Design of Military Applications with EAs
(Extended Abstract)

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1 Introduction

The Air Force Institute of Technology applies evolutionary computational methods to a variety of design problems. Examples presented include wireantenna geometry Design, protein structure prediction, and laser system design. Each section includes a limited discussion on problem domain background and evolutionary algorithm application. Detailed papers exist on these applications if definitive insight is desired.

2 Wire-Antenna Geometry Design

Problem dimensionality and function complexity in determining antenna electromagnetic properties make standard deterministic methods inadequate for the task. Current development practices use simple wire structures for inductive processes followed by mathematical calculations in determining wire current distributions. Once current distributions are calculated, the electromagnetic properties are rendered. This process is time consuming and unreasonably complex - especially when testing a multitude of antenna shapes. Fortunately, computers have made this process easier. Programs like the Numerical Electromagnetic Code (NEC) ver 4.1, have dramatically increased the ability of designers to quickly test different proposals of wireantenna designs to determine their effectiveness.

The analytical complexity of finding a good antenna design induces a large search space making it so approaches, be they deterministic or stochastic, are incapable of finding optimal solutions. Classical antenna design approaches require starting positions that are close to the global optimum; otherwise, they tend to get stuck in local minimums. This situation drives the need for using a stochastic algorithm, an evolutionary algorithm. While various forms of EAs are made for dealing with antenna optimizations, the most common implementation technique is with the use of genetic algorithms. Antenna configuration properties are examined with regard to trade-offs for specific application requirements and intended purpose. This translates to multiple objectives that must be examined in order to create the best antenna possible for each situation. This effort uses a single aggregate objective as well as examining two different multiobjective genetic algorithm approaches.

Remote Intrusion Monitoring System (RIMS) is a practical military example of where antenna design is critical to mission success. The RIMS is based on the concept of a remote sensor being dropped into a location that requires monitoring. A distant receiving system records sensor disposition to detecting if changes around that sensor occur. In order for RIMS to work the remote antennas must be robust enough to be able to work without user interaction. Because of the nature of these systems it is imperative that they be as inconspicuous as possible. At the same time, without the required electromagnetic performance to transmit to the repeaters, the antennas are ineffective. One has to weigh the decision of how high a frequency is needed so that it is powerful enough to penetrate its cover, yet not so large as to be able to be seen. Other criterion that must be weighed for the RIMS problem include omnidirectional azimuth for widespread transmission, robust components for zero maintenance, and low level voltage source. Each of these tradeoffs represent a different objective that can be examined by the researcher individually, or in a multiobjective formulation. The sponsors of this effort include AF operational commands.

Many antenna fitness evaluation functions use a weightedsum approach to combine the multiple objectives of power gain, symmetry, resistance, and reactance as well as possible penalty functions related to constraints into a single scalar fitness value. The objectives themselves are computed using an electromagnetic code such as the Numerical Electromagnetics Code (NEC) ver 4.1, then appropriately combined via a userspecified EANEC interface and returned as the fitness value. Because the GEA itself may not make distinctions between feasible and infeasible designs (constraints) prior to requesting a fitness evaluation, the interface is capable of detecting instances when NEC determines the geometry is infeasible.

One should also consider the general fitness landscape being searched. An optimal antenna fitness value does not necessarily mean the associated geometry is desirable. What is desired is a geometry fitness to be located within a fitness plateau and not to be sensitive to small genotype perturbations. Additionally, one must analyze any optimal geometry as to its physical implications, ensuring its feasibility in the “realworld.” Direct comparison of aggregate and a posteriori Pareto implementations are difficult due to the fact that one produces a single answer while the other produces a vector of solutions. If the entire Pareto Front is enumerated, on it the aggregate result can be found. However, this actually happening is improbable due to the size of the search space and the large Pareto Front that would exist due to the four objectives in the antenna design problem.

Implementation of Pareto Operators on top of existing realvalued GA systems, such as GENOCOP III, is an effective way of finding good antenna configurations quickly. With the Pareto modifications we give the decision maker the ability of choosing from a vector of equally nondominated solutions for the antenna’s desired attributes. This vector may or may not include the most optimal solution that the decision maker (DM) desires due to searching over the entire landscape. If the DMs know exactly how they want the objectives to compare in terms of overall quality, they can specify that using the a priori techniques. This motivates the genetic algorithm to search specifically in that area of the problem landscape.

The Pareto GENOCOP-III finds solutions across the Pareto Front, allowing the DM to choose what trade-off of objective values would be best for the system. Also illustrated is the fact that this approach can match the results of an aggregate approach as well for simpler problems. When dealing with complex problems, like the 13 wire implementation, a directed search, such as an aggregate approach, is beneficial in reducing computation time when the weights are known.

3 Protein Structure Prediction (PSP)

Interest in protein structure prediction is widespread and has been previously addressed using evolutionary algorithms: Simple genetic algorithm (GA), messy GA (mga), fast messy GA (fmGA), and Linkage Learning GA (LLGA). However, past research used off the shelf software such as GENOCOP, GENESIS, and mGA. Our modified fmGA, is “good” at finding semioptimal solutions in a reasonable time. The study focuses on tuning this fmGA in an attempt to improve the effectiveness and efficiency of the algorithm in solving a protein structure and in finding better ways to identify secondary structures. Note that that this material design research was initiated over ten years ago and many papers are available covering this topic. The Air force sponsor of our work is the AF Research Laboratory, Materials & Manufacturing Directorate, WPAFB, OH.

Protein structure prediction is a Grand Challenge problem. Solving this problem involves finding a methodology that can consistently and correctly determine the configuration of a folded protein without regard to the folding process. A variety of algorithmic approaches have been proposed, ranging from GAs, SA, to hybrids between deterministic and stochastic methodologies using nonlinear opti mization techniques and maximum likelihood approaches. We focus on modifications to the fmGA, such as multiobjective implementation of the fmGA (MOfmGA), residue integrated Ramachandran plots, and a farming model for the parallel fmGA (pfmGA) to improve on previous GA applications for protein structure determination.

This investigation utilizes the CHARMm (version C22) energy model as a fitness function. Good protein structures are found by minimizing protein potential energy. A choice between real and binary values is required. In the past both of these encodings yielded similar results. Thus, a binary encoding was chosen, and the angles discretetized into 1024 (1 MB or 2^{10}) sections for every $360°$ is used.

Fast Messy GA: Following our previous sGA and mGA work, the fmGA is our explicit BB GA of choice. The mGA’s advantage over the sGA is in its ability to explicitly create tightly linked building blocks for defeating deception by insuring that there is a good solution in the population of building blocks created in the initialization phase. However, it is extremely expensive to build every combination of a particular building block size to put into a population. The fmGA is designed to reduce this expense by replacing the initialization phase and primordial phase with a probabilistic complete initialization (PCI) and primordial phase, consisting of selection and building block filtering (BBF).

Parallel fast messy GA: The pfmGA is an extension of the fmGA and is a binary, population based, stochastic approach that exploits Building Blocks (BB)s within the population to find solutions to optimization problems. Our pfmGA may be executed in a single program single data (SPSD) or a single program multiple data (SPMD) mode.

Multiobjective fmGA (MOfmGA): A modified Multiobjective fmGA (MOfmGA) executes using the same algorithm structure as the fmGA. The differences include the use of a multiple competitive template design where each objective function is assigned a competitive template. This competitive template evolves to "optimize" that particular objective function. Overall, the fmGA used in this investigation is programmed to run in serial and parallel on various commercial platforms. The algorithm's generic performance metric is two fold goodness of the structure (effectiveness) and the time to converge (efficiency).

Studied is both effectiveness and efficiency for the fmGA when used to determine a protein structure. Included tests are competitive template generation, a building block size, Ramachandran constraint and a multiobjective experiment. Efficiency is tested using a Farming Model. The "goodness" of solutions are evaluated using RMS differences.

Competitive Template Generation: The fmGA explicitly manipulates BBs in search of the global optimum and uses the idea of speciation through successive phases of the algorithm. The fmGA uses a competitive template, which is a fully specified population member, to evaluate these partially defined strings or building blocks. By focusing on modifying the process that the fmGA uses to create and update the competitive template during the execution of the algorithm the algorithm's effectiveness is increased.

Building Block Experiment: The BB analysis is performed in an attempt to identify the building block sizes that result in the fmGA finding better solutions. A BB is a partial string representing bits from one, some, or all of the dihedral angles that each chromosome represents. The BBs are not restricted to be contiguous bits from the chromosomes but instead can be noncontiguous bits from the chromosome. Constraints based on Ramachandran Maps Search algorithms having constrains on search space by a feasibility function statistically, overtime, must find better solutions. This premise also applies to this experiment, by constraining the search space to have only feasible solutions it is expected that better solutions are found.

Multobjective Experiment: In the single objective implementation of the fmGA, the CHARMm energy function is utilized and consists of a summation of several terms. In the multiobjective approach, the objectives are drawn from each of the terms within the CHARMm energy function, defined in terms of bonded and nonbonded interactions.

Farming Model Experiment: Alternate efficiency models, such as the island model, have been previously applied in parallelizing GAs. Due to the computational expense of our energy fitness function calculation in the PSP problem, the addition of a farming model is proposed as discussed. The Component Under Test for efficiency is the fitness function calculation. The farming out of a computationally expensive fitness evaluation should realize speed up in efficiency without affecting the effectiveness. Wall clock time is measured by system clock time to complete.

Multiple Competitive Templates: The multiple CT modification requires the fmGA to have the ability to compute a panmetic competitive template in addition to having multiple competitive templates present during computational search. Statistical techniques used are the Kruskal-Wallis (KW) and ttest for paired and unpaired observations

(PO). There is a clear difference between the random, betasheet, and all alphahelix related templates (alphahelix, multiple, and panmetic competitive template). Similar results are reported with the PO test. Finally, the KW test also confirmed that the alphahelix related, betasheet, and randomly generated competitive template methods are different.

Farming Model Experiment: The pfmGA utilizes an island model paradigm to conduct parallel communications between processors. At each stage of the communications, all processors communicate their best found population member to processor 0. Processor 0 then determines which is the “best” and communicates that population member back to all of the processors who then update their CT. After the update, all of the processors continue to execute the algorithm independently with independent population members until the next update communication is necessary. Due to the complexities associated with the energy fitness function calculation, the addition of a farming model in combination with the island model is proposed. Farming out the fitness calculations to another set of slave processors allows for a decrease in the overall processing time as long as the computation time is greater than the communications time required. As the slave processors calculate fitness values, the masters can do the same or conduct other computations. In addition to speedup gained for the peptide selected in this investigation, the addition of these slave processors allows for the MOfmGA to handle larger proteins.

The BB analysis is performed in an attempt to identify the building block sizes that result in finding better solutions for $Polyanline_{16}$. A BB is a partial string representing bits from one, some, or all of the dihedral angles that each chromosome represents. The BBs are not restricted to be contiguous bits from the chromosomes but instead can be noncontiguous bits from the chromosome. This analysis covers a variety of BB sizes and compares the results to determine which size produces the best statistical results. The BB ranges chosen for testing included: 1618, 1820, 2022, . . ., and 3840. The results of the BB size experiment show that different BB sizes yielded the best results for each protein.

Ramachandran Experiment: The Ramachandran experiment takes advantage of problem domain information in restricting the search space (not size) for the algorithm. In the preliminary results the MOfmGA is executed three times for each of the methods to provide statistical results. Results indicated that Ramachandran constraints achieve better structures.

4 QC Laser Design

A quantum cascade (QC) laser is a specific type of semiconductor laser that operates through principles of quantum mechanics. The unipolarity of a QC laser indicates that electrons are solely responsible for releasing energy in the form of photons which emit light. These electrons transition from one energy state to another within a layer of semiconductor material releasing energy in the form of photons during their descent. The binding to these energy states is a result of the semiconductor layers being extremely thin. A Unlike the earliest form of semiconductor lasers where the energy bandgap determines the wavelength of the light emitted with QC lasers the thickness of the layers determines the wavelength. This is a critically important property of QC lasers because it allows them to be tuned to a desired frequency.

Because there is a genuine lack of compact and coherent devices which can operate in the far-infrared area of the electromagnetic spectrum the motivation exists for designing a terahertz QC laser. Additionally, the QC laser is expected to be more efficient and cost effective than currently existing devices operating in the terahertz frequency range. It has potential applications in the fields of spectroscopy, astronomy, medicine and free-space communication as well as applications to near-space radar and chemical/biological detection due to the unique signatures of biomolecules in the terahertz frequency range. Terahertz frequency emission has the ability to permeate paper, ceramic and cardboard membranes. A single or multiple detectors with a reasonable level of power producing an acceptable signal-to-noise ratio may be tuned for detection of a specific agent. In addition to chemical and biological detection terahertz emission has demonstrated the ability to detect a concealed weapon using 2-D fast fourier transforms to produce an image array. The AFRL Sensors directorate is supporting this effort.

The overarching goal of this current research is to optimize a quantum cascade laser which experiences continuous wave operation in the terahertz frequency range. Generally, laser optimization requires tuning parameters solely to increase the overall gain. In this case, the optimization of the quantum cascade laser given simulation is a multiobjective problem because in addition to being concerned about the gain it is also necessary to ensure the laser is operating in the terahertz frequency range. For optimization of the QCL operating in the terahertz frequency range being designed a multi-objective algorithm which can handle real values is required. Parallelization is desired because of the intensive computation required to correctly simulate the operation of the QCL given specific parameters. The particular search algorithm used has been named general multi-objective parallel genetic algorithm (GENMOP). GENMOP is a pareto-based algorithm that utilizes real values for crossover and mutation operators. Additionally, the algorithm employs fitness sharing through a niche radius.

Communication time and data rate, or throughput, are two of the most important measures used for comparison of paralleled processes. The communication time for a program running in parallel can be significant overhead thus increasing the overall computation time appreciably. The data rate is a measure of the peak number of bytes of data that can be transferred per second and is a direct reflection on the chosen interconnection network for communication. Also, a measurement of the parallel speedup is important. The experiments are all designed so the efficiency metrics for parallelized programs can be gathered. The QC laser simulation is designed, so that both the target frequency and number of layers needed to form the laser structure can be provided at runtime.

Conclusions

We have describe various AFIT research focused on specific AF design problems. As indicated, the application of our EA software to these problems has resulted in acceptable solutions. Due to the limitation of this abstract, other successful EA applications to real-world AF design problems such as groundwater remediation design, antenna placement on aircraft, network intrusion detection, dynamic UAV communication structure organization, and priority satellite communication were not included.