order to provide a wider range of features. For instance, the Strength Pareto Evolutionary Algorithm 2 (SPEA2) as well as the epsilon and the hypervolume indicators have been incorporated in a modular way. Likewise, an easy-to-use SPEA2 has been added to the library.

5.1.3. Paradiseo-MO

ParadisEO-MO (Moving Object) is dedicated to the design of solution-based metaheuristics. It is based on C++ template and is problem independent. The first version of ParadisEO-MO provided three algorithm schemes: the hill climbing, tabu search and simulated annealing schemes. It provided also an application example on the symmetric traveling salesman problem (TSP). During this year, this platform has been greatly improved. On the one hand a new algorithm scheme has been added: the iterated local search (ILS); and a lot of "ready-to-use" box have been provided: stopping criteria, cooling scheduler schemes... On the other hand, a complete set of documentation has been added: a source code documentation, two combinatorial concept presentations, a report that full describes the platform and four lessons, respectively for each algorithm scheme, solving the symmetric TSP problem.

5.1.4. Paradiseo-G

ParadisEO has been coupled with Globus GT4 to tackle optimization problems on Grids. The coupling of ParadisEO with Globus consisted in two major steps: design and implementation, and deployment on the Grid, in particular Grid'5000. The first step consisted in the gridification of the parallel and hybrid models provided in ParadisEO meaning their adaptation to the properties of grids (large scale, heterogeneous and dynamic nature of the resources and multi-administrative domain). The MPICH-G2 communication library has been considered. The second step consisted in building a system image for Globus 4 including MPICH-G2. This image allows to build a virtual Globus grid able to deploy and execute the parallel hybrid meta-heuristics provided by ParadisE0. This year, a new archive containing ParadisEO has been built and it can be used either under classical environments either with Globus. From the user point of view, ParadisEO consists now in a single package that can be deployed to best suit to the environment.

5.1.5. New technical features

The solution-based metaheuristic part of ParadisEO (ParadisEO-MO) has been extended this year in order to include a new advanced algorithm: the *variable neighborhood search* (VNS). With the VNS scheme, the other algorithms included in ParadisEO-MO but also the mutation operators of ParadisEO-EO can be used as different neighborhoods. The current version of the VNS has been already applied on the *docking* problem and gives promising results. New tutorials are available, including a lesson on the hybridizing between ParadisEO-EO and ParadisEO-MO in order to design cooperative metaheuristics.

5.2. Docking@Grid

Participants: Jean-Charles Boisson, Laetitia Jourdan, Arnaud Liefooghe, Nouredine Melab, El-Ghazali Talbi [correspondent], Alexandru Tantar.

Docking@GRID is a software dedicated to the flexible conformational sampling and docking on the computational grid. The goal of the software is to help users to perform such processes in a friendly way. In other words, the software provides a web portail for remote job submission, importation/preparation of proteins, access to protein data bank, visualization, efficient sampling and docking. The project could be later integrated into the larger platform of chemioinformatics tools under construction around the site of the ”Chimiothèque Nationale”-project of the CNRS (Prof. Hibert, Strasbourg). This platform, designed as a portail for the display of the collections of molecules synthesized in French academic labs might offer predicted affinities of these compounds with respect to various biologically interesting targets, in order to facilitate compound selection.

The current version considers only sampling and visualization of conformations. A registration step requiring a reduced amount of information is demanded in order to access the provided resources. The software offers a hierarchical perspective, allowing to group different tasks into projects. A new project can be created by accessing the Ligands/ActiveSite section - following this initial phase, the project is displayed in a hierarchical manner. After creating the project, the user has the possibility of creating a new molecule file by employing the Msketch application (Chemaxon), which is provided in the form of a Java applet. Following this process, a conformational sampling step can be applied on the specified file. The sampling process relies on a hybrid genetic hierarchical algorithm executed in a distributed environment and making use of different parallelization strategies. The underlying framework is ParadisEO-G which is a Globus based version of the ParadisEO framework. The parallelization of the algorithm is transparently achieved by making use of the ParadisEO models - asynchronous island model, parallel evaluation of the population and parallel synchronous multi-start model. As middle-ware an MPICH-based distribution of MPI is used, the execution being performed on a dedicated set of machines.The results are displayed at the end of the sampling process, a notification mail being sent in case the processing step takes longer than 5 seconds. The obtained conformations may be visualized by using the MView tool (Chemaxon). Each conformation can be further subjected to rigid transformations (translations, rotations), animations can be constructed, etc.

This year, from a first new model, we have designed and tested seven other models for the flexible docking problem. All these models have been validated on instances of the CCDC-Astex dataset thanks a multi-objective genetic algorithme based on IBEA (Indicator Based Evolutionnary Algorithm) proved to be better than NSGA-II (Non dominated Sorting Genetic Algorithm). We use twelve different configurations of the GA for each model. The configurations using local searches as mutation operator and making a full flexible docking give the best results. According to the result gained, the surface and robustness objectives improve the docking efficiency.

All this work has been funded by the ANR Dock project and the "PPF Bio-Informatique" of the USTL.

6. New Results

6.1. Hybrid Metaheuristics for Multi-objective Optimization

Participants: Arnaud Liefooghe, Laetitia Jourdan, El-Ghazali Talbi.

Designing metaheuristics is generally a matter of intensification and diversification. This is even more pronounced for multi-objective optimization problems where the goal is to find a well-converged and well-diversified Pareto set approximation. Instead of trying to improve a method in term of intensification or another one in term of diversification, a common approach is to make them cooperate in order to benefit of their respective behaviors. Hybridizing metaheuristics is known to be efficient to solve different kinds of optimization problems. we proposed two cooperative models for multi-objective optimization combining an evolutionary algorithm called SEEA (Simple Elitist Evolutionary Algorithm)and a population-based local search called IBMOLS (Indicator-Based Multi-Objective Local Search)SEEA and IBMOLS are quite different to each other and do not explore the search space in the same way. Furthermore, both methods maintain a secondary population (the archive) in parallel of the main one to store non-dominated solutions. This archive is not only used as an external storage, but also takes part in the evolution engine. Thus, each method can manage its own population and can use the archive as a single shared memory. The general idea of our Hybrid Metaheuristic (HM) is to run SEEA and to lunch IBMOLS regularly by using a subset of archive items as an initial population. Therefore, two versions can be imagined: a *periodic version*, in which IBMOLS is launched at each step of the HM, and an *adaptive version*, in which IBMOLS is launched at a specific step only if a condition is verified, with regards to the search scenario. The resulting algorithms are general-purpose search methods and have been suited for the particular case of the bi-objective ring star problem.

we introduced another HM for the same problem. Indeed, an interesting property of the bi-objective ring star problem is that a lot of Traveling Salesman Problem (TSP) generally need to be solved. Moreover, a large number of approaches to solve the TSP has been proposed and this problem has been widely investigated in the literature. This new HM successfully integrates a problem-specific heuristic, initially proposed for the TSPinto a multi-objective evolutionary algorithm.

6.2. Using a Top-Tree structure to solve constrained spanning tree problems

Participants: Jérôme Brongniart, Clarisse Dhaenens, El-Ghazali Talbi.

Even if efficient methods exist for the classical spanning tree problem, constrained spanning tree problems are NP-hard problems that have to be considered with attention and exact and heuristic methods can be developed.

Knowing that most of the existing meta-heuristics for the spanning tree based optimization problems can be described in terms of edge swap, where an edge of the current solution is permuted with a non-tree edge, this edge swap procedure is worth to be deeply studied. It appears that in a constrained context, the computational cost of updating these information can be prohibitive, due to the non-local nature of the additional requirements tackled in these problems,

Hence, in order to reduce this computational time, we have adapted a dynamic algorithm - based on the Top-Tree structure - firstly designed for updating tree information, in order to take into account edge swap. Thanks to the genericity of this new dynamic approach, new exact algorithms and meta-heuristics will be able to be developed to solve a large class of constrained problems.

6.3. A new P2P approach for branch-and-bound on grids

Participants: Malika Mehdi, Nouredine Melab, El-Ghazali Talbi.

The Branch and Bound (B&B) algorithm is one of the most used methods to solve in an exact way combinatorial optimisation problems. In a previous article, we proposed a new approach of the parallel B&B algorithm for distributed systems using the farmer-worker paradigm. However, the new farmer-worker approach has a disadvantage: some nodes of the B&B tree can be explored by several B&B processes. To prevent this redundant work and speed up, we propose a new P2P approach inspired from the strategies of existing P2P systems like Napster and JXTA. Validation is performed by experimenting the two approaches on mono-objective flow-shop problem benchmarks using 500 processors belonging to the French national grid, Grid5000. The obtained results prove the efficiency of the proposed P2P approach. Indeed, the execution time obtained with the P2P version, even if more communicative, is better than the farmer-workers one.

6.4. A constraint programming method for a cutting problem, based on a new graph-theoretical model

Participant: François Clautiaux.

We considered the problem of determining if a given set of rectangular items can be cut in a large rectangle, using a certain type of cuts only, namely *guillotine cuts*. This problem is a crucial issue in many real-world applications.

We proposed a brand new model to take into account the guillotine-cut constraint. We introduced a new class of arc-colored and oriented graphs, named guillotine graphs, which model guillotine patterns. Then we showed that an uncolored and non-oriented multigraph is sufficient to obtain any guillotine pattern. We proposed linear algorithms for recognizing these graphs, and computing the corresponding patterns.

We have embedded our model into a constraint-programming scheme. The obtained results improve the previous best results of the literature by a wide range.

6.5. Mixing graph-decomposition, dynamic-programming, heuristics and linear-programming duality for packing problems

Participants: Ali Khanafer, François Clautiaux, El-Ghazali Talbi.

We considered the one- and two-dimensional variants of the bin packing problem with conflicts. Given a set of items, an unlimited number of bins and a conflict graph, the goal is to find a conflict-free packing of the items minimizing the number of bins used. The concepts of *dual-feasible functions* (DFF) and *data-dependent dual-feasible functions* (DDFF) have been used in the literature to improve the resolution of several cutting/packing problems.

We have proposed a general framework for deriving new DDFF as well as a new concept of *generalized data-dependent dual-feasible functions* (GDDFF), a conflict generalization of DDFF. The GDDFF takes into account the structure of the conflict graph using the techniques of graph triangulation and tree decomposition.

Finally, we present new lower bounds that take good use of DFF and GDDFF. Computational experiments show that our bounds are always faster than the previous best bound and they lead to improved results for several instances.

6.6. SSO model for the "de novo protein sequencing" problem

Participants: Jean-Charles Boisson, Laetitia Jourdan, El-Ghazali Talbi.

During this year, the SSO model (Sequence, Shape, Order) dedicated to the "de novo protein sequencing" problem has been fully implemented and tested. Each step consists on a metaheuristic collaborating sequentially with the next one. For the "Sequence" step, a greedy algorithm has been designed. It allows, from MS/MS spectra, to gain a model from the sequence of each peptide. For the "Shape" step, the initial population of the genetic algorithm is initialized thanks to the peptide models from the "Sequence" step. During the evolution, each individual is evaluated according to an experimental MS spectrum. For the "Order" step, several local searches have been compared and the chosen one is an iterated local search. Consequently, each individual of the final population of the GA from the "Shape" step is intensified thanks to this local search according to an other MS spectrum.

The current metaheuristic collaboration has been tested on experimental data and each time large sequences of the right experimental protein have been found. These results have been obtained by comparing result sequences with the protein to find thanks to the blast program.

All this work has been funded by the "PPF Bio-Informatique" of the USTL.

6.7. Study of local search algorithms and intensification for the conformational sampling problem

Participants: Alexandru Tantar, Nouredine Melab, El-Ghazali Talbi.

An assessment of local search algorithms and intensification, diversification operators has been performed for the conformational sampling problem. A parallel implementation of OCBA (Optimal Computing Budget Allocation), a powerful statistical selection procedure, has been developed in order to sustain the comparison of the different algorithms and operators. A survey on selection procedure has been previously presented by Branke et al.

The Nelder-Mead Simplex local search method has been first addressed due to simplicity considerations, along with the Solis and Wets algorithm, which introduces adaptive search mechanisms. Additionally, gradient based methods were included, namely, the Conjugate Gradient, the Adaptive Simulated Annealing (ASA - adaptive exploration technique, gradient-based parameters adjustment and the L-BFGS (second order method employing Hessian approximations).

Variance annealing schemes have been used for the mutation operators, inducing a dynamic behavior where variance is scaled as to adapt the search with the exploration advancement. Further, a Pearson-system based mutation operator has been introduced, setting the basis of a powerful and flexible operator.

The study has been conducted at the different phases encountered during an evolutionary approach exploration, having as input random solutions, in a first phase, second, optimized solutions, and last, near-global solutions. Thus, the behavior of the different addressed local search algorithms and operators has been analyzed at multiple stages, aiming in identifying the components to be employed on a per exploration phase basis. Both conformational energy and RMSD (Root Mean Square Deviation) criteria were employed for comparison.

As a first outcome, the study revealed different patterns in the ranking of the components. A constant ranking including the ASA, the Solis and Wets and the L-BFGS algorithms has been obtained. ASA has been ranked first on random and optimized solutions while a shift in rank has been obtained for the near-global solutions where L-BFGS scored best. In this scenario the Solis and Wets algorithm, while being ranked second, represents an intermediate solution, with a constant behavior on different quality solutions. No correlation between the energy and RMSD rankings has been observed.

Similarly, for the diversification operators the Pearson type III mutation ranked first in most of the cases. Due to its flexibility the operator has been later adapted in order to be used in self-adaptive exploration algorithms. The back-bone of a self-adaptive parallel exploration algorithm has been thus developed, initial results showing significant improvement when using the adaptive mechanisms.

Complementary to the afore described study, generic parallel components were introduced in ParadisEO. As a first outcome, a hybrid package including AutoDock and ParadisEO has been constructed, introducing several parallel exploration strategy into the AutoDock framework.

6.8. Landscape analysis in multi-objective optimization and its role in adaptive and interactive methods

Participants: Emilia Tantar, Clarisse Dhaenens, El-Ghazali Talbi.

The main challenge of the last decade in Evolutionary Multi-objective Optimization (EMO) was to supply well-distributed and well-converged Pareto-approximate sets and the goal was nearly achieved since a large spectrum of efficient results are reported for multi-objective optimization problems both for theoretical and practical problems. The new context allowed to broader the research interests for more in depth approaches, where performance guarantee factors are added to the search process, as convergence studies and interactive tools are provided to the user in order to help the decision maker to explore the landscape of efficient solutions. Another important aspect tackled by our studies concerns the structure of the provided approximation set.

In order to provide a higher level of accuracy, for multi-objective optimization methods, landscape analysis studies were entailed on the structure of the ϵ-efficient set. For a specific combinatorial problem ($\{0,1\}$-knapsack problem) the non-connectedness between the ϵ-efficient set and the Pareto set was outlined in our studies The role of these in depth studies is to enlighten the connection between the complexity of MOCO problems and the associated (approximate) Pareto set and to establish the types of approximation sets needed for these new types of landscape characteristics. In this direction, a new ϵ-adaptive approach is proposed.

The novelty of the proposed approach consists - besides the approximation of the entire set of $-\epsilon$ efficient solutions - in the proposed mechanism used for adapting the values of ϵ during the search as to ensure convergence towards the desired level of accuracy, in the limit and in a probabilistic sense. The adaptation of ϵ during the search was chosen as to speed up the search process by reducing the number of iterations needed in order to achieve a desired ϵ accuracy level.

Furthermore, following the path of integrating the decision maker in the optimization process proposed in [42], a new interactive procedure is proposed. The method is intended to help the decision maker to explore the landscape of proposed efficient solutions, and thus to ease his or her task to find the "right" solution according to the current situation. The decision maker has at its disposal two perspectives, the decision and variables spaces in order to fully entail the non-connectedness aspects.

6.9. Material design for the shielding of electric devices

Participant: Laetitia Jourdan.

Common work with Ecole des Mines de Douai, CINVESTAV-IPN Mexico.

In the design of materials for the shielding of electric devices there is a recent trend to use multi-layer compounds due to some restrictions in the making process of the materials but also since they are supposed to have a higher potential to offer better characteristics than the related mono-objective materials. In this work we investigate the possible impact of the number of layers in a compound critically. It will turn out that at least for the general objectives we study here and for conducting polymer composites multi-layered materials are suitable to only a limited extent. To be more precise, when "just" aiming for a high shielding efficiency the task can be accomplished with merely one layer. If in addition the cost of material comes into play, however, a second layer may be helpful, but further layers do not seem to have a significant impact on the performance of a material.

6.10. Dynamic vehicle routing problem

Participants: Laetitia Jourdan, El-Ghazali Talbi, Mostepha-Redouane Khouadjia.

We study the dynamic Vehicle Routing Problem which is a dynamic and real-time version of the conventional Vehicle Routing Problem (VRP). In the classical VRP, the planning of tours is accomplished before the working day, whereas in the dynamic version of this problem the planning of tours is made in a dynamic or real-time way. The purpose is to try to insert the new customer orders in the already planned tours, when the vehicles are already on routes, and in minimizing the tours cost. The dynamic property of this problem makes that it cannot be effectively resolved by classic insertion heuristics. Furthermore, proposed metaheuristics in literature do not exploit enough the information about the problem. This information change during the time, and must be treated as fast as possible before a change happens in the global optimum.

Actually, we lean on the self-organization theory and the concept of adaptive memory to deal with the dynamism of a problem. The self-organizing theory can inform us about the structure to be used to design flexible metaheuristics, and able to follow the evolution of the global optimum during all the time of optimization. The adaptive programming informs us about the mechanisms to be used for updating the information gathered by the algorithm during its search. To put together these two points, we test the Adaptive Particle Swarm Optimization metaheuristic (APSO) for the resolution of the DVRP.

7. Contracts and Grants with Industry

7.1. SOGEP - REDCATS

(2006-2008): The cooperation with SOGEP, the logistic and delivery subsidiary company of REDCATS (PINAULT PRINTEMPS REDOUTE) consists in solving a logistic and transportation problem. The objective here is the design and implementation of a decision aid framework for solving complex vehicle routing problems including different constraints.

7.2. CEA

(2006-2009): The cooperation with the CEA intervenes in the ANR project ”DOCK” (Docking on Grids).

8. Other Grants and Activities

8.1. Regional Actions

- COLIVAD project (Pilotage Optimal des processus de Livraison en Vente à Distance (2006-2008): This project is part of "Pole de compétitivité" PICOM (*Industries du commerce*). It deals with solving a logistic and transportation problem.

8.2. National actions

- Decrypton project, AFM-CNRS-IBM: ”Conformational sampling and docking on Grids and application to neuromuscular disease” (2006-2008): collaboration with INSERM and IBL (Lille Institute of Biology). he objective of this project is the development and assesment of our Docking@GRID software platform for a physiopathological problem related to myotonic dystrophy.
- ANR DOCK (Docking on Grids) (2006-2009): collaboration with IBL (Institut de Biologie de Lille) and CEA (Grenoble). The challenge in this project is a new model and grid-enabled optimization algorithm for the structure prediction and docking of molecules.
- ANR CHOC (Challenges on Combinatorial Optimization on Grids) (2006-2009): collaboration with Prism (Univ. of Versailles), MOAIS (INRIA Rhones-Alpes), GILCO (Grenoble). he project deals with the design and implementation of grid-enable software frameworks for exact and metaheuristic optimization algorithms.
- PPF (Bioinformatics) (2006-2009): This national program within the university of Lille (USTL) deals with solving bioinformatics and computational biology problems using combinatorial optimization techniques.
- CONS-PACK project (study of constrained packing problems) 2007-2009: collaboration with Université de Technologie de Compiègne and Ecole des Mines de Nantes, supported by GDR RO (GDR on Operational Research). his project explores the multi-objective modeling of cutting and packing problems.

8.3. International actions

- INRIA project 3+3 Méditerrannée PERFORM (2006-2009) involving the University of Malaga (Spain), University of Constantine (Algeria), and University of Tunis (Tunisia). This project deals with multi-objective optimization.
- University of Constantine (2004-2008): CMEP program with the University of Constantine (Algeria) on "Metaheuristics for optimization of hard problems".
- NEGST (NExt Grid Systems and Techniques - 2006-2009): International Collaboration and Promotion on interoperability and advanced technologies of Grid. program between CNRS (France) and Japan on optimization on Grids.

8.4. Visits and researcher invitations

The project had visitors during the year 2008:

- E. Alba (Malaga, Spain)

9. Dissemination

9.1. Services to the scientific community

9.1.1. Research Management

- Co-fondator and chair of the group META (Metaheuristics: Theory and Applications, http://www.lifl.fr/~talbi/META). This group is associated with the ROADEF (French Operations Research Society), and the CNRS research groups GDR ALP and MACS.
- Chair of the group PM2O (Multi-objective Mathematical Programming, http://www.lifl.fr/PM2O). This group is associated with the ROADEF (French Operations Research Society), and the CNRS research group GDR RO (Operations Research).

- Secretary of ROADEF (the French Operational Research Society - http://www.roadef.org).
- Direction of the CIB (Bioinformatics Center) of the Genopole of Lille.
- Scientific Committee of the Genopole of Lille.
- Member of the Steering Committee of INRIA ALADDIN Project.
- Steering Committee of the INRIA ADT Aladdin-G5K.
- Co-leader of an ALADDIN working group on scalability of Grid-enabled algorithms and applications.
- Member of the Scientific Committee of High-Performance Computing of Université de Lille1.

9.1.2. Participation to Working Groups

- EURO-PAREO (European working group on Parallel Processing in Operations Research).
- EURO-EU/ME (European working group on Metaheuristics).
- EURO-ESICUP (European Working Group on Cutting and Packing).
- ECCO (European Chapter on Combinatorial Optimization).
- ERCIM (European Research Consortium for Informatics and Mathematics) working group on Soft Computing.
- JET national group on evolutionary computation.
- PM2O national group on Multi-objective Mathematical Programming.
- META national group on Metaheuristics: Theory and Applications.
- KSO national group on cutting and packing.

9.1.3. Organizations of sessions, workshops and conferences

- Co-organization of JOBIM'2008, Journées ouvertes biologie informatique, mathématiques
- Organization of the International Conference on Metaheuristics and Nature Inspired Computing (META 2008)
- Organization of sessions in ROADEF'2008, 9th conference of the French Operational Research Society, Clermont-Ferrand, Feb 2008.
- Organization of "2èmes Journées Aladdin-Grid5000" in Lille, Nov. 5-6 2008

9.1.4. Editorial boards

- Editorial board of the International Journal of Data Mining, Modelling and Management

9.1.5. Reviews

- Review of journal papers:
  - IEEE Transactions on Systems Man and Cybernetics
  - IEEE transactions on Computational biology and Bioinformatics
  - IEEE Transactions on Parallel and Distributed Systems
  - IEEE Transactions on Evolutionary Computation
  - Parallel Computing
  - Calculateurs Parallèles
  - Journal of Supercomputing
  - Parallel and Distributed Computing Practices
  - Journal of Parallel and Distributed Computing

  - Genetic Programming and Evolvable Machines
  - Journal of Heuristics
  - European Journal of Operational Research
  - Annals of Operations Research
  - 4'OR
  - International Journal of Production Economics
  - Computers and Operation Research
  - Discrete Applied Mathematics
  - Journal of Computational Optimization and Applications
  - Information Processing Letters
  - Extraction de connaissances et apprentissage
  - European Physical Journal B
  - Journal of Mathematical Modelling and Algorithms
  - Bioinformatics
  - Jouranl of Artificial Evolution and Applications
  - Knowledge based systems
  - ...
- Review of a research project:
  - Evaluation of a four year project for the Israel Scientific Foundation

9.1.6. Program Committees

- International Conferences on Evolutionary Computation:
  - GECCO'08
  - NISCO'07
  - EMO'09
- International conferences on Operations Research and Production Management
  - CPAIOR08 - workshop on bin-packing and placement problems, Integration of AI and OR Techniques in Constraint Programming for Combinatorial Optimization Problems, 5th International Conference, CPAIOR 2008, Paris, France, May 2008
  - MOSIM'08
- Other conferences
  - ISPDC'2008
  - HPC&S'2008
  - NIDISC'2008 (in conj. with IPDPS'2008).

9.1.7. Phd and HdR committees

Pr Dhaenens was referee of the following thesis:

- Rémy Chevrier, "Optimisation de transport à la demande dans des territoires polarisés", thèse soutenue le 18 novembre 2008 à l'Université d'Avignon et des Pays de Vaucluse.

Jury : Philippe Canalda, Clarisse Dhaenens, Michel Gendreau (Rapporteur), Loic Grasland, Didier Josselin, Robert Laurini (Raporteur), Isabelle Thomas (Raporteur)

- Louis-Philippe Kronek, "Analyse combinatoire de données appliquées à la recherche médicale", thèse soutenue le 12 décembre 2008 à l'Institut Polytechnique de Grenoble.

  Jury : Nadia Brauner, Vand Dat Cung, Clarisse Dhaenens (rapporteur), Pierre Lemaire, Francis Sourd (rapporteur).
- V. Derrien, "Utilisation de méthodes heuristiques pour la résolution de problèmes combinatoires en bioinformatique", thèse soutenue en Mars 2008 à l'Université d'Angers.

  Jury: R. Andonov (rapporteur), C. Dhaenens (rapporteur), J-K. Hao, B. Levrat, J. Nicolas, J-M. Richer.

9.2. Teaching

- Postgraduate (IEEA, USTL): "Optimization methods" (L. Jourdan).
- Postgraduate (IEEA, USTL): "GRID computing", (N. Melab, B. Derbel).
- Undergraduate (IEEA, USTL): "Distributed Systems" (N. Melab, B. Derbel).
- Undergraduate (IEEA, USTL): "Operations Research" (N. Melab).
- Undergraduate (Polytech'Lille): "Operations Research" (C. Dhaenens).
- Undergraduate (Polytech'Lille): "Graphs and combinatorics" (C. Dhaenens).
- Undergraduate (Polytech'Lille): "Data mining" (L. Jourdan, C. Dhaenens).
- Undergraduate (Polytech'Lille): "Advanced Optimization" (L. Jourdan).
- Undergraduate (Polytech'Lille): "Production Management" (C. Dhaenens).
- Undergraduate (IUT, USTL): "Graphs and Modeling" (F. Clautiaux).

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Major publications by the team in recent years

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[2] N. JOZEFOWIEZ, F. SEMET, E.-G. TALBI. *Target Aiming Pareto Search and its application to the vehicle routing problem with route balancing*, in "Journal of Heuristics", vol. 13, 2007, p. 455-469.

[3] J. LEMESRE, C. DHAENENS, E.-G. TALBI. *An exact parallel method for a bi-objective permutation flowshop problem*, in "European Journal of Operational Research", vol. 177, n^o 3, 2007, p. 1641-1655.

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[5] M. MEZMAZ, N. MELAB, E.-G. TALBI. *An efficient load balancing strategy for grid-based branch and bound algorithm*, in "Parallel Computing", vol. 33, n^o 4-5, 2007, p. 302–313.

[6] J.-M. PIERSON, J. GOSSA, P. WEHRLE, Y. CARDENAS, S. CAHON, M. E. SAMAD, L. BRUNIE, C. DHAENENS, A. HAMEURLAIN, N. MELAB, M. MIQUEL, F. MORVAN, E.-G. TALBI, A. TCHOUNIKINE. *GGM: Efficient Navigation and Mining in Distributed Genomedical Data*, in "IEEE Transactions on Nanobioscience", vol. 6, n^o 2, 2007, p. 110-116.

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[10] L. VERMEULEN-JOURDAN, C. DHAENENS, E.-G. TALBI. *Evolutionary Feature Selection for Bioinformatics*, in "Computational Intelligence in Bioinformatics", G. FOGEL, Y. PING, D. CORNE (editors), To appear Dec. 2007, IEEE CS/Wiley, 2007, p. 117–139.

Year Publications

Doctoral Dissertations and Habilitation Theses

[11] J.-C. BOISSON. *Modélisation et résolution par métaheuristiques coopératives : de l'atome à la séquence protéique*, Ph. D. Thesis, Université des Sciences et Technologie de Lille, 2008.

Articles in International Peer-Reviewed Journal

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