

**OPTIMIZATION FRAMEWORK FOR A RADIO  
FREQUENCY GUN BASED INJECTOR**

by

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# ABSTRACT

## OPTIMIZATION FRAMEWORK FOR A RADIO FREQUENCY GUN BASED INJECTOR

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Linear accelerator based light sources are used to produce coherent x-ray beams with unprecedented peak intensity. In these devices, the key parameters of the photon beam such as brilliance and coherence are directly dependent on the electron beam parameters. This leads to stringent beam quality requirements for the electron beam source. Radio frequency (RF) guns are used in such light sources since they accelerate electrons to relativistic energies over a very short distance, thus minimizing the beam quality degradation due to space charge effects within the particle bunch. Designing such sources including optimization of its beam parameters is a complex process where one needs to meet many requirements simultaneously. It is useful to have a tool to automate the design optimization in the context of the injector beam dynamics performance. Evolutionary and genetic algorithms are powerful tools to apply to nonlinear multi-objective optimization problems, and they have been successfully used in injector optimizations where the electric field profiles for the accelerating devices are fixed. Here the genetic algorithm based approach is extended to modify and optimize the electric field profile for an RF gun concurrently with the injector performance. Two field modification methods are used. This dissertation presents an overview of the optimization system and examples of its application to a state of the art RF gun. Results indicate improved injector performance is possible with unbalanced electric field profiles where the peak field in the cathode cell is larger than in subsequent cells.

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To my husband, Geoff, and our children, Athena and Konrad,

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# CHAPTER 1

## INTRODUCTION

### 1.1 INTRODUCTION

For linear accelerators (linacs), the injector, where the particles to be accelerated originate, sets the beam performance characteristics of the machine. This makes the beam parameters at the injector a critical aspect of the final beam characteristics of the machine. The focus of this research is, first, to develop a tool to automate the design of injectors based on radio frequency (RF) guns and, second, to apply this tool to examine possible improvements that can be made to an existing state of the art RF gun.

There are two main types of electron sources or guns for photo-injectors used in particle accelerators. The first is a direct current (DC) gun which accelerates photo-emitted electrons using a fixed electric field between a cathode and an anode. These guns can produce a continuous stream of electrons and are limited by field emission [1]. They can provide the very high vacuum environments required by some cathode photo-emitter materials [2]. A DC gun design to produce 19-77 pC electron bunches at 1300 MHz [3] operating at a target high voltage of 750 kV is under development at Cornell University for an energy recovery linac (ERL) based x-ray light source [4]. It has achieved 425 kV gap voltages but operates at an administrative limit of 250 kV [5]. Jefferson Lab's Free Electron Laser (FEL) DC photocathode gun has operated routinely at 320 kV, delivering 135 pC per electron bunch at 74.85 MHz [6]. The second source type is an RF gun where a time varying electric field established in a resonance cavity structure accelerates the electrons. RF guns are capable of accelerating 1 nC bunches of electrons to  $\sim 4.7$  MeV/c in 20 cm [7]. Due to heat losses into the cavity walls sufficient to melt the cavity, RF guns are limited to pulsed operation. They are also susceptible to field emission. RF guns are used mainly in FEL light sources [8,9].

There exist no tools to evaluate the optimality of RF gun designs thoroughly especially with regard to the overall injector performance (beam dynamics). This research project develops and applies an automated optimization method based on the genetic algorithm (GA) approach to improve RF gun cavity shape based on

beam dynamics performance. Note that portions of this dissertation work have been published in three conference proceedings [10–12].

## 1.2 INJECTOR DESIGN PROCESS

The injector for a particle accelerator typically has three main components: particle source, beam transport system, and acceleration system. Figure 1 presents a generic injector and its components. The overall purpose of these systems is to create a beam at the exit of the injector that meets the specific beam quality requirements imposed by the accelerator’s application. While it is easier to treat these systems as independent, the reality is that the effects of these various systems become intertwined as the beam moves from rest at the source to typically relativistic energies at the end of the injector. The results are systems that serve more than one function, such as acceleration and beam transport together. This often nonlinear interplay of effects combined with the large number of beam parameters and requirements that sometimes conflict makes designing and optimizing an injector difficult [13]. Historically, injector optimization has been a manual process where the injector designer concentrates on one or two beam quality requirements, designs injector components to meet those requirements, and makes trade-offs with the balance. While injectors designed this way are successful, it is understood that the designs may not be globally optimal, flexible, or robust over a large range of beam parameters. A system to automate the design process could allow more than a handful of beam parameters to be considered carefully.

The geometries of accelerating components in an injector are often selected and optimized in an early phase of an injector design. These designs typically build on the successes of previous machines where success is defined in terms of field characteristics, mechanical stability, and manufacturability. The development cycle for these elements is quite long. Once chosen, the injector designer must work within the confines of the capabilities of the structures. On the other hand, it may be advantageous to have the ability to explore alternative accelerating structure geometries and their field profiles in the context of the injector design to ensure that the available accelerating fields are best optimized to meet the injector beam requirements.

## 1.3 PROPOSED APPROACH USING GENETIC ALGORITHMS

Automation of the injector design and optimization process has been slow to come

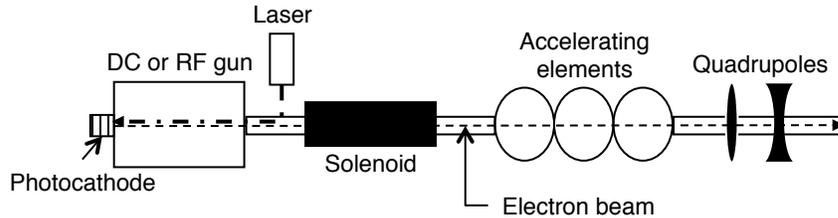


FIG. 1: Generic injector layout (not to scale). The particle source is comprised of the gun, laser, and photocathode. The gun and accelerating elements (RF cavities) are the acceleration system. The beam transport consists of the magnets, but the accelerating elements also contribute to the beam transport for non-relativistic beams.

about for two main reasons. The first is due to the general nonlinear interdependence of beam quality parameters making it difficult to separate the variables and treat them independently. In some cases, the relationships between parameters are not known exactly. Posing an optimization problem using the classical methods under these conditions is extremely difficult or impossible [13]. The other reason is that the beam dynamics codes are computationally intensive. Gains in computer processor power and speed have helped enormously allowing injector designers to simulate many variations of a machine design in the time it took to simulate only one or two designs over a decade ago. As is true with many physics and engineering problems today, these simulations which were once performed on very specialized supercomputers or large mainframe computers can now be performed on desktop computers [14, 15]. These same gains in compute power have led to the growth of affordable parallel computer architectures consisting of desktop class machines connected with dedicated high speed networks [16]. With these dedicated distributed computing resources, a different approach to the optimization problem taking advantage of evolutionary algorithms (EAs) or GAs can be used [17] to automate the injector design and optimization process [13].

GAs solve problems by mimicking the way living organisms in a population pass traits from one generation to the next through the recombination and mutation of genes to increase the viability of the population [18, 19]. The GA approach is very much in the vein of Darwin’s notion of “survival of the fittest” [20] where individuals

with the best chances of survival breed offspring with similar characteristics thereby increasing the odds that the offspring will survive to reproduce.

GAs can be used to study problems posed as a multi-objective optimization problem (MOOP). A MOOP has several bounded inputs and more than one desired outcome or objective. A general statement of a MOOP is [17]

$$\begin{aligned} &\text{Minimize/Maximize } f_m(\mathbf{x}), & m = 1, 2, \dots, M; \\ &\text{subject to } g_j(\mathbf{x}) \geq 0, & j = 1, 2, \dots, J; \\ & h_k(\mathbf{x}) = 0, & k = 1, 2, \dots, K; \\ & x_i^{(L)} \leq x_i \leq x_i^{(U)}, & i = 1, 2, \dots, n; \end{aligned}$$

where  $M$ ,  $J$ ,  $K$ , and  $n$  are, respectively, the numbers of functions to minimize or maximize (objective functions), inequality constraint equations, equality constraint equations, and independent or decision variables. The  $x_i^{(U)}$  and  $x_i^{(L)}$  are the upper and lower bounds for the decision variables. GAs are suited for MOOPs [13,17] for several reasons. First, unlike classical optimization methods, GAs do not require derivative information. This is helpful for injector optimization problems where functional information (let alone derivative) is often not available [13]. Second, they provide a way to manage and characterize the inputs ( $\mathbf{x}$ ) and outputs of a MOOP through decision vectors which represent different sets of values for  $\mathbf{x}$  and fitness assignments that indicate how well different  $\mathbf{x}$ 's meet the constraints and optimization objectives. Third, they can search for a set of decision vectors,  $\mathbf{x}$ 's, that meet the objectives and satisfy the constraints in a population if they exist.

The Platform and Programming Language Interface for Search Algorithms (PISA) [21] provides a convenient way to merge application problems and GAs. It separates the GA selection algorithm processing from the decision variable creation and model evaluation processing into two programs that work in a coordinated fashion using a well defined set of interface files. With this design, stand alone programs that implement different standard GAs can be developed independently of the program responsible for model processing. The only requirement is adherence to the file interface, and if that is followed, the implementation details for each program are hidden. The result is a flexible test environment where different GAs and problem models can be used together at run time without changing the source code of either program.

Alternate PISA (APISA) [13] is PISA where the model evaluation program has been customized to study injectors with an interface to a beam dynamics code, viz.,

A Space Charge Tracking Algorithm (ASTRA) [22]. APISA is the first step towards automating the injector design process. It allows designers to find appropriate settings, magnet strengths, RF phases, and amplitudes for injector beam line elements and the physical distances between them without changing the element geometries. It also allows the designer to study the effect of bunch shape coming off the cathode. For a photocathode gun, the bunch shape directly relates to the laser pulse shape and duration. APISA has been used to determine that a high voltage DC photocathode gun operating in the 500-750 kV range can serve in an injector delivering beam meeting all of the beam quality requirements for Cornell's proposed ERL light source [13,23].

This study develops a framework that allows an injector designer to optimize the accelerating fields of an RF based electron gun concurrently with the overall injector design. This framework, based on APISA, provides two paths for gun design development. Both approaches assume that the desired accelerating field resembles the  $TM_{010}$   $\pi$ -mode of a multi-cell pillbox cavity in which the phase of the accelerating field changes by  $180^\circ$  in adjacent cells. The first path is a purely theoretical exercise that searches for the on-axis accelerating electric field profile that provides the best injector beam characteristics independent of the geometry of the gun. It approximates the  $\pi$ -mode with a sine wave. It, then, changes the sine's features by multiplying it with a variable function described by a truncated Fourier series whose coefficients can be changed by the GA. In reality, the fields produced by a gun depend on the geometry of the gun cells. The second path modifies a cylindrically symmetric cavity description and uses a field solver, viz., Poisson Superfish [24], to find the attendant field profile information. The GA framework varies aspects of the cavity description to change the field profile as dictated by the desired beam characteristics of the injector.

An important beam characteristic for accelerators and light sources is emittance. The particles in a charged particle bunch can be treated as a statistical ensemble. It is more convenient to refer to the properties of the ensemble instead of the individual particles, and the emittance is one such property. At each point in time, each particle has six coordinates associated with it, three spatial  $(x, y, z)$  and three momenta  $(p_x, p_y, p_z)$ . One way to view the ensemble of particles is in phase space. There is an emittance for each two dimensional projection of the six dimensional phase space, and the emittance is a measure of the area occupied by the particles in the projection.

The emittance is important because it is preserved under linear forces [25]. Once set in the injector, in a linac where the linear force model applies, the emittance cannot be improved, only degraded. The transverse rms emittance normalized with respect to energy [26] is

$$\varepsilon_n = \beta\gamma\sqrt{\langle(x - \langle x \rangle)^2\rangle\langle(x' - \langle x' \rangle)^2\rangle - \langle(x - \langle x \rangle)(x' - \langle x' \rangle)\rangle^2}$$

where  $\beta$  is  $v/c$ ,  $v$  is the velocity,  $c$  is the speed of light,  $\gamma$  is the relativistic Lorentz factor  $\gamma = (\sqrt{1 - \beta^2})^{-1}$ ,  $x$  is the spatial coordinate, and  $x'$  is the angle ( $x' = p_x/p_z$ ). An alternative formulation that can be used to calculate both transverse and longitudinal emittances [27] is

$$\varepsilon_n = \frac{1}{m_0c}\sqrt{\langle(p_x - \langle p_x \rangle)^2\rangle\langle(x - \langle x \rangle)^2\rangle - \langle(p_x - \langle p_x \rangle)(x - \langle x \rangle)\rangle^2} \quad (1)$$

where  $m_0$  is the particle rest mass. The emittance is fundamental to some characteristics of an accelerator. In an FEL, the transverse emittance must be less than  $\lambda_{FEL}/(4\pi)$  where  $\lambda_{FEL}$  is the FEL wavelength to efficiently produce radiation [28]. For light sources, emittances determine the full six dimensional normalized brightness of the source defined as [29]

$$B_n = \frac{N}{\varepsilon_{n,x}\varepsilon_{n,y}\varepsilon_{n,z}} \quad (2)$$

where  $N$  is the number of electrons in the bunch, and  $\varepsilon_{n,x}$ ,  $\varepsilon_{n,y}$ , and  $\varepsilon_{n,z}$  are the normalized transverse emittances ( $x,y$ ) and the normalized longitudinal emittance ( $z$ ), respectively. The brilliance of the light produced depends on the brightness of the source. Higher brightness leads to higher brilliance, and to increase brightness for a fixed bunch charge, the emittances of the beam must be minimized.

The Photo Injector Test Facility Zeuthen (PITZ) [7] has developed an RF gun based injector, and this state of the art gun is studied in this research. Its RF gun is a 1.5 cell 1300 MHz cavity operating at 40 MV/m peak at the Cs<sub>2</sub>Te photocathode wall. The RF cavity is located between two solenoids. The downstream solenoid is used for emittance compensation counteracting emittance growth due to space charge effects that develop as the electron bunch is accelerated in the cavity [30,31]. The upstream solenoid is used to ensure that the magnetic field at the cathode is zero. The main requirement of this gun system is to deliver 1 nC bunches of electrons with 1-2  $\pi$  mm mrad normalized transverse emittance approximately 1 m downstream of the gun. To this end, the cavity has been tuned to produce a balanced field profile, meaning that the amplitude of the peak field value is the same in both cells. The

optimizations performed in this research indicate that better transverse emittance near the end of the injector may be achieved if the gun is operated with an unbalanced field profile where the peak amplitude of the gun cell is twice that of the full cell.

## 1.4 DISSERTATION LAYOUT

This dissertation begins with an overview of GAs that covers the general terminology and mechanisms. A description of the specific algorithm used in this research project is included in the overview. Next, the first contribution of this dissertation research is presented, the design and implementation of the components that automatically generate RF cavity field profiles in APISA. This is prefaced with overviews of the PISA and APISA systems that form its basis. Also, operational issues that impact the design are outlined. The second contribution of this research, the analysis of the PITZ RF gun design using this augmented version of APISA, follows. The conclusion discusses the viability of using a GA approach in designing an RF gun based injector and future improvements for the system. Appendices are provided for reference. The first two describe how ASTRA, the beam dynamics simulation code, and Poisson Superfish, the field solver, work. The third serves as a user's guide for PISA and APISA.

## CHAPTER 2

### EVOLUTIONARY ALGORITHMS OVERVIEW

#### 2.1 MULTI-OBJECTIVE OPTIMIZATION OVERVIEW

When discussing MOOPs, it is helpful to understand how the problem statement and its solutions are characterized [17]. An objective function in a MOOP is the same as in a single objective problem. Strictly speaking, it is a function that is to be minimized or maximized, but it can be a calculated value from a numerical model of the system under consideration. In a multi-objective optimization, there are two or more objectives, and they form a vector. In turn, the collection of vectors form a space called the objective or search space. The objectives depend on a set of variables or inputs that also form a vector known as the decision vector. Each element in the decision vector is a decision variable with upper and lower limits on its value. There is a corresponding decision space for the decision vectors. The mapping between the decision and objective spaces is the mathematical model of the system and is typically the set of objective functions to be optimized. The results of a multi-objective optimization are presented in terms of these two spaces.

Single and multi-objective optimizations both can have constraints, and the constraints are used to restrict the set of candidate solutions for the optimization problem. An instance of a decision vector that falls within the limits of the decision variables, satisfies the constraints of the problem, and is a solution of the objective functions produces a feasible solution for the optimization. The set of all feasible solutions for a MOOP contains both optimal and suboptimal solutions [17].

Solutions can be additionally characterized in terms of dominance. This can be used to differentiate between the optimal and suboptimal solutions in the feasible set. Unlike feasibility that is determined from the evaluation of the problem statement, dominance is a relative description. It is a comparison of the objective values for two solutions against the optimization goal. One objective value is said to be better than another if, in the case of a minimization, its value is less than the other's [17]. Further, an objective value is said to be no worse than another if it is equal to or better than the other [17,32–34]. Again, for a minimization, a solution is no worse than another if it is less than or equal to the other. A solution, a set of objective values, dominates

another when all of its objective values are no worse than those of the other, and it has at least one objective value that is better than the corresponding objective value of the other solution. For example, in a maximization problem with six objectives, if solution 1 has five objective values that are the same as those of solution 2 and the remaining one is better (has a larger value), then solution 1 dominates solution 2, and solution 2 is suboptimal relative to solution 1. Alternatively, solution 1 is said to be non-dominated by solution 2. It is this non-dominance characteristic that is so important in multi-objective optimization.

Because the objectives often conflict in a multi-objective optimization, it is possible to have more than one feasible optimal solution. The classic illustrative example of conflicting objectives is car price versus features [17]. Carmakers produce cars with a variety of interior, exterior, comfort, and safety features, and the price of a car varies with the features provided. Why do the carmakers do this? One reason is that they want to sell cars to as many buyers as possible, but each car buyer uses his or her own set of criteria for choosing a car to buy. Not every car buyer can afford nor wants a luxury car. On the flip side, there are buyers who will pay handsomely for many features. This means there is no single best car for the carmakers to produce in terms of cost or features. For each set of features, though, there is a price that a buyer is willing to pay. Conversely, for each price, there is a set of features that the carmakers are willing to provide. This leads to a set of cars not a single car to produce. The set of cars that represents the best trade-off between cost and features for each combination of the two is the optimal set. Ironically, there is an additional conflict defining this best set. For the buyer, the best set may consist of the least expensive cars for each set of features to minimize how much the buyer pays for the most number of features. The carmaker may want to maximize profits, and the best set may be the most expensive cars providing the least features. In reality, the optimum where the carmaker sells the most number of cars with reasonable profits lies in between.

Whatever the criteria for forming the best set, the optimal set has two characteristics. The main one is that the members of the set are non-dominated relative to each other. Each car price and feature pairing is the best possible for that combination. Comparing two cars in this set means their prices and features are different, but relatively speaking, neither one is clearly better than the other. A more expensive car from the set has the best features for that price. A cheaper car may provide

fewer features but still provides the best features possible at that price. Another characteristic of the optimal set is that each member dominates at least one member of the set of feasible solutions. In the car example, for a car buyer looking to buy the cheapest car with the most features, an optimal car compared to the various available cars will for the same price have more features, for the same features have a cheaper price, or have a cheaper price and more features. This non-dominated set is called the Pareto-optimal front [17,34]. Looking at the Pareto-optimal front in the objective search space, it is part of the boundary surrounding the feasible solutions, but it is not the entire boundary [17]. In the car example, the car buyer's front represents a different part of the search space than the carmaker's front.

Since there may not be a single optimal solution for a MOOP, the goal of a multi-objective optimization method is to find the Pareto-optimal front or an estimate of it [17]. This points to the need for a method that can evaluate and process multiple solutions concurrently to find the multiple optimal solutions and identify candidate members of the Pareto-optimal front [17]. EAs are an appropriate choice because they operate on populations or collections of solutions [34], and as a result, some EAs have been specifically designed to find a broad representative sample of the Pareto-optimal front for MOOPs.

## 2.2 GENETIC AND EVOLUTIONARY ALGORITHMS OVERVIEW

EAs apply processes in nature to optimization problems. GAs, a type of EA, mimic the competition between prospective organisms to mate and the exchange and change of genes in chromosomes during sexual reproduction to search a decision space for optimal solutions [17]. EAs use the population and environmental pressure concepts from evolution to direct the search toward the Pareto-optimal front. Historically, GAs operated on binary string representations of the decision variables [18], but that limitation seems to have eased since there are real valued vector analogs of the processes originally designed to operate on binary strings [17]. Unless referring specifically to the historic GAs, EA will be used throughout this discussion.

A major difference between EAs and classical optimization techniques is, as mentioned previously, that EAs operate on populations, a set of solutions. Classical techniques in both single and multiple objective optimization methods are iterative and produce a single new decision vector at the end of an iteration based on information from a small set of previously generated solutions. In contrast, EAs produce

and evaluate several decision vectors per iteration, and the population of decision and objective vectors produced during an iteration is called a generation [17]. Each decision and objective pair is sometimes referred to as an individual [34]. Because EAs are population based, they, also, have very novel ways to create new decision variables.

The initial population of decision vectors is typically created by randomly selecting the decision variable values within the limits imposed by the optimization [17]. The general EA process starts when the decision vectors are, then, used to produce the objective vectors, and each individual is assigned a fitness value. The fitness metric is defined differently for each EA, and the metric is, at a minimum, a function of the objective values. Fitness is a measure of how “good” an individual is.

The next stage is to create the next population [35]. This is a multi-step process that mirrors to some degree what happens in biological populations. The first step is called selection, or reproduction, where individuals deemed worthy of being parents are identified and placed in an intermediate population known as the mating pool. The source population from which parents are chosen varies with the algorithm but usually is some incarnation of the previous generation. Individual worthiness is determined by competition using fitness. There are several standard methods of competition or selection, and each algorithm elects which one to use. Generally, though, a selection process involves picking two individuals from a population at random, comparing their fitness values, and putting a copy of the winner, the one with the better fitness value, in the mating pool. The main goals of this step are to pick the best individuals from a population to place in the mating pool, and to ensure that better individuals have more opportunities to participate in the next step where offspring are produced than lesser individuals. This second goal is achieved with the number of copies a particular individual has of itself in the mating pool [17]. A better, fitter, solution should, in practice, have more copies in the mating pool and thereby have a greater influence on the characteristics of the offspring. The net effect of this step is to reduce the overall diversity in the offspring population [17]. Because the initial population is randomly created, it is diverse and has no preference for any particular regions of the decision or objective space, but this is not true for subsequent populations. The selection process introduces preferences for the regions in the search space where the parents reside and thereby reduces the diversity of the population [17]. This is the mechanism EAs use to identify promising regions in the

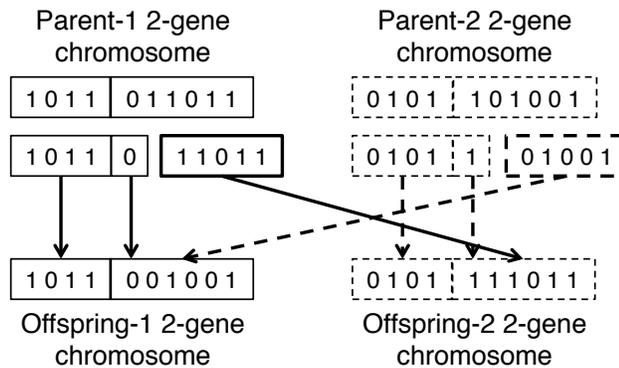


FIG. 2: Binary crossover example. The genes in Parent-1 in decimal are 11 and 27, and the genes in Parent-2 are 5 and 41. The first gene in each parent is transferred directly to the offspring. The second gene for Offspring-1 is 9 and for Offspring-2 is 59.

search space.

Once the mating pool is formed, offspring are produced from the parents. Since the original processes and terminology were developed for GAs, the discussion here will follow suit. Recall that historically a GA works on a binary string. This string is called a chromosome and has a fixed length [18]. The string is subdivided into contiguous sections according to the number of decision variables, and the subsections are called genes. Note that the string does not have to be divided into equal parts [17] as shown in Figure 2. In this example, the chromosome is 10 bits long and has two genes. The first gene uses 4 bits while the second uses the remaining 6 bits. Dividing the chromosome into unequal sized genes allows one to customize the precision of each decision variable since the number of bits allocated to a decision variable determines the number of different available values, i.e. for an allocation of  $m$  bits, there are  $2^m$  different values [17].

As in sexual reproduction, the chromosomes from two parents are combined to create two new chromosomes through a process called crossover. Crossover is also referred to as recombination. In crossover's simplest form, single-point crossover, two parent chromosomes are broken at the same randomly selected point in the chromosome, and parts exchanged [18]. The break point is not confined to gene boundaries, so whole and partial genes are exchanged in this process [17]. Figure

2 shows a single break occurring between bits 5 and 6 located in the second gene. Breaking within genes creates two new chromosomes with genes that are similar to but may not be exactly the same as the genes in the parent chromosomes. When a partial gene is exchanged, gene information from one parent is blended with the corresponding gene from the other parent, and the resulting offspring are variations of the parents as is the case in Figure 2. Crossover allows GAs and EAs to move around the decision space [17, 19]. It is analogous to swapping the  $y$ -coordinates between two points on a 2D Cartesian plot. The two new points are displaced relative to the original points. This is a naïve and imperfect way to create a real valued version of this form of crossover since it respects the inherent gene boundaries in the decision vector [17], unlike the binary version.

The other genetic process is mutation. Here, again in its simplest form, a randomly selected individual bit is flipped from on to off or vice versa [17]. For a real valued decision vector, mutation slightly adjusts a randomly picked decision variable in the decision vector. Mutation allows the GA to increase diversity balancing the decrease in diversity due to selection [17].

### 2.3 STRENGTH PARETO EVOLUTIONARY ALGORITHM 2

The algorithm used in this research, Strength Pareto Evolutionary Algorithm 2 (SPEA2) [36, 37] follows the basic processes outlined above with some variations. SPEA2 is classified as an elite preserving algorithm. In elitist strategies, individuals with special desirable characteristics are treated differently than members of the standard parent and offspring populations [17]. Non-dominated individuals are preferred in SPEA2 since it strives to find a broad representative sample of the Pareto-optimal front. Because individuals are normally chosen at random from the population to participate in the selection competitions, it is possible that promising individuals are overlooked and lost if they are not chosen to compete. Elitism addresses that. Since these individuals have desirable characteristics in terms of the problem objectives, they are kept in a reserve and allowed to outlive the generations in which they are created. This gives them opportunities to produce offspring in subsequent generations as long as they continue to qualify as elite. They are also given preference during the selection process for the mating pool. In SPEA2, only members of the elite population, also known as the archive, are candidates for the mating pool [36, 37].

SPEA2 uses a fixed size archive [36, 37]. It is limited to  $\overline{N}$  individuals. For each

new generation, after evaluating the decision vectors and assigning fitness values, it fills the archive first with all of the non-dominated individuals from the previous contents of the archive and the latest population. If the number of non-dominated individuals is larger than  $\overline{N}$ , SPEA2 systematically removes less desirable non-dominated individuals from the archive until the number of individuals matches  $\overline{N}$ . Because its archive is also the latest and best estimate of the Pareto-optimal front and is supposed to be a diverse representation of the front, less desirable non-dominated individuals are those that are clustered near other individuals. Clustering of solutions is a direct consequence of the way the search in a EA focuses more tightly on the promising regions of the search space as it progresses from one generation to the next approaching the optimization goals [17]. To identify clustered individuals, SPEA2 uses the  $k$ -th nearest neighbor distance,  $\sigma^k$  [36, 37]. Fundamentally,  $\sigma^k$ , in SPEA2, is a Euclidean distance calculated in the objective space. In a list of distances calculated between an individual  $i$  of the bloated archive and each other member of the bloated archive sorted in increasing order,  $\sigma_i^k$  is the  $k$ -th element. In SPEA2,  $k$  is taken to be  $\sqrt{N + \overline{N}}$  where  $N$  is the maximum size of the current population. The truncation of the archive proceeds in rounds removing one individual each time. First,  $\sigma_i^k$  is calculated for each individual  $i$  in the archive. Individuals that are either duplicates of other individuals (have identical  $\sigma^k$  for all  $k$ ) or have the same smallest  $\sigma^k$  are identified. If a single individual is found, it is removed. Otherwise, the  $(k - 1)$ -th distances and so on are considered until a single individual is identified. If the number of non-dominated individuals is less than the archive size, the remaining slots are filled with the better dominated individuals from the population. Conveniently, the fitness metric used in SPEA2 provides an indication of whether or not an individual is non-dominated or dominated (and to what extent).

Fitness in SPEA2 is to be minimized and is calculated from three quantities [36]. The first is the strength,  $S(i)$ . Strength is a tally of the number of individuals in the archive and the current population that individual  $i$  dominates. The strength values are then used to calculate the raw fitness,  $R(i)$ , for each individual  $i$ .  $R(i)$  is the sum of strength values,  $S(j)$ , of the individuals in the archive and current population that dominate individual  $i$ . It is zero for non-dominated individuals. The third quantity needed for the final fitness calculation is used to differentiate between individuals with equivalent raw fitness values. It is an estimate of the density of solutions in the vicinity of each solution. As with the archive, the preference is to keep individuals

from sparser regions of the search space to maintain diversity. The density estimate for individual  $i$ ,  $D(i)$ , uses  $\sigma_i^k$  as

$$D(i) = \frac{1}{\sigma_i^k + 2}$$

where the offset 2 is used to ensure that  $0 < D(i) < 1$ . The fitness,  $F(i)$ , is defined as  $F(i) = R(i) + D(i)$ . Referring back to the archive truncation process, for a non-dominated individual,  $F(i) < 1$ . For dominated individuals,  $F(i) > 1$ , and because SPEA2 fitness is to be minimized, when comparing dominated individuals, the dominated individual with  $F(i)$  closer to 1 is better.

Since dominance ranks solutions based on objective values only, SPEA2 is an unconstrained optimization algorithm. Constrain-dominance is a ranking system that extends the dominance definition to include the effects of inequality constraints [17]. It can be used instead of dominance in the strength and raw fitness calculation above to change SPEA2 into a constrained optimization algorithm [13,17]. In a constrained optimization problem, the search space is a subset of the unconstrained search space because some feasible solutions in the unconstrained problem become infeasible in the constrained problem [17]. Failing to satisfy one or more constraints of the constrained problem makes these solutions infeasible in the constrained problem. Some of these solutions may lie near the boundary between the feasible and infeasible solutions in the constrained problem. The Pareto-optimal front for the constrained problem is a subset of this boundary between the feasible and infeasible regions, and an infeasible solution near the boundary can provide useful constraint related information to guide the optimization to the Pareto-optimal front. Constrain-dominance uses this nearness to the boundary between feasible and infeasible solutions to rank infeasible solutions [17]. An individual constrain-dominates another if any of the following three conditions is true [17]. If its solution dominates the other under the original dominance definition, constrain-dominance preserves that, and it constrain-dominates the other. If its solution is feasible and the other is not, it constrain-dominates the other. Lastly, if both are infeasible, then as with dominance, the constraints are compared individually. If all of its constraints are no worse than those of the others, and it is better in at least one constraint, then it constrain-dominates the other. Since the original definition of dominance is preserved, the raw fitness and strength values are unchanged for non-dominated solutions. The net effects of the change, then, are to possibly increase the raw fitness values of dominated solutions and to provide counts

for infeasible solutions [17]. Since dominated solutions are feasible, their raw fitness values will be less than the raw fitness values for the infeasible solutions. This maintains the relative ranking of the solution groups: first, non-dominated solutions; second, dominated solutions; and third, infeasible solutions.

To create offspring, this implementation of SPEA2 [21, 38] uses simulated binary crossover (SBX) [17, 39, 40] and uniform crossover [18] between two parents from the mating pool, and polynomial mutation to mutate the offspring [17, 39, 40]. Uniform crossover is an extension of the naïve single-point crossover for real valued decision vectors discussed above in 2.2 [17]. Instead of one break point in the decision vector, the number of possible break points is the same as the number of elements in the decision vector. Each element of the decision vector is considered in turn and has the opportunity to be swapped with 50 % probability [21, 38, 41].

SBX [17, 39, 40] is a better implementation of the binary form of single-point crossover for real valued decision vectors since it incorporates the variation aspect of binary single-point crossover. It also factors in the distance between the two parents and creates similarly spaced offspring and, as a result, is an adaptive process. Initially, the distance between pairs of parents is large since they are randomly generated, but as the search proceeds, the spacing between pairs of parents becomes smaller as the overall population becomes less diverse. SBX defines a spread factor,  $\beta_i$ , between two generation  $t$  parent decision vector elements,  $x_i^{(1,t)}$  and  $x_i^{(2,t)}$ , and the corresponding offspring elements,  $x_i^{(1,t+1)}$  and  $x_i^{(2,t+1)}$ , of the next generation  $t+1$  as [17]

$$\beta_i = \left| \frac{x_i^{(2,t+1)} - x_i^{(1,t+1)}}{x_i^{(2,t)} - x_i^{(1,t)}} \right|.$$

The probability density function shown in Figure 3 for achieving these spread values based on the user configurable tuning parameter,  $\eta_{SBX} \geq 0$ , is [17]

$$p(\beta_i) = \frac{1}{2} (1 + \eta_{SBX}) \begin{cases} \beta_i^{\eta_{SBX}}, & \beta_i \leq 1; \\ \beta_i^{-(2+\eta_{SBX})}, & \beta_i > 1, \end{cases}$$

This probability density function is not symmetric about  $\beta_i = 1$ , and its cumulative distribution function is

$$P(\beta_i) = \frac{1}{2} \begin{cases} \beta_i^{(1+\eta_{SBX})}, & \beta_i \leq 1; \\ -\beta_i^{-(1+\eta_{SBX})}, & \beta_i > 1. \end{cases}$$

The Monte Carlo inverse transformation technique [42] with  $u_i = P(\beta_i)$  where  $u_i$  is a uniformly distributed random number between 0 and 1 is used to generate random [17, 39, 40]

$$\beta_i^r = \begin{cases} \{2u_i\}^{\left(\frac{1}{1+\eta_{SBX}}\right)}, & u_i \leq \frac{1}{2}; \\ \{2(1-u)\}^{\left(\frac{-1}{1+\eta_{SBX}}\right)}, & u_i > \frac{1}{2}. \end{cases}$$

Finally, the offspring  $x_i^{(1,t+1)}$  and  $x_i^{(2,t+1)}$  are linear combinations of the parents with  $\beta_i^r$  scaling factors [40]

$$x_i^{(1,t+1)} = \frac{1}{2} \left\{ \left( x_i^{(1,t)} + x_i^{(2,t)} \right) + \beta_i^r \left( x_i^{(1,t)} - x_i^{(2,t)} \right) \right\}, \quad (3)$$

$$x_i^{(2,t+1)} = \frac{1}{2} \left\{ \left( x_i^{(1,t)} + x_i^{(2,t)} \right) - \beta_i^r \left( x_i^{(1,t)} - x_i^{(2,t)} \right) \right\}. \quad (4)$$

This assumes the decision vectors are not bounded [40]. For bounded decision vectors, the spread is redefined to ensure that the offspring created fall within the bounds of the decision variable. The bounded version of the spread,  $\bar{\beta}_i$ , is defined relative to the upper and lower bounds on the decision variable,  $x_i^{(U)}$ , and  $x_i^{(L)}$  as [39, 40]

$$\bar{\beta}_i = 1 + 2 \frac{\min \left( x_i^{(1,t)} - x_i^{(L)}, x_i^{(2,t)} - x_i^{(L)}, x_i^{(U)} - x_i^{(1,t)}, x_i^{(U)} - x_i^{(2,t)} \right)}{\left| x_i^{(2,t+1)} - x_i^{(1,t+1)} \right|}.$$

The randomly generated  $\bar{\beta}_i^r$  is [39, 40]

$$\bar{\beta}_i^r = \begin{cases} (\alpha u_i)^{\left(\frac{1}{1+\eta_{SBX}}\right)}, & u_i \leq \frac{1}{\alpha}; \\ \{2 - \alpha u_i\}^{\left(\frac{-1}{1+\eta_{SBX}}\right)}, & u_i > \frac{1}{\alpha}. \end{cases}$$

where  $\alpha = 2 - \bar{\beta}_i^{-(1+\eta_{SBX})}$ , and  $\bar{\beta}_i^r$  is used in (3) and (4) instead of  $\beta_i^r$ .

Polynomial mutation is similar to SBX in that it uses a customizable probability density function to create a small offset that is added to a randomly selected variable in the decision vector [17]. Polynomial mutation, also, has bounded and unbounded implementations. The unbounded probability density function shown in Figure 4 is a polynomial function with the user defined tuning parameter,  $\eta_{pm} \geq 0$ , [17, 39, 40]

$$p(\delta_i) = \frac{1}{2} (1 + \eta_{pm}) (1 - |\delta_i|)^{\eta_{pm}}.$$

This function is symmetric about  $\delta_i = 0$ . For uniformly distributed  $u_i$  between 0 and 1, the randomly generated [17, 40]

$$\delta_i^r = \begin{cases} (2u_i)^{\left(\frac{1}{1+\eta_{pm}}\right)} - 1, & u_i < \frac{1}{2}; \\ 1 - \{2(1-u_i)\}^{\left(\frac{1}{1+\eta_{pm}}\right)}, & u_i \geq \frac{1}{2}. \end{cases}$$

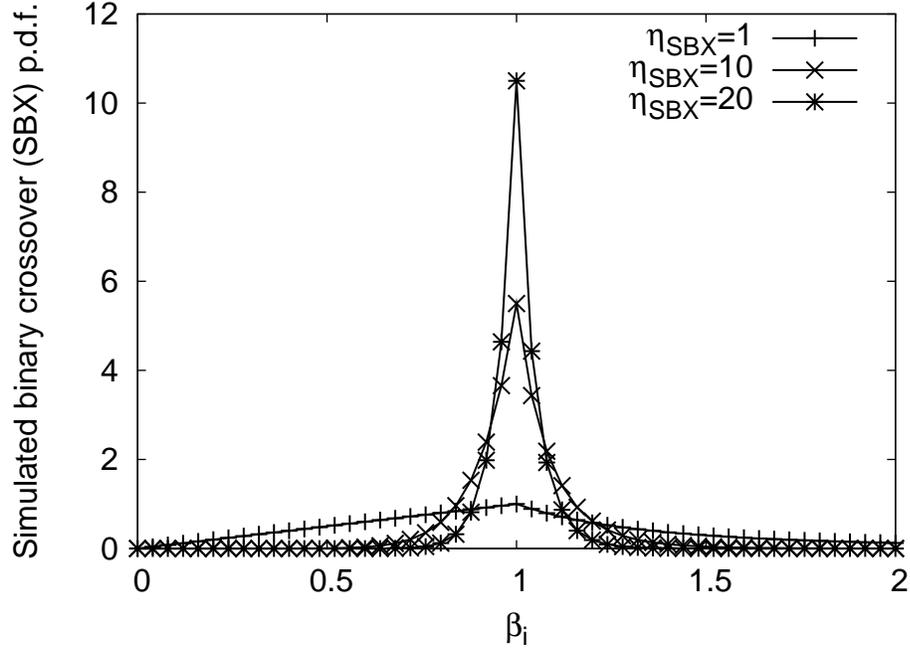


FIG. 3: Probability density function for SBX.

are used in

$$\underline{x}_i^{(1,t+1)} = x_i^{(1,t+1)} + \delta_i^r \Delta_{\max}$$

to create the mutated,  $\underline{x}_i^{(1,t+1)}$ , from  $x_i^{(1,t+1)}$  where  $\Delta_{\max}$  is the maximum change allowed. The next generation index,  $t + 1$ , is used on both sides of the equation because mutation occurs after crossover, and crossover creates two new individuals for the next generation. This means that mutation is modifying a member of the next generation. The bounded versions are [39, 40]

$$\Delta_{\max} = x_i^{(U)} - x_i^{(L)}$$

and

$$\bar{\delta}_i^r = \begin{cases} (2u_i + (1 - 2u_i)(1 - \delta)^{1+\eta_{pm}})^{\left(\frac{1}{1+\eta_{pm}}\right)} - 1, & u_i < \frac{1}{2}; \\ 1 - \{2(1 - u_i) + 2(u_i - \frac{1}{2})(1 - \delta)^{1+\eta_{pm}}\}^{\left(\frac{1}{1+\eta_{pm}}\right)}, & u_i \geq \frac{1}{2}. \end{cases}$$

where

$$\delta = \frac{\min(x_i^{(1,t+1)} - x_i^{(L)}, x_i^{(U)} - x_i^{(1,t+1)})}{x_i^{(U)} - x_i^{(L)}}.$$

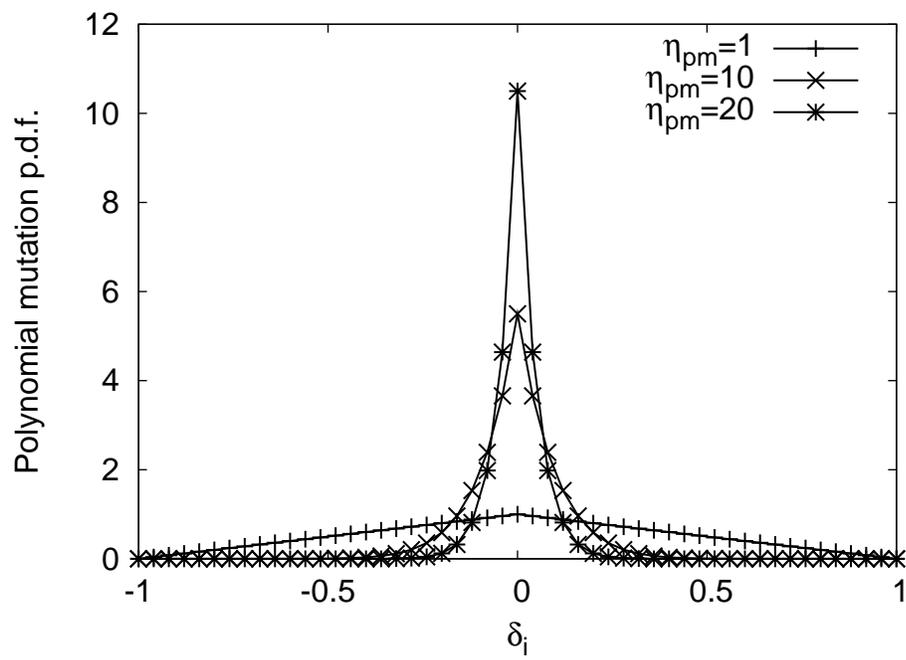


FIG. 4: Probability density function for polynomial mutation.

## CHAPTER 3

### METHODS

#### 3.1 PURPOSE

This study develops a framework that allows an injector designer to optimize the accelerating fields of an RF based electron gun concurrently with the overall injector design. This framework, based on APISA [13] from Cornell University, provides two paths for the gun design. Both approaches assume that the desired accelerating field resembles the  $\pi$  mode ( $TM_{010}$ ) of a multi-cell pillbox cavity where the phase of the accelerating field changes by  $180^\circ$  in adjacent cells. Two ancillary goals of this project are to make a system that is of general use and to use free or freely available software solutions.

#### 3.2 OPTIMIZATION TOOL HISTORY

In this section, the foundations for the optimization software design and operation are described. APISA is an extension of PISA [21] from the Computer Engineering and Networks Laboratory (TIK) of the Swiss Federal Institute of Technology (ETH) Zurich. Therefore, PISA is discussed first followed by APISA.

##### 3.2.1 PISA

PISA is a software package to use for easily evaluating the performance of various GAs and EAs against known or standard academic unconstrained MOOPs [36]. For reference, the general statement of this type of MOOP is

$$\begin{aligned} &\text{Minimize/Maximize } f_m(\mathbf{x}), & m = 1, 2, \dots, M; \\ &\text{subject to } & x_i^{(L)} \leq x_i \leq x_i^{(U)}, \quad i = 1, 2, \dots, n; \end{aligned}$$

where  $\mathbf{x}$  is a vector of  $n$  decision variables with upper and lower bounds,  $x_i^{(U)}$  and  $x_i^{(L)}$ , and  $f_m(\mathbf{x})$  are the  $M$  objective functions to optimize. While EAs differ in implementation and strategy for searching a decision variable space, they share a basic function to identify individuals in a population to seed the next generation of decision variable vectors. PISA takes advantage of this commonality to divide the process into two state machines that communicate through files [21, 38, 41] as shown

in Figure 5. One state machine identifies individuals for the mating pool and archive, and the other performs problem evaluations and generates individuals. These state machines operate under the assumption that only one state in one state machine is active at a time, and processing is coordinated with a file that acts like a semaphore.

The identification state machine, referred to as the selector [21,38,41], is the key to the success of the optimization despite its relative simplicity. Its main function is to identify individuals in the population to put in the mating pool. At a minimum this process involves calculating a fitness value for each individual in the population and selecting potential parents based on fitness and other criteria outlined in the algorithm. For algorithms like SPEA2, the selector also identifies members of the archive. All of the steps in the selector can be performed without specific knowledge of the problem under consideration because the fitness calculation is based on dominance, the relative comparison of objective values only. This means that the selector needs only objective value related information to complete its task. Specifically, it needs the total number of objective functions to consider and, for each individual, the identity information (i.e., index identification number) and the objective values.

The variator state machine provides overall control of the progression of the optimization and does the bulk of the work [21,38,41]. It keeps track of the number of generations that have run and checks for completion. It creates individuals for the population either randomly for the first generation or through recombination and mutation applied to the contents of the mating pool. Each new individual then translates into a problem model evaluation to obtain new objective values. Other information from the selector state machine such as the contents of the archive may require the variator to prune individuals from the population.

Since PISA's purpose is to study benchmark unconstrained MOOPs [41], the variator has a list of predefined problems with known multi-variable objective functions that it can optimize. The limits of the decision variable values are automatically generated for each problem. The predefined problems and generated decision vectors simplify the optimization problem configuration. Running an optimization requires the name of the problem to solve, the numbers of decision variables and objective functions to use, the maximum number of generations to produce, and quantities related to population size. The maximum number of generations is used to stop optimization processing, and the output is the decision and objective information for the individuals that form the best approximation of the Pareto-optimal front.

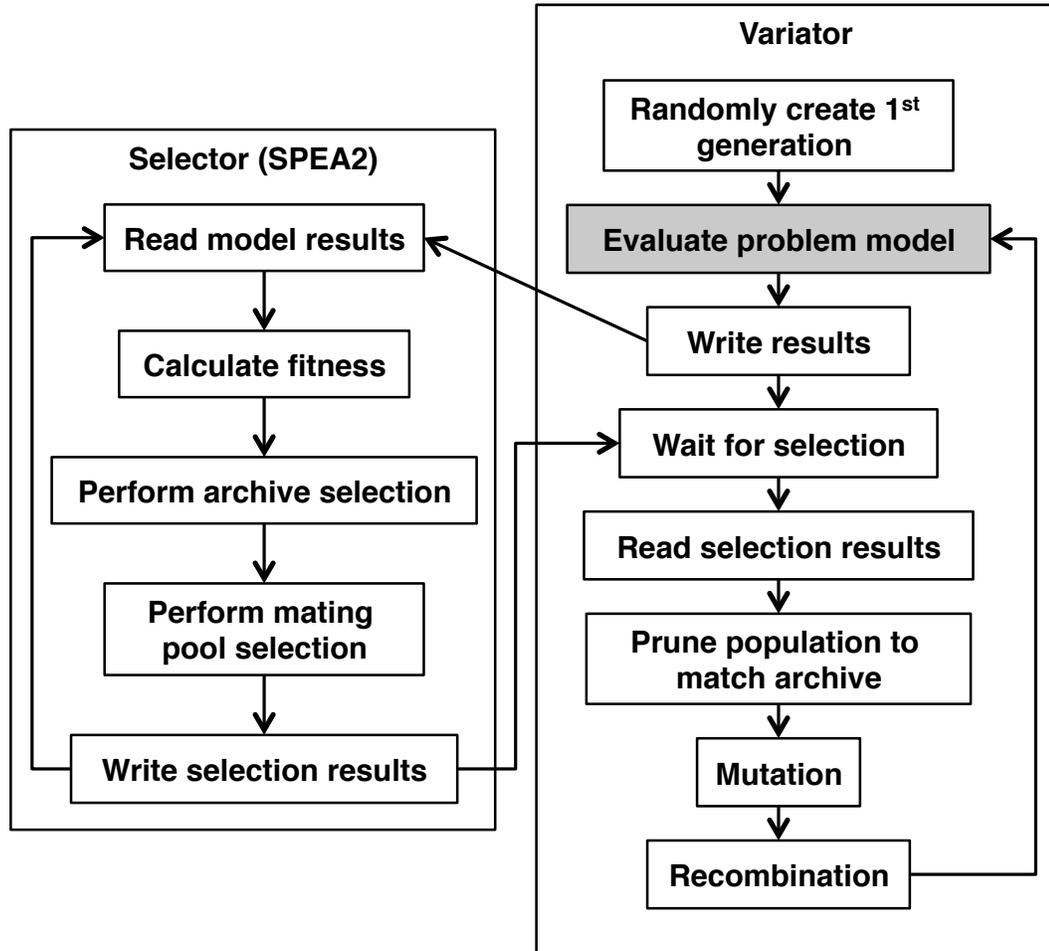


FIG. 5: The PISA state machine processes, selector and variator, communicate through a series of files. The general internal processing that takes place in each state machine is also shown. Here, the problem model evaluation is a tractable mathematical function evaluation.

PISA allows the user to control aspects of these randomized processes used in creating new individuals. There are gatekeeper parameters that are used to determine whether or not a process such as recombination or mutation will occur at all for an individual. In each application of the process, a random number is generated and compared to the gatekeeper threshold provided. If the generated number is less than or equal to the threshold, the process is allowed. The  $\eta$  parameters used in probability density functions for operations like SBX and polynomial mutation are user configurable.

The basic purpose, design, and operation of PISA have been covered.

### 3.2.2 CORNELL'S APISA

APISA [13] is PISA that has been customized for accelerator injector design since its variator runs ASTRA, an accelerator beam dynamics simulation program, and it uses ASTRA results to compute its objective function values. Figure 6 shows the details of the problem evaluation block in APISA that interfaces to ASTRA. Merging PISA and ASTRA enables injector designers to vary several parameters including the characteristics of the bunch emitted from the source, operating settings for beam line elements (e.g., amplitudes and phases), and the relative spacing of the elements in the beam line simultaneously to find optimized injector designs. Because APISA allows constraints [13], it solves a more general MOOP for injector designs

$$\begin{aligned}
 & \text{Minimize/Maximize} && f_m(\mathbf{x}), && m = 1, 2, \dots, M; \\
 & \text{subject to} && \tilde{g}_j(\mathbf{x}) > \tilde{g}_j^{(L)}, && j = 1, 2, \dots, J'; \\
 & && \tilde{g}_j(\mathbf{x}) < \tilde{g}_j^{(U)}, && j = (J' + 1), (J' + 2), \dots, J \\
 & && x_i^{(L)} \leq x_i \leq x_i^{(U)}, && i = 1, 2, \dots, n;
 \end{aligned}$$

where  $\tilde{g}_j^{(L)}$  and  $\tilde{g}_j^{(U)}$  are the bounds used in the strict inequality constraints.

PISA is designed to work with small and relatively simple problems that can be evaluated easily and very quickly, so it performs all calculations serially without a noticeable impact on execution time. Beam dynamics simulations are more CPU intensive by nature because they model the response of many charged macro-particles to the electromagnetic fields in an injector beam line. The execution time of a beam dynamics simulation increases with the number of macro-particles, the length of the beam line modeled, and the complexity and number of electromagnetic fields. For this reason, APISA takes advantage of the fact that once defined all individuals

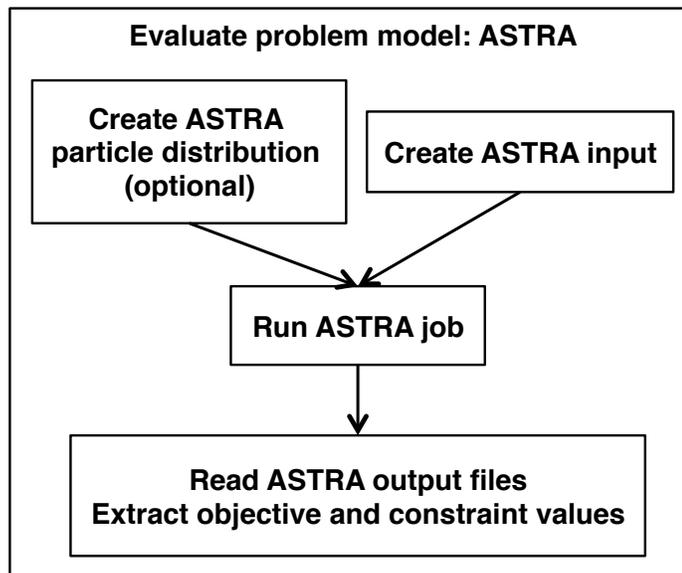


FIG. 6: APISA keeps the state machines of PISA and changes the model evaluation to run ASTRA to simulate the beam dynamics.

in a population are independent of each other [17]. Individuals can be evaluated in parallel, so APISA is designed to run in a parallel computing environment [17]. While this requires more available computer processors, it can significantly reduce the wall clock time for the evaluation of each generation in the optimization process.

ASTRA is a general-purpose injector beam dynamics simulation package and can be used to model many different injector designs. In order to retain the flexibility of ASTRA and to give the injector designer the ability to customize the optimization set up for each injector design, APISA allows the user more control of the MOOP than PISA. Because the decision variables directly translate into settings in the ASTRA input file or features of optionally APISA generated macro-particle distributions, decision variable names and their upper and lower value bounds are configurable. Decision variables may be independently varied or offset relative to another variable. The user also specifies the objective variables and the optimization goal, minimization or maximization, for each objective. Lastly, strict inequality constraints are supported, and the fitness calculation in the SPEA2 selector is expanded to incorporate the constraint related information.

As an aside, APISA employs simple arithmetic tricks [17] to concurrently accommodate minimization, maximization, and both kinds of strict inequality constraints [17]. A maximization problem can be converted into a minimization problem by multiplying the objective value by -1 and looking for the corresponding minimum objective value. Similarly, a less than constraint can be converted to a greater than constraint by first changing the constraint to be relative to zero and then again multiplying through by -1. Stated more explicitly for an arbitrary constraint variable,  $\tilde{g}_j(\mathbf{x})$ , whose value must be less than  $\tilde{g}_j^{(U)}$ :

$$\begin{aligned}\tilde{g}_j(\mathbf{x}) &< \tilde{g}_j^{(U)} \\ \tilde{g}_j(\mathbf{x}) - \tilde{g}_j^{(U)} &< 0 \\ -(\tilde{g}_j(\mathbf{x}) - \tilde{g}_j^{(U)}) &> 0 \\ \tilde{g}_j^{(U)} - \tilde{g}_j(\mathbf{x}) &> 0.\end{aligned}$$

With these two conversions, APISA reduces all problems to minimizations that are subject to strictly greater than constraints. Thus the same fitness calculation can be used for any combination of objective goals and constraints types.

### 3.3 RESEARCH ADDITIONS TO APISA

The two cavity field generation extensions to APISA and additional minor features developed for this research are covered in this section. Also, an overview of the operating environment and its impacts on the design and execution of the optimization system are provided.

To provide APISA with the ability to modify the fields provided by an RF based gun as part of an injector optimization, APISA has two methods for creating field profiles. Figure 7 shows where in the problem evaluation block the field creation systems have been added. The first method, called field morphing, morphs an idealized field profile using a truncated Fourier series [11]. This creates nonphysical field profiles since boundary conditions are ignored, but it can find field profile shapes that can be used to guide cavity geometry development. The second method, called geometry morphing, modifies a cavity geometry and uses a field solver to generate the field profile [11, 12]. For each field generation method, relevant characteristic information that can be used in the optimization as constraints or objectives is provided. These two field generation methods and additional supporting features are discussed next.

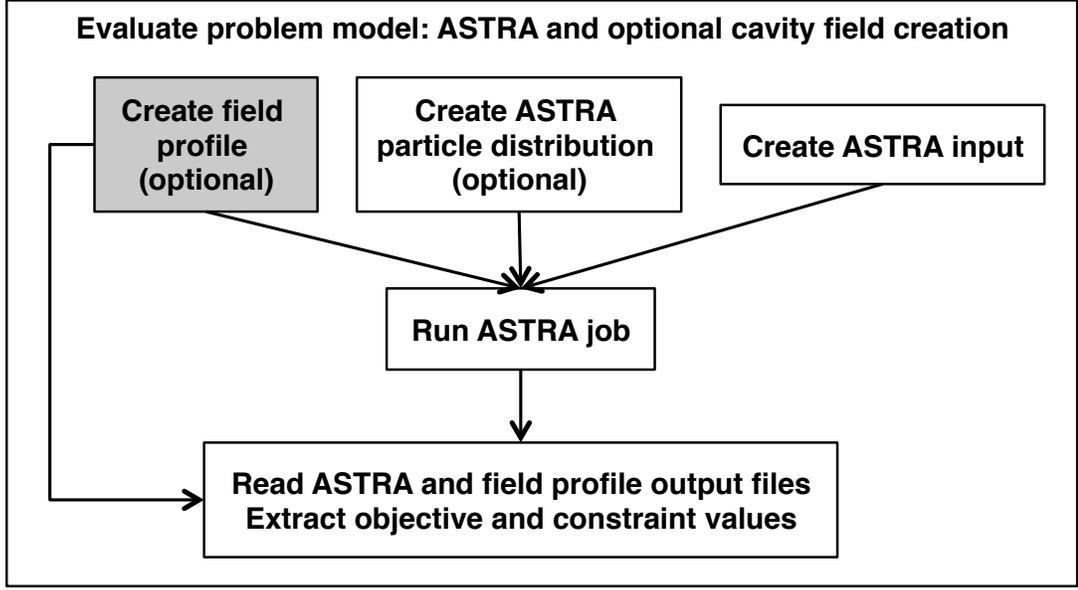


FIG. 7: APISA has been changed to now optionally produce a field profile for an RF cavity based gun.

### 3.3.1 FIELD MORPHING

In this purely theoretical method, the field profile for the field morphing method is derived from a sine wave with frequency,  $f_{source}$ . This sine wave,  $E_{\pi_{approx}}$ , roughly approximates the accelerating  $\pi$  mode in a cavity and is defined as

$$E_{\pi_{approx}}(z) = \sin\left(2\pi\frac{z}{\lambda_{source}}\right)$$

with free space wavelength,  $\lambda_{source} = c/f_{source}$ .  $E_{\pi_{approx}}(z)$  is combined with a truncated Fourier series to create an on-axis field profile,  $E_z(z)$ , to use in ASTRA. The truncated Fourier series is

$$f_{morphing}(z) = 1 + \sum_{n=1}^{15} a_n \cos\left(2\pi n \frac{z}{L_{cavity}}\right) + \sum_{n=1}^{15} b_n \sin\left(2\pi n \frac{z}{L_{cavity}}\right)$$

where  $L_{cavity}$  is the length of the cavity. The 1 in the  $f_{morphing}(z)$  expression ensures that the resulting field profile reproduces  $E_{\pi_{approx}}(z)$  when all of the Fourier coefficients are zero.  $L_{cavity}$  is found from  $\lambda_{source}$  and the number of cells in the RF cavity,  $n_{cells}$ , so

$$L_{cavity} = n_{cells} \frac{\lambda_{source}}{2}.$$

The resulting on-axis field profile is

$$E_z(z) = f_{morphing}(z) E_{\pi_{approx}}(z).$$

All parameters,  $f_{source}$ ,  $n_{cells}$ , and the Fourier coefficients, may be fixed by the user or varied by the optimization. Any unspecified Fourier coefficients default to zero. This system is intended to simulate the field in superconducting RF (SRF) and RF guns where the cathode is located at the center of the upstream wall of the first cell of the cavity. Therefore, if  $n_{cells}$  has a fractional part, it is assumed to be the gun cell and precedes any full cells. The input and output flow for the field morphing field creation block is detailed in Figure 8.

Characteristics of the resulting Fourier series function and the field profile generated are provided to the optimization and can be used in constraints or objectives. Table 1 shows some characteristics provided and the full listing is in C.5.1. An example constraint use relates to  $f_{morphing}(z)$ .  $f_{morphing}(z)$  can move the frequency of the field profile away from  $f_{source}$  by introducing additional zero crossings [11]. Since  $f_{morphing}(z)$  and  $E_{\pi_{approx}}(z)$  are multiplied together, wherever there is a zero crossing in either function, a zero crossing will appear in the result. If the optimization is to produce a cavity with a certain fixed frequency, this change is undesirable. Provided some decision variables are Fourier coefficients, a constraint requiring that  $\min[f_{morphing}(z)] > 0$  guides the optimization towards sets of Fourier coefficients that result in  $f_{morphing}(z)$ s that are positively offset from the  $f_{morphing}(z) = 0$  axis [11]. This is, of course, subject to the limits of the decision variables. These functions can still alter the frequency of the resulting field profile but not as drastically. Similarly, the frequency of  $E_z(z)$ ,  $f_{E_z}$ , can be used as a constraint and an objective simultaneously to further limit  $f_{morphing}(z)$ . If the constraint is  $f_{E_z} > f_{E_z}^{(L)}$  where  $f_{E_z}^{(L)}$  is the lower bound on the desired  $f_{E_z}$  and an objective is to minimize  $f_{E_z}$ , the optimization will, subject to the limits placed on the Fourier coefficients, move toward Fourier coefficient settings that result in  $f_{morphing}(z)$ s that produce field profiles with frequencies as close to  $f_{E_z}^{(L)}$  as possible [11].

### 3.3.2 CAVITY GEOMETRY MORPHING

In reality, the fields produced by a gun depend on the boundary geometry of the gun cells [47]. The second path follows the approach of modifying a cylindrically symmetric cavity description and using the field profile information generated by

TABLE 1: Example field profile characteristics provided by the field morphing method

Characteristic	Method of Calculation
Maximum of $E_z(z)$	$\max [E_z(z)]$
Minimum of $E_z(z)$	$\min [E_z(z)]$
Frequency of $E_z(z)$ , $f_{E_z}$	Frequency of $E_z(z)$ determined via Fast Fourier Transform [43–46]
Maximum of $f_{morphing}(z)$	$\max [f_{morphing}(z)]$
Minimum of $f_{morphing}(z)$	$\min [f_{morphing}(z)]$

the field solver Poisson Superfish [24] from Los Alamos National Laboratory. Since this method uses solutions to Maxwell’s equations for physical cavity geometries and boundary conditions, the field profiles produced are more realistic than the idealized field profiles of the field morphing method. This section discusses how Poisson Superfish is incorporated into APISA. There are three parts. The first is a general cavity geometry description with named parts that can be easily modified by the optimization software. The second component is a translation that converts the geometry description to Poisson Superfish’s geometry description. Lastly, there is a set of programs that encapsulates the Poisson Superfish processing to produce a field profile to use in ASTRA simulations and a list of cavity field characteristics and figures of merit for the optimization to use in constraints and objectives. These will all be discussed in turn following a brief overview of Poisson Superfish and its suitability for this optimization system.

### Poisson Superfish overview

Poisson Superfish [48] is a field solver commonly used in accelerator physics to calculate electromagnetic fields for RF cavities and magnets. It is written in FORTRAN. It uses the FORTRAN namelist input format and produces binary formatted and text output. For RF cavities, it assumes the geometry is cylindrically symmetric. This means it only needs a description of the cross-section of the top half of the cavity geometry to find the fields in the cavity. It creates physical and logical triangular meshes on which it solves the Helmholtz equation to calculate the fields (discussed in B.2). A fictitious magnetic current density is used to excite the fields in the cavity.

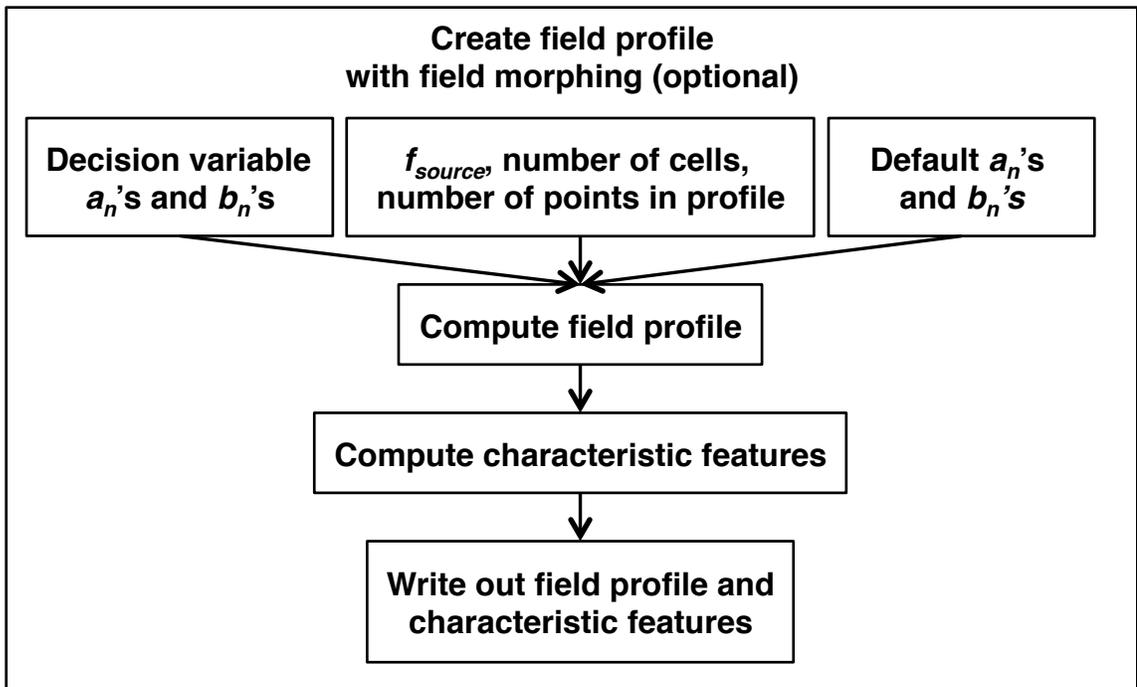


FIG. 8: Field morphing flow chart.

On resonance, when the energy transfer between the electric and magnetic fields is balanced, this magnetic current density goes to zero as it should. It, also, calculates several characteristics of the field and figures of merit.

There are several benefits to using Poisson Superfish. The first is that it is freely available in the United States [24]. This satisfies a goal of this optimization software design to use free or essentially free software. It is a standard in the accelerator community and has long been used to design and model RF cavities. It computes the fields and characteristics fairly quickly making it a good candidate field solver to use in a system that needs to calculate the fields for hundreds of cavity geometries per generation in a timely fashion.

From the standpoint of running the optimization, the main drawback to Poisson Superfish is that, while it once ran on several different platforms including linux, it now runs only in a Windows environment [15]. The optimization software is designed to run in a linux environment since at present virtually all large-scale computing facilities are linux based. This means some software framework is needed to enable

Poisson Superfish to run under linux. The solution to this using Wine [49,50], a freely available environment for running Windows executables in other operating system environments, and Xvfb [51,52], the X Windows virtual frame buffer, is discussed in detail subsequently.

### **Cavity description**

A Poisson Superfish geometry description is essentially an ordered list of points, lines, and curves that form a set of closed areas that represent a cross-section of the electromagnetic field producing device [48]. The very general nonspecific nature of the description poses challenges for incorporating it into the optimization software. Examples of the challenges and the solution used in this research to address them are presented.

Without plotting the lines and curves in a Poisson Superfish geometry description, it is not always obvious what shape or shapes the geometry description represents. Further, for RF cavity representations, matching the lines and curves of the geometry description to the physical parts of a cavity can be difficult, even for simple designs, because the geometry description provides no clues as to what part of the cavity structure a set of lines and curves depicts. For the optimization software to change the geometry description directly, it needs to be able to automate this identification process. For example, to change the radius of one cell in a multi-cell cavity, the optimization first needs to know which parts of the description are associated with the particular cell to be changed. It then needs to know which subset of those lines and curves depend on the radius of the cell. Finally, it has to compute changes for each of these elements and generate a new geometry description. This requires some a priori knowledge of the desired final cavity shape and restrictions on how the lines, points, and curve elements are used to create it. This can lead to limitations on the types of cavities that the optimization can be applied to since the specifics of each cavity type have to be translated into a set of rules that the optimization can use to identify the cavity type and its components [48].

Because the lines and curves in the ordered list use a combination of absolute and relative position information [48], another complication is that adding or making a change to one part of the description may require changes to all downstream components. For example, increasing the length of a cavity cell shifts the positions of downstream elements, and those positions must also be updated. Unlike the radius

change example above where the changes are limited to the cell to be changed, this simple cell length change is not localized. This can be further complicated if there is interplay resulting from other changes.

These challenges can be recast differently. Although not explicitly stated, the optimization needs a name for what it will change in the cavity geometry to fit in the decision vector model [12]. It also needs to know how to propagate that named change into the many possible required changes in the geometry description. The foregoing discussion outlines the challenges related to designing the optimization to directly manipulate the Poisson Superfish geometry description. The solution then is to separate the details of Poisson Superfish’s geometry description from the optimization software. This can be accomplished with a cavity description based on cavity structural elements and their dimensions that can be translated into a Poisson Superfish geometry description.

This cavity geometry description assumes cavities are built from two elements, tubes and cells [12]. The cell parameters are shown in Figure 9. Each self-contained element is named and is described by a list of named dimensions, offsets, and angles. The cavity is, then, described with an ordered list of these cavity building blocks that are together converted to a Poisson Superfish file. The first benefit of this description approach is that each aspect of the cavity geometry has a name. It also makes it easy to change or add elements to the description since the individual elements are independent of each other. Adding or changing a building block element may require minor changes to neighboring elements, but the changes only involve simple value substitutions and are limited to the elements on either side. For example, if the radius of a beam tube is changed, it may be necessary to change the exit iris radius of the upstream cavity element and the entrance iris radius of the downstream element. Otherwise, adding an element is just a matter of inserting the building block describing the element in the appropriate position in the description. The optimization though does not add or remove building blocks. For each optimization, the number, types, and order of the building blocks are fixed. However, the optimization can change settings in the description, and using a feature described in 3.3.3 and C.5.2, it can perform any related substitutions as directed in the optimization decision variable configuration.

Although the geometry translation only produces straight-line cavity geometries [11,12], the cavity geometry description is flexible and allows the geometry of a cavity

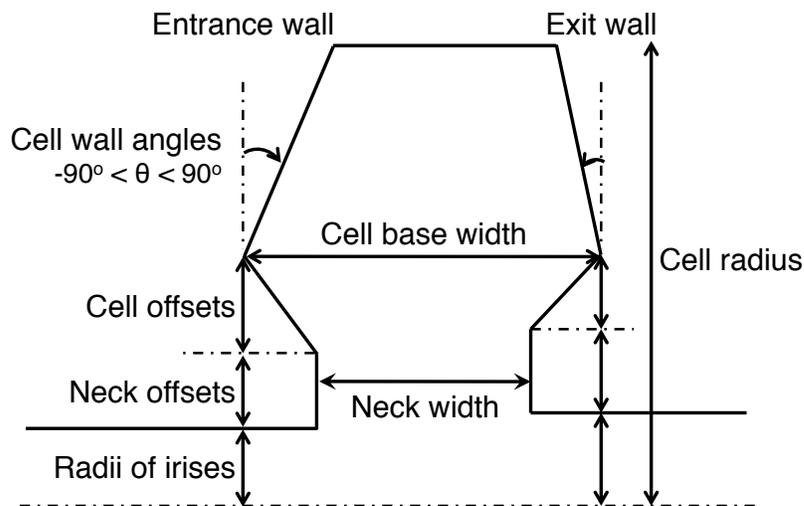


FIG. 9: Cell geometry parameters and cavity layout [12].

to morph easily from one general form to another. The main cavity cell type used in this research is the pillbox cavity used in RF guns, and it can be extended easily to its elliptical cavity counterpart used in SRF guns. Both of these geometries produce simple accelerating mode fields. A pillbox cell can be described simply by its radius and length since it is a right cylinder. Because the cavity description is designed to produce the features of several cavity types, it contains more dimensions than the radius and length, and these have to be set for completeness. A rough approximation of an elliptical cavity can be made from a pillbox cavity if the walls or end caps are allowed to tilt toward each other. Another cavity type, called re-entrant, can be modeled with the end cap cones tilted away from each other. Examples of all three are shown in Figure 10.

Some Poisson Superfish specific information is included in the geometry description because the information is necessary to the operation of Poisson Superfish [48]. The first is related to frequency. In Poisson Superfish, the `FREQ` namelist variable is often thought of as the desired resonance frequency of the geometry, but it is subtly different from that. In reality it is used by Poisson Superfish to decide where to search for the resonance frequency [48]. Often, it turns out that this search frequency is the resonance frequency, but it is not guaranteed. The frequency building block in this description is used in the same way and is referred to as the search frequency.

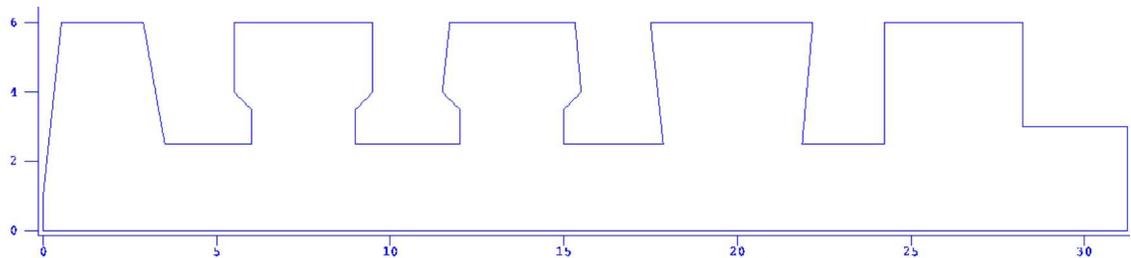


FIG. 10: Straight line approximations of various cavity cell types. Here are an elliptical (far left), three re-entrant (middle three), and pillbox (far right) cell geometries for Poisson Superfish. These cavities are cylindrically symmetric about the x-axis. Length units are cm for both axes. The radius for each cell is 6 cm, and the total length of the structure is 31.2 cm.

It is a required block in the geometry description. The other relates to the fictitious magnetic current density used in Poisson Superfish [48]. This magnetic current density needs to have an identified source location in the geometry. This source location is called the drive point because it is used to drive the field excitation in the cavity. The geometry translator calculates the exact position of the drive point location, but there is a building block that can be used to indicate in which element the drive point should be placed initially. The program discussed below that APISA uses to run Poisson Superfish uses this block. This block is not required because Poisson Superfish will generate a drive point location if one is not provided, but it may not choose the best location.

The translation of the high-level cavity geometry description to the Poisson Superfish description presently creates cavity geometries constructed with straight lines and sharp corners using a list of points. Physical cavities have rounded corners and are composed of curved and straight lines, but straight-line cavities while not practical to build and operate can be used to perform preliminary design studies. Poisson Superfish requires the cross-section described in its geometry description file to be a simple closed surface [48]. Simple means that the lines and curves that make up the cross-section do not intersect each other except at endpoints where two are connected [53]. The outline or perimeter of a five-pointed star is a simple polygon, but a hand-drawn five-pointed star as shown in Figure 11 where each side of the star crosses two other sides of the star is not a simple polygon. Clearly, one determining

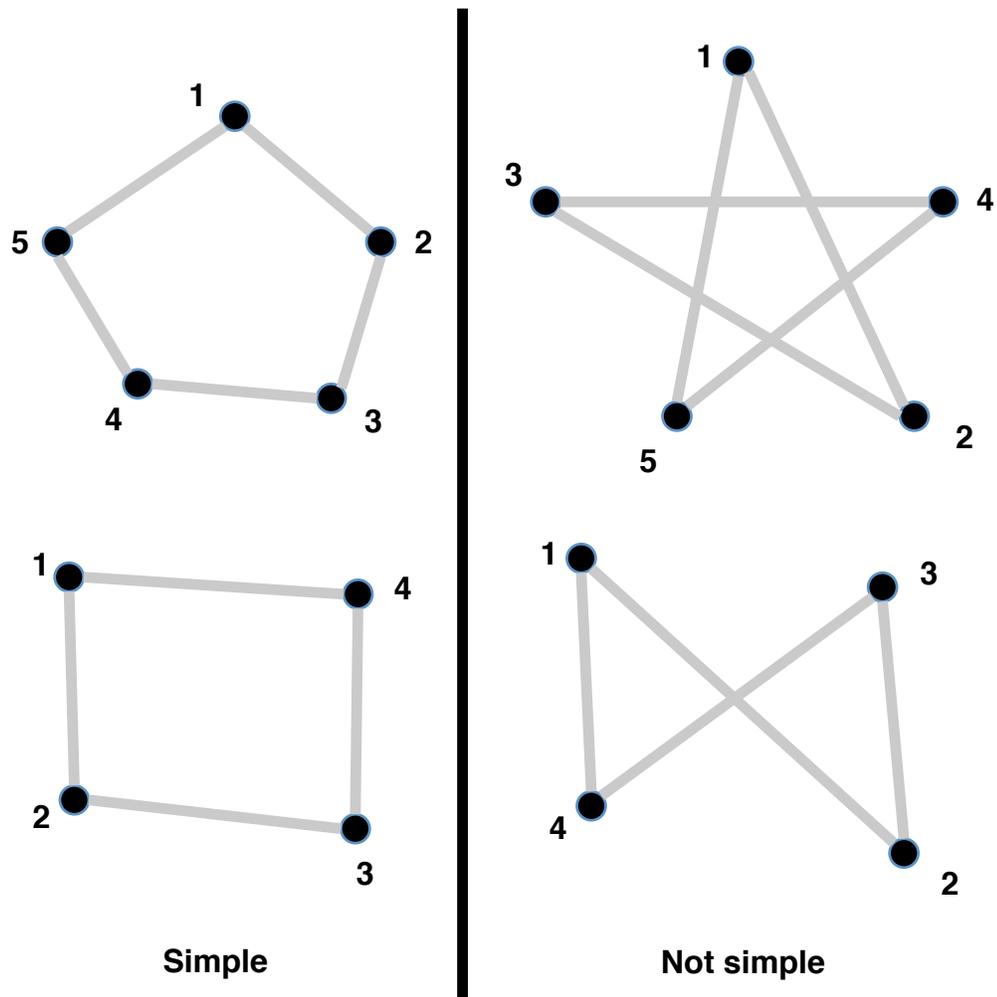


FIG. 11: Examples of simple and not simple polygons.

factor for simplicity is the order in which the points are connected. The translator checks that the points calculated from the high-level geometry description form a simple polygon [53] and writes out the Poisson Superfish geometry file only if the polygon is simple.

The translator has additional features. The first is that it converts the units named in the high-level description to the defaults preferred by Poisson Superfish (namely MHz for frequency and cm for length) and the translator (radians for angles). A second is that it adds spool pieces (beam tubes) to the cavity irises as necessary to minimize the possibility of the cell profile overlapping an adjacent cell

and creating a non-simple cross-section. This is useful for re-entrant style cavities that have dumbbell shaped cross-sections. Lastly, it identifies potential cavity sections for drive point placement and calculates drive point positions.

For APISA, the geometry translation and Poisson Superfish processing are combined into one program called `ps_tuner` [12]. The field creation block with `ps_tuner` for cavity morphing is shown in Figure 12. Basically, this program takes a geometry description as an input and produces a field profile and relevant characteristics. It aims to find a  $\pi$  mode, but if it is unsuccessful, it provides a minimal  $E_z(z) = 0$  profile. The search for the  $\pi$  mode is a multi-step process. First, it determines which elements in the geometry description can be used for drive point locations. If a drive point location is provided, it is placed first in the list of candidate drive point elements. The frequency block information is used to produce a list of five candidate search frequencies to use in Poisson Superfish. The first is taken from the frequency block, and the other four are at 50 MHz intervals centered on that designated frequency. For each combination of drive point element location and search frequency, the program generates a Poisson Superfish geometry description, calls the necessary Poisson Superfish programs, extracts the field profile and other related information from the Poisson Superfish output files, calculates any additional characteristics, and then checks for a  $\pi$  mode. The on-axis profile for a  $\pi$  mode has one fewer zero-crossings than cells. A 1.5 cell cavity is considered to have two cells, and its  $\pi$  mode field profile has one zero-crossing. The cycle stops once a  $\pi$  mode is found or the drive point and search frequencies combinations are exhausted. In the latter case, the  $E_z(z) = 0$  profile is produced. Otherwise the  $\pi$  mode field profile and its characteristics are written to files.

As mentioned previously, Wine [49], formerly known as “Wine is not an emulator,” and Xvfb [51] are used together to create an environment under linux [54] to run Poisson Superfish [11]. In keeping with the goal of using free software, Wine and Xvfb are freely available and often provided as part of a standard linux installation. A brief overview of each product and how it works with Poisson Superfish is provided, followed by a description of the system used in APISA.

Wine creates a Windows like environment including a Windows file system structure [49]. Files may be accessed using the Windows or linux path conventions. Installing a Windows program under Wine is the same as under Windows. The installer that comes with the Windows compatible program such as Poisson Superfish is used

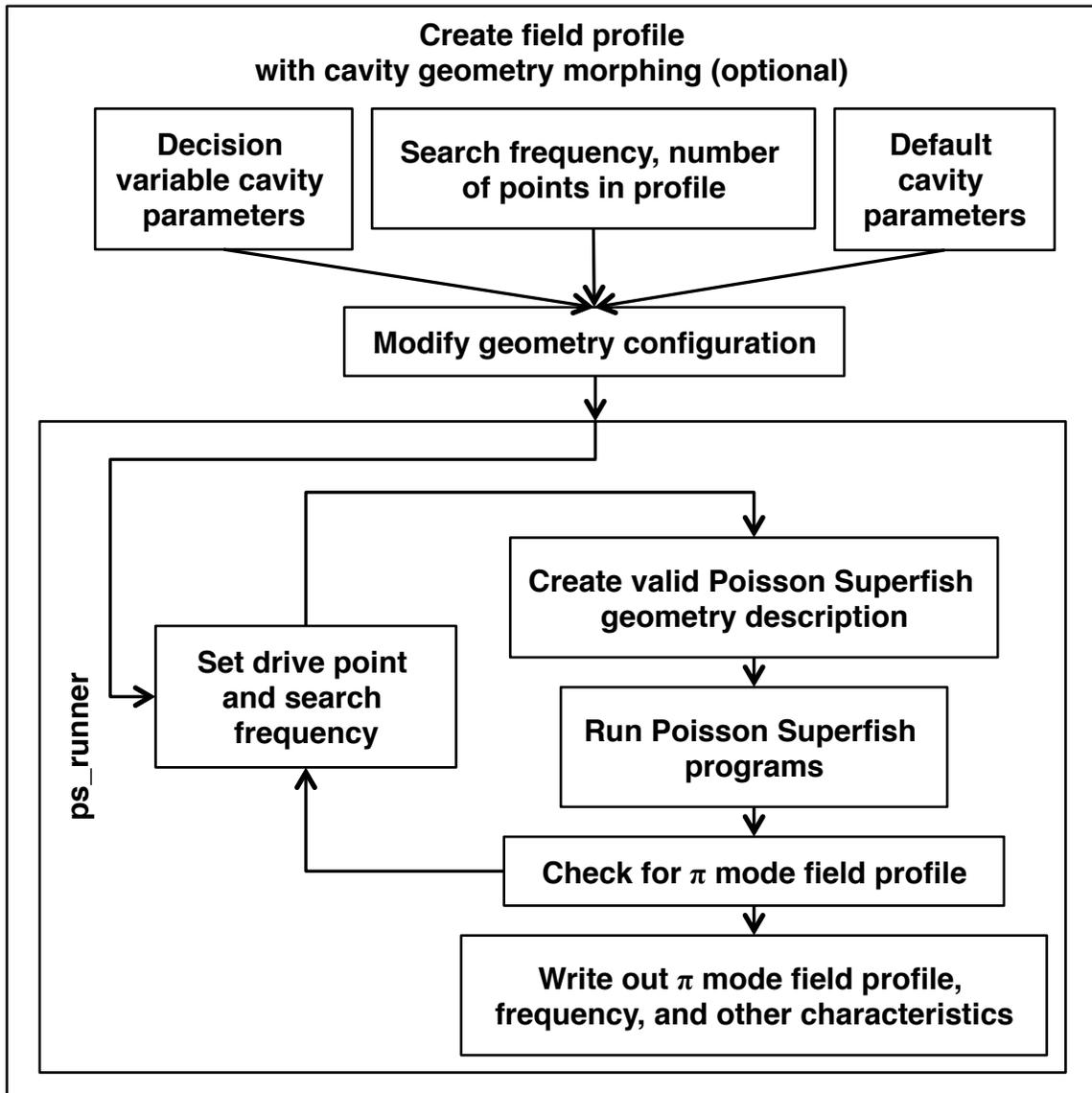


FIG. 12: Cavity morphing flow chart.

in both cases. Wine translates the Windows calls including the graphics ones to compatible calls for the host operating system. For linux systems, the non-graphics calls are mainly converted to linux system calls, and the graphics calls are translated to X Windows calls; the low-level windowing graphics package that is available on linux. Poisson Superfish runs in Wine, albeit more slowly than in its native Windows environment. The performance impact is noticeable but not significant. Wine is sufficient to run Poisson Superfish in a linux environment.

Poisson Superfish runs with a graphical interface, and it is not possible to run it without the graphical interface. The graphics output must be handled in order for Poisson Superfish to run in the monitor-less linux environment commonly used for large-scale high performance computer systems. Xvfb can be used as a monitor for Poisson Superfish [55]. As part of the X Windows system, it is normally used in tests of the X Windows software. It acts just like an X Windows display with the added benefit that a display number can be assigned to it when it is launched. It can receive X Window graphics directed to its display number without displaying them. It can even be used as a bit bucket for graphics output! Given the display number attached to an Xvfb process, Wine can run Poisson Superfish and redirect the graphics output to Xvfb.

With the basic issues of running Poisson Superfish in a linux environment addressed, the focus switches to the challenges of running these programs on a large scale. One limitation of Wine is that its low level server can only direct its graphics output to a single display, regardless of the number of graphics producing programs it is running [52]. This means when multiple instances of Poisson Superfish in Wine are running on a computer, only one Xvfb process can be used to receive all of the graphics. Since ASTRA and Poisson Superfish are single threaded programs, a single running instance of either program cannot use more than one processor in a multi-processor computer. However, multiple concurrently running instances can consume several processors. That is how APISA distributes processing to best take advantage of the multi-processor nodes in a cluster computer environment. This means, though, that APISA must start only one Xvfb process for each set of Poisson Superfish runs on a multi-processor computer. In reality, it launches multiple `ps_tuner` programs, but the Xvfb restriction remains. The launching of Xvfb is managed with a program called `xvfb_manager`. This program takes care of launching Xvfb, searching for an available display number to use, and writing the display

information to a file. If `xvfb_manager` is run subsequently, it will check for an Xvfb process using the recorded display information and relaunch it if it is not running. The program can also be used to kill an Xvfb process. The display information in the file is also used by the program `ps_tuner` when it launches Poisson Superfish with Wine. To ensure that Xvfb is running before launching a `ps_tuner` run, APISA launches an `xvfb_manager`. This leads to several concurrently running instances of `xvfb_manager`, but they avoid interfering with each other through the use of a lock file.

### 3.3.3 OPTIMIZATION OPERATION CUSTOMIZATIONS

This section covers minor additions made to APISA to support this research effort.

#### Particle loss allowances

ASTRA simulates the electron bunch using macro-particles. Depending on how an injector is configured either in physical layout or settings (gradient, amplitude, and phase setpoints), particles in the bunch may traverse the entire beam line, or they may be lost at various points. In most cases, all of the beam particles are supposed to transport through the beam line, but sometimes beam loss is deliberate as in a beam chopping slit system. ASTRA tracks five particle loss mechanisms [22]. One is loss due to particles intercepting apertures in the beam line. One is specific to ASTRA processing. There is a subset of particles in the particle distribution that ASTRA designates as passive particles. The loss of any of these particles is tracked separately from the rest of the particles in the distribution. Losses due to improper RF phasing errors are tallied either as backward traveling particles or particles that travel backwards past the starting position of the simulation. The last mechanism is due the cathode field. At the end of the simulation, ASTRA reports the number of particles lost due to each mechanism.

For most beam lines, particle losses indicate that the settings for the electromagnetic elements in the beam line are not set properly, and APISA from Cornell adheres to that model. It marks simulations with particle losses as invalid and sets all ASTRA related results to a large value. Unfortunately, if every individual in a generation is invalid, then the optimization has no useful information to guide its search since all individuals independent of the decision variable settings look the same from the objective and constraints perspective. For a beam line where full

beam transmission is expected, all invalid individuals indicate that the choice of decision variables is wrong, their ranges are incorrect, or some fixed parameters are set incorrectly. For beam lines that expect losses, the decision variable and fixed settings may be correct, but the optimization will fail. Allowing particle losses is useful for these cases. This version of APISA provides access to the particle loss tallies from ASTRA. Each loss mechanism can be independently allowed or disallowed, and the tallies for the allowed loss mechanisms can be used in constraints and objectives in the optimization.

### **Peak field rescaling**

Cornell’s APISA uses the same field profiles in the beam line for each individual throughout the optimization. It can vary the amplitude scaling for these profiles, and for RF cavity fields, it can change phases. The amplitude scaling in ASTRA is changed with a peak amplitude scale factor. The field profile is scaled so that the largest peak in the profile matches the scale factor. The relative shape of the field profile, though, is fixed. When APISA changes the peak amplitude scale factor for a fixed field profile, the same peak in the same relative position in the field profile is scaled each time. The change scales the field profile in a deterministic way for each individual. This is not necessarily true for fields generated using either the field or geometry morphing method developed for this research. It is very likely that the field profiles are different for each individual. For fields produced using these methods, the relative amplitudes of the peaks can be different. This complicates the effect of the peak amplitude scale factor even when the scale factor is fixed. This is because, unlike in the fixed field profile case, the relative location of the largest peak can be different for each individual. The sameness of the fixed field case is lost. A feature added to APISA addresses the ambiguity introduced with the different field profiles [44–46]. APISA can now optionally rescale the peak amplitude scale factor. The peak amplitude scale factor can be increased or decreased to ensure that a particular peak, for example the first peak, is scaled to the original desired setting of the amplitude scale factor. Thus, for an optimization where the peak scale factor is fixed (i.e. not a decision variable), the actual value used in the ASTRA input file may change to guarantee that a selected peak, which may not be the largest in amplitude, has a fixed value.

### **Fixing the field profile frequency in ASTRA input files**

Another option related to the difference in possible fields applies to the frequency of the field used in the ASTRA simulations. As the optimization changes parameters that affect the cavity field profile, the frequency of the field profile can change. This may not be desirable, for example, if the purpose of the optimization is to consider the effect of field profile shapes for a fixed frequency. ASTRA does not crosscheck the frequency provided in the input file against the frequency of the field profile. This means that the frequency in the ASTRA input file can be held fixed while the field generation method produces various field profiles of different frequencies. For the cavity geometry morphing method, the cavity geometry for the desired fixed frequency can be created from the geometry of the cavity that produced the field profile. Scaling the dimensions of the source geometry by a ratio of the desired fixed frequency and the source cavity frequency results in a geometry with the same field characteristics as the source geometry but at the desired frequency. This version of APISA can be directed to update the ASTRA file with the frequency of the field profile or leave it fixed.

### **Linear relationships for decision variables**

The last new feature pertains to setting decision variables. Cornell's APISA allows a decision variable to be offset relative to another decision variable [13]. This capability is extended to allow linear relationships with the addition of a slope factor, but there are two minor differences between these methods. The first is that each variable set using Cornell's offset method is counted as an optimization decision variable since the offset is generated by the optimization. This can cause problems for optimizations with a large number of related input parameters to change because the number of optimization decision variables is limited. Variables set using the linear relationship method are not counted as optimization decision variables. The slope and offset for the linearly set variables are fixed, so these linearly set variables do not change independently in a randomized fashion as with the offset variables. For two variables where one is linearly dependent on the other, the decision variable count is one since only one variable is set using the randomized processes of the optimization. The other difference is that the offset method has user configurable upper and lower bounds that the optimization must obey. There are no explicit limits for the linearly set

variables. They are instead determined by the limits of the independent variable and the linear relationship.

The linear relationship method for setting variables opens up the optimization to allow variables to track decision variables. This means that a variable can be set to the negative value of a decision variable. This is useful for creating, for example, re-entrant or elliptical cavity approximations with walls that have the same but opposite tilt angles. The tilt angle of one wall is a decision variable set directly by the optimization, and the angle of the other wall is calculated from the linear relationship where the slope is -1 and the offset is zero. This is the mechanism mentioned previously in 3.3.2 that directs the optimizer to propagate cavity dimension decision variable changes such as the beam tube iris to neighboring elements.

### 3.4 COMPUTATION ENVIRONMENT CONSIDERATIONS

Cornell's APISA is written in C++ and is designed to run in a linux environment. Since individuals in a generation are independent, it parallelizes the problem evaluation portion of the variator processing by dispatching each problem evaluation to a computer that shares a file system with the computer running the variator and selector state machines. The common file system is necessary because the information used by the various parts of the system is stored in or conveyed through files [13]. For each generation, several problem evaluations are needed to compute the objective values for the individuals in the population, and this points to the need for access to many processors. APISA can operate in different environments that meet these requirements. For example, for small problems with only a few individuals in each generation, APISA can run on a single multi-processor computer. For large problems, though, cluster computers are a more suitable choice.

Cluster computer designs vary in the details with regard to how the hardware is connected together, but they all have a common basic design [56]. They take advantage of the low-cost yet powerful computing capabilities of PC processors. The basic design connects thousands of these low-cost processors together with dedicated high-speed, high-throughput networks. These machines are designed to tackle computationally intensive problems like weather modeling, weapons simulations, or lattice gauge calculations in quantum chromodynamics [57]. For these problems, calculations are analyzed to see if they can be parallelized to speed up the overall

computation, and the programs are written accordingly using specialized software libraries to parallelize the computations and to move and share data among the nodes quickly [16].

APISA is not that kind of parallel computing program. It is a distributed computing program, and it uses a cluster computer as a dedicated single user computer batch farm [13]. A batch farm is a collection of stand-alone processors to which users submit jobs for execution. In a traditional batch farm, the job dispatch system acts as a gatekeeper. It schedules jobs for a user based on the user's available time allotment and usage history, and at Jefferson Lab this is known as Fairshare allotment [58]. This guarantees that access to the batch farm, a shared resource, is reasonable for all users. If a user submits many jobs over a short period of time after a long period of inactivity, the dispatch system will give preference to scheduling these jobs over those from another user who submits jobs regularly. While the regular user's jobs may spend more time than usual in the job queue during this period of time, in the long term, the access for both users is the same. This job throttling makes a traditional batch farm unattractive for running APISA. To work with a traditional batch farm, the variator and selector state machines run outside the batch farm, and the variator state machine submits the problem evaluation jobs to the batch farm. APISA needs to run many problem evaluation jobs for each generation, and depending on the number of individuals per generation, the job dispatch system can introduce extended periods of inactivity holding APISA jobs in queues. Thus, the throttling can extend the time it takes APISA to complete a generation and the entire optimization.

Cluster computers also have job dispatch management systems that operate under the same guidelines. The difference is that since the number of available processors is so high—thousands, compared to hundreds—each user can ask for a larger number of processors for each job, and during the time the job is running, the user's application has unfettered access to all of the processors assigned to the job [59,60]. This means a properly configured APISA optimization will run to completion in the time allotted to the job without interruption.

Two APISA parameters that need to be balanced against the available cluster computer resources are the number of individuals per generation and the number of generations. The number of individuals influences the number of processors requested, and the number of generations impacts the time requested. There are several

cluster resource factors to consider.

One consideration is how the processors are grouped (quad core or dual core). For Jefferson Lab's cluster computers, if one core of a multi-core processor is assigned to a job, the remaining processors are unavailable to other jobs until the one core job is finished. For most efficient use of the cluster computer processors, it is best to adjust the number of individuals to be an even multiple of the processor groupings.

To minimize delays between submitted jobs due to the Fairshare system, the total number of processors in use at anytime should not exceed the number of processors owned by the user. At Jefferson Lab, when groups pay for time on the cluster computers, they are buying access to a given number of processors, and the processors for the various cluster computers carry different usage weights. Processors in a newer cluster computer are more expensive to use than those in an older cluster computer. Since processor performance is not critical to APISA processing, an APISA job can run on an older cluster computer and have access to a larger number of processors. For example, successive optimizations for this research can run without delays from the Fairshare system on a maximum of 96 processors of the older (7n) cluster [60]. This number of processors takes into account the fact that 7n computers each contain two quad core processors.

The last cluster computer related factors are job time limits. The maximum time that a single job can run continuously is 48 hours. Time limits tie into the maximum number of generations that APISA can run in a single job.

The basic game for sizing an APISA job to the limits imposed by the cluster computer system is to ensure that the product of the number of generations, the number of individuals per generation, and the time to evaluate one individual is less than or equal to the product of the number of Fairshare allotment CPUs for the particular computer and the maximum time limit. Using this research's Fairshare allotment, if it takes 30 minutes to evaluate one individual on average, then at most 96 generations can be run on the 96 cores in a 48 hour long job. To double the number of individuals, the number of generations must be halved.

## CHAPTER 4

### VERIFICATION

#### 4.1 BENCHMARK INJECTOR MODEL

Before proceeding with optimization, it is prudent to ensure that the model of the target injector used in the optimization is reasonable. The PITZ RF gun is well documented with simulations and measurements. It also has a simple beam line with only three electromagnetic elements, the RF gun cavity and two solenoids. Combined these features make the PITZ gun a good candidate for study. To verify the simulation model, this research reproduces a solenoid magnet strength and RF phase parameter scan published in [7].

In this numerical experiment, the beam emittance is calculated at a beam diagnostic location downstream of the gun cathode while the RF gun phase and main solenoid strength are varied [7]. Its purpose is to identify the RF gun phase and main solenoid strength settings to achieve minimum transverse emittance at the beam diagnostic for a fixed peak RF gun amplitude or gradient. The RF gun gradient is 40 MV/m. The layout used in simulations is shown in Figure 13. The beam enclosure is removed as shown, and the particles travel through fields and free space. The RF gun cavity is 0.265 m in length, and the 1.5 cells occupy the first 0.175 m followed by a beam tube and coaxial coupler. The gun cathode and beam diagnostic are 1.618 m apart. The main solenoid is after the full cell of the gun, and its center is located 0.276 m from the cathode. The bucking solenoid located just upstream of the gun is off and not used in this experiment. The emittance in the ASTRA simulation is available at any point along the beam line because it can be calculated from statistical moments of the particle distribution using (1). In the physical machine, it is measured with a slit device.

The reference phase in this experiment for the RF gun is the phase that gives the beam the most energy gain. RF guns do not operate at this phase [7]. Nonetheless, it is a useful reference because it can be easily found with beam based measurements in a physical machine using a magnetic spectrometer. This reference phase is often referred to as the crest phase, and operating a cavity for maximum energy gain is termed running on crest. In the experiment, the RF phase is varied  $\pm 10^\circ$  from the

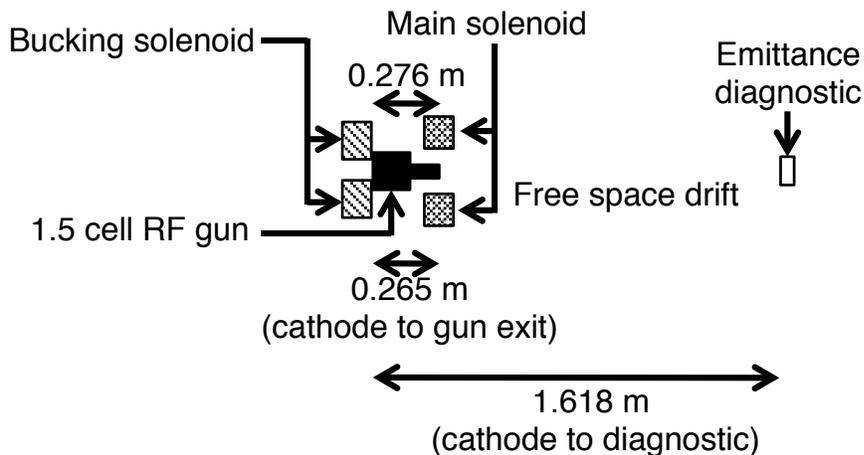


FIG. 13: Layout of front end of the PITZ diagnostic beam line [7].

TABLE 2: Main solenoid settings

Solenoid setting	Amps	Tesla
Start	285	-0.1676876
Focus at emittance diagnostic [10]	290	-0.1706231
End	305	-0.1794296

crest phase. The results presented here follow this convention.

The reference setting used for the solenoid focuses the beam to a small spot at the location of the downstream emittance beam diagnostic [7]. To facilitate comparisons with different published results for this parameter scan, the solenoid setpoint is quoted in Amps. In the APISA optimizations to follow, though, the setpoint is in Tesla. Based on measurements at PITZ, the calibration between the two is linear [61, 62], and Table 2 shows some representative values used in these parameter scans. The 20 A solenoid setting variation is not symmetric like the RF phase variation. Instead, it varies from 5 A below the reference to 15 A above.

An initial report of this benchmark effort appears in [10]. The parameter scan presented there matches the patterns and trends in the PITZ work [7]. It does not

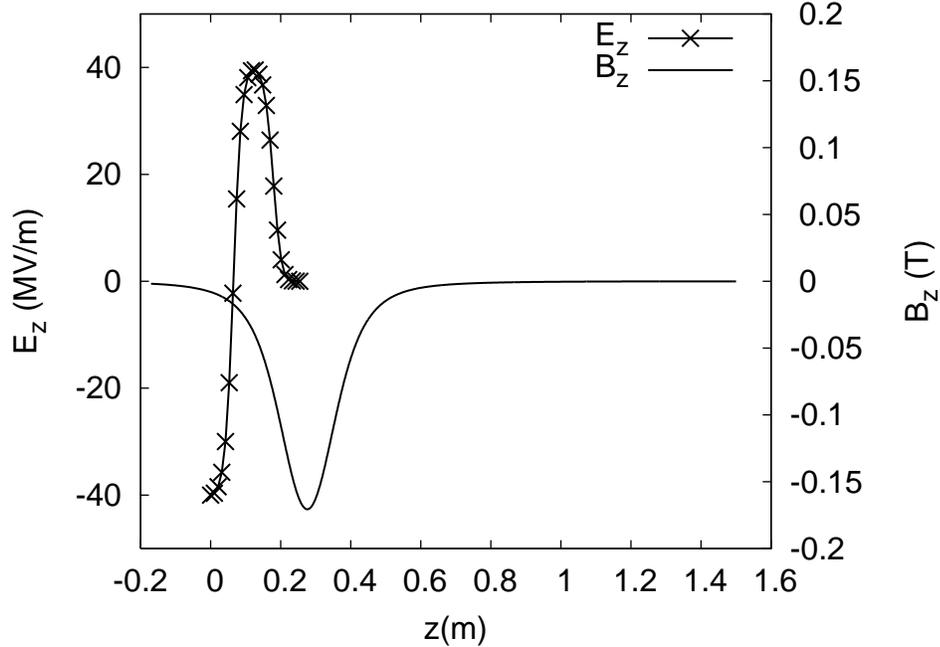


FIG. 14: Field profiles used in previous work [10,63]. The  $E_z$  vs.  $z$  on-axis profile is for the RF gun and is a snapshot of the time varying field. The  $B_z$  vs.  $z$  on-axis profile is for the main solenoid and is static. Its peak value is scaled to the setting that focuses the beam on the emittance diagnostic in Table 2. The solenoid profile is used elsewhere in this research.

exactly reproduce the original but is sufficiently close to validate the model. The model in [10] uses the same geometry information for the RF gun and solenoid as the PITZ work [63] to create the field profiles used in the simulations. These profiles are shown in Figure 14. Some discrepancies in the initial work may have affected the results. These include using a higher bunch charge and slight differences in the ASTRA macro-particle distributions. Also, macro-particles losses during the simulations are significant but may be present in the PITZ work based on another simulation study presented in [7,10].

Two sets of parameter scans are presented here to address these issues and to justify additional changes to the model in this research. The two sets are differentiated by the particle distribution used to model the electron bunch. The distributions are characterized in bunch charge, time, position, and momentum. In both cases, the

TABLE 3: Particle distribution configuration parameters

	<b>ASTRA Distribution type [22]</b>	<b>1 nC Bunch Charge</b>	<b>800 pC Bunch Charge</b>
time	plateau	flattop 25 ps rise time 5 ps	flattop 24 ps rise time 6 ps
position	radially uniform	0.45 mm rms	0.485 mm rms
momentum	isotropic	$E_k = 0.55$ eV	$E_k = 0.55$ eV

form of the distributions used for each dimension is the same, but their configurations for charge, time, and position are different. The momentum distribution is the same. The first set follows the distribution configuration used in PITZ simulations while the second uses some parameters that match experimental PITZ results. The distribution parameters are summarized in Table 3 and discussed below. To reduce simulation time, the number of macro-particles in each distribution is 2000.

In the PITZ simulations, the bunch charge is 1 nC [7], lower than the 1.65 nC used in [10]. Spatially, the macro-particle particle distribution represents a cylindrically symmetric beam emitted from a photocathode. The beam radius is 0.45 mm rms [7], and the distribution is shown in Figure 15. The temporal profile is known as a flat top or plateau [22]. It resembles a rectangular pulse with sloped sides but has smooth transitions in slope. The flat top region is 25 ps FWHM. The sloped sides represent the rise and fall time of the beam due to laser turn on and off. The rise and fall times are assumed to be mirror symmetric and are set to the same value. This value is called the rise time, and it is 5 ps [7] for this distribution. A histogram of the temporal distribution is shown in Figure 16. The momentum distribution simulates the average momentum of the electrons after emission from the Cs<sub>2</sub>Te photocathode using a laser producing 262 nm wavelength light in the PITZ RF gun [7, 61]. It is known as an isotropic distribution [22] because the momenta of the particles are distributed across the surface of a half-sphere. The momentum components in the beam propagation direction,  $p_z$ , are uniformly distributed, and the transverse components,  $p_x$  and  $p_y$ , are calculated to ensure the average kinetic energy is 0.55 eV, the net average energy

after cathode emission. The calculation is based on [64]

$$E_k = E_{total} - E_0$$

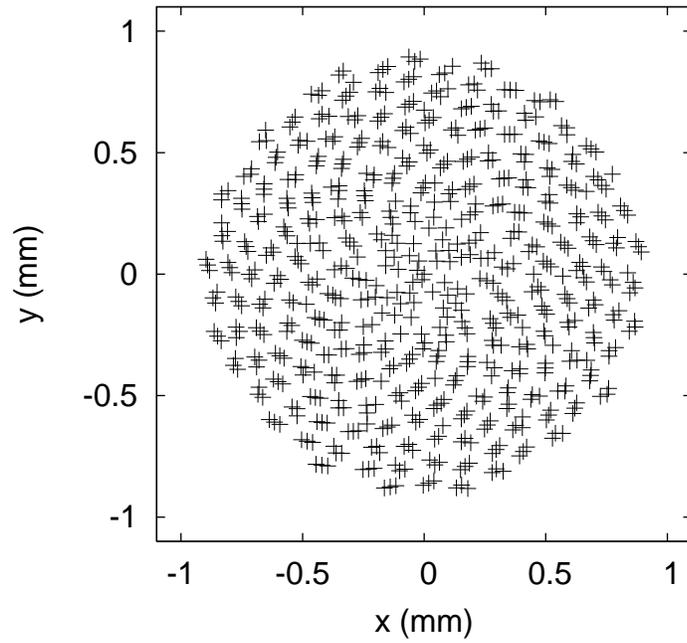
$$E_k = \sqrt{p_x^2 + p_y^2 + p_z^2 + E_0^2} - E_0$$

where  $E_k$  is the kinetic energy,  $E_{total}$  is the total energy,  $E_0 = m_0c^2$  is the electron rest energy, and  $p_x$ ,  $p_y$ , and  $p_z$ , are the momentum components. Two views of the distribution are shown Figures 17 and 18. Combined, these show that the momenta are distributed across the surface of the half-sphere.

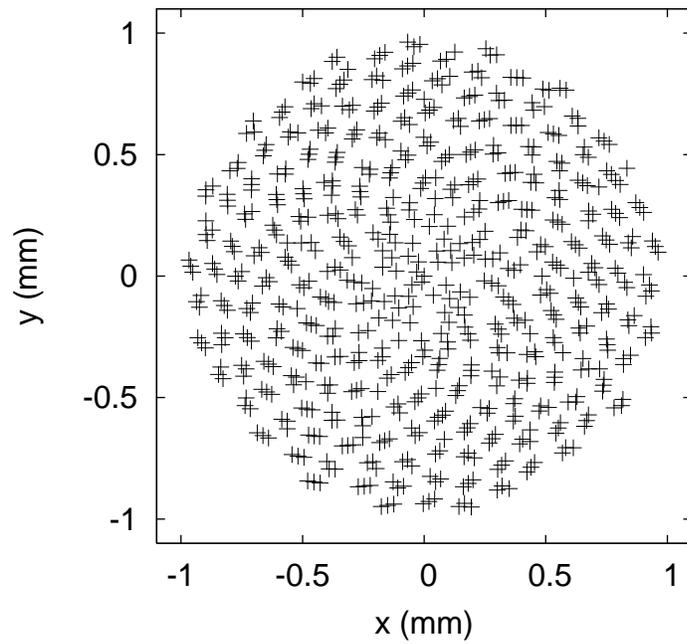
For the second distribution, the bunch charge is further reduced to 800 pC to mitigate particle losses as is shown below. Reflecting measurements with a beam, the beam radius is increased to 0.485 mm rms, and the temporal distribution has a 24 ps flat top region with 6 ps rise [7]. This profile is used throughout this research and is shown with the PITZ simulation distribution in Figures 15, 16, 17, and 18. As an aside, except for the bunch charge, this is the same distribution used in [10].

Each set of parameter scans is performed for three different geometry descriptions. The first is the curvilinear PITZ cavity geometry with a 1300.1361 MHz resonance frequency in Figure 19. Two straight-line approximations of the original PITZ geometry are introduced as reasonable models for study. One straight line geometry uses the same dimensions as the original PITZ geometry and has a 1288.6149 MHz resonance frequency. The second straight line geometry takes advantage of the fact that the first straight line geometry is a solution to Maxwell's equations meeting the boundary conditions [47]. Provided all of the geometry dimensions are scaled uniformly by the ratio of the actual geometry resonance frequency to the desired resonance frequency, the first straight line geometry can be used to create another straight line cavity with the same resonance frequency as the curvilinear PITZ geometry. The frequency of the scaled geometry is 1300.1391 MHz. In general though its field characteristics will match those of the straight line cavity but at a different resonance frequency. The straight line geometries are shown in Figures 20 and 21, and Table 4 summarizes the differences in physical dimensions of the three geometries. The resulting on-axis field profiles are shown in Figure 22. Despite the differences in the geometries, the field profiles are very similar to each other. In the cavity geometry figures, the isolines are along constant magnetic field values [48] of the magnetic field.

Before discussing the parameter scan results, it is worth noting that the 800 pC

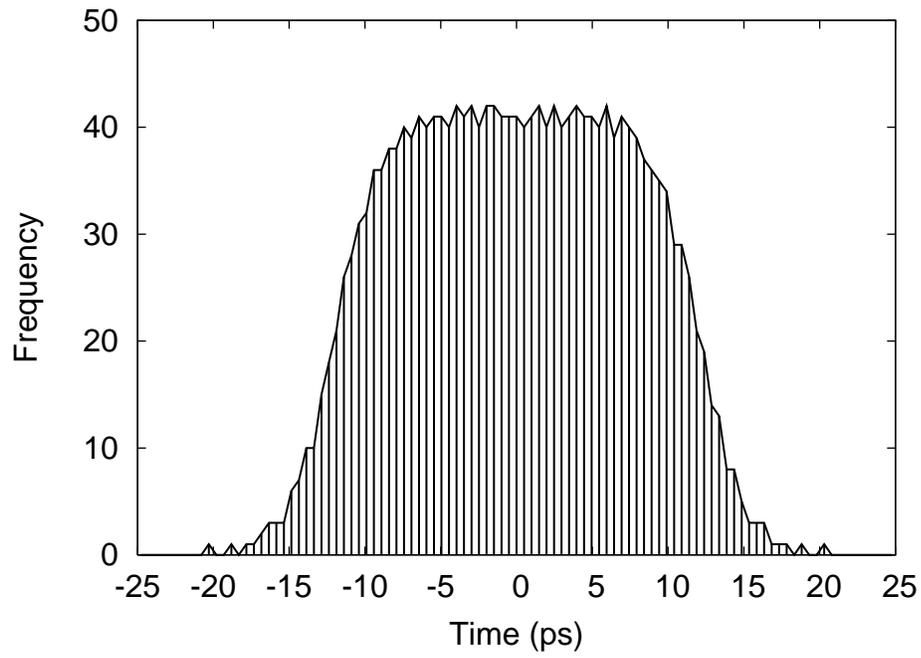


(a)

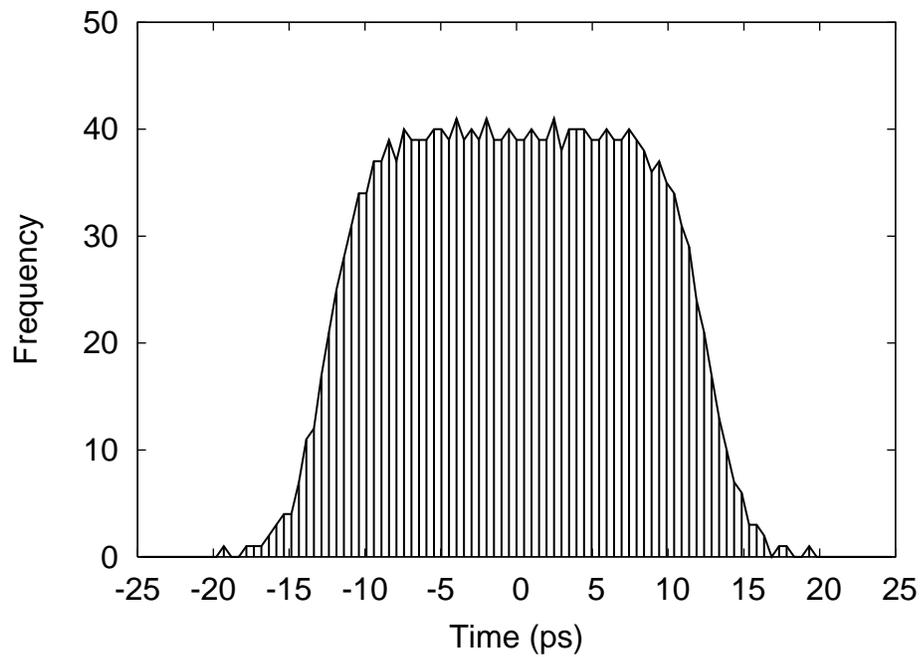


(b)

FIG. 15: Spatial distributions viewed in the  $x - y$  plane for 0.45 mm rms and 0.485 mm rms transverse beam sizes: (a) 0.45 mm rms; (b) 0.485 mm rms. Increasing the number of particles in the distribution fills in the space between the spiral arms.



(a)



(b)

FIG. 16: Histograms of the plateau temporal distributions: (a) 24 ps flat top with 6 ps rise time; (b) 25 ps flat top with 5 ps rise time.

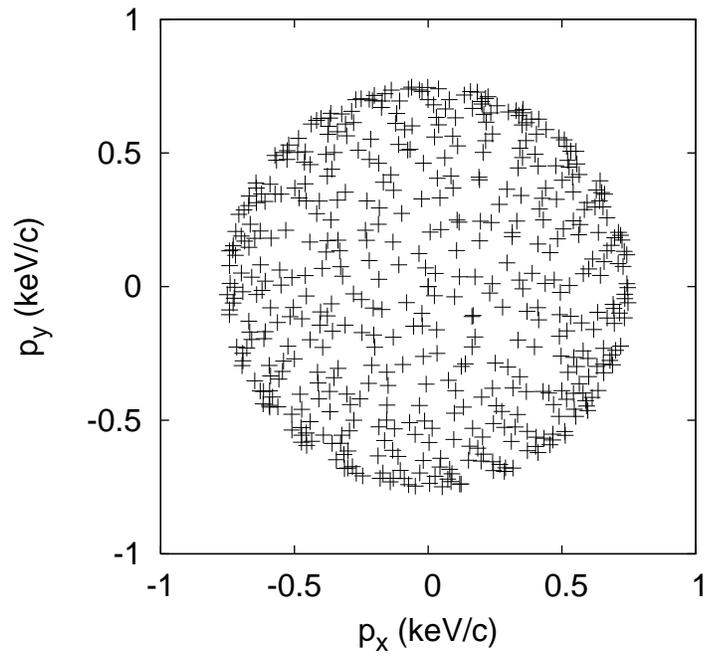


FIG. 17: Momentum distribution viewed in the  $p_x - p_y$  space.

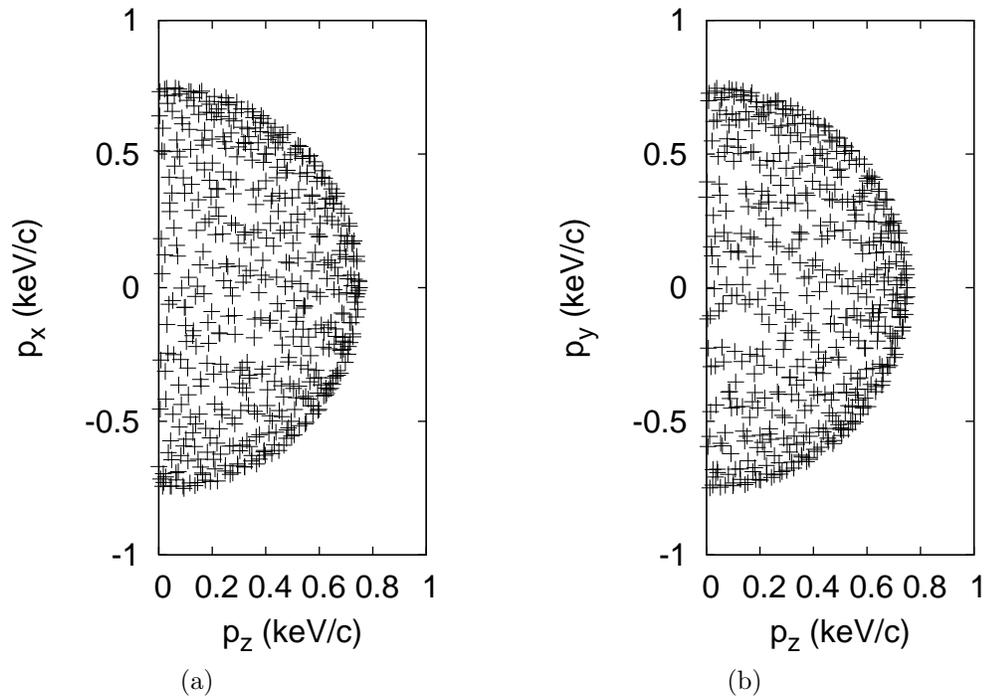


FIG. 18: Momentum distribution viewed in the  $p_z - p_x$  and  $p_z - p_y$  spaces: (a)  $p_z - p_x$ ; (b)  $p_z - p_y$ .

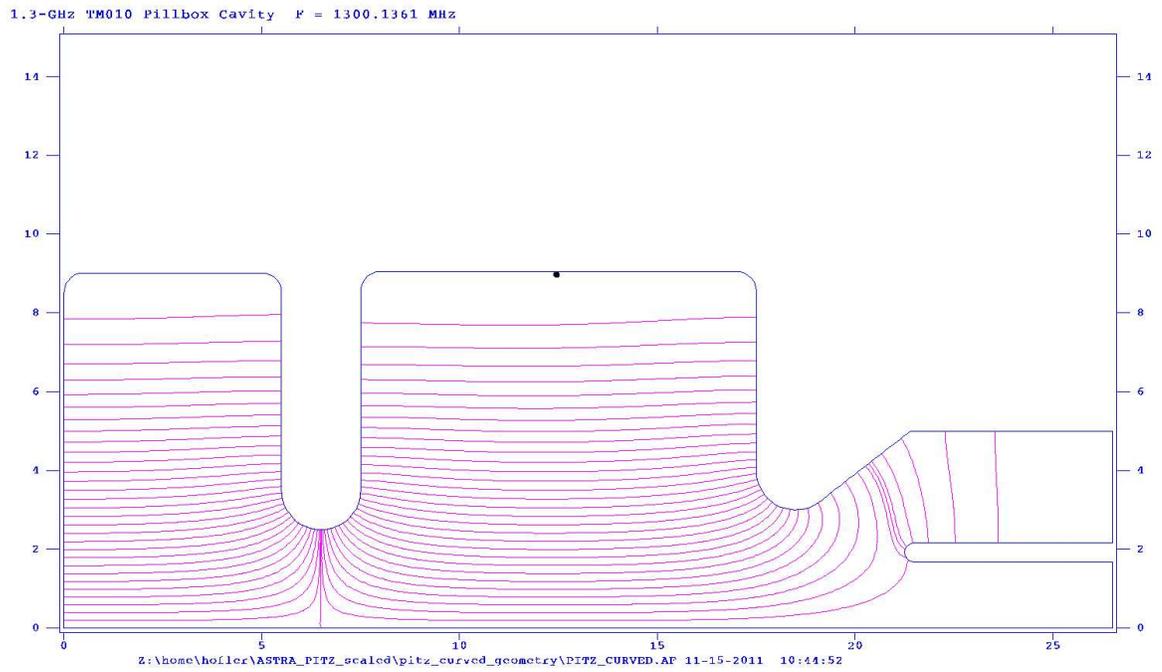


FIG. 19: PITZ curvilinear geometry [63]. Axes units are cm.

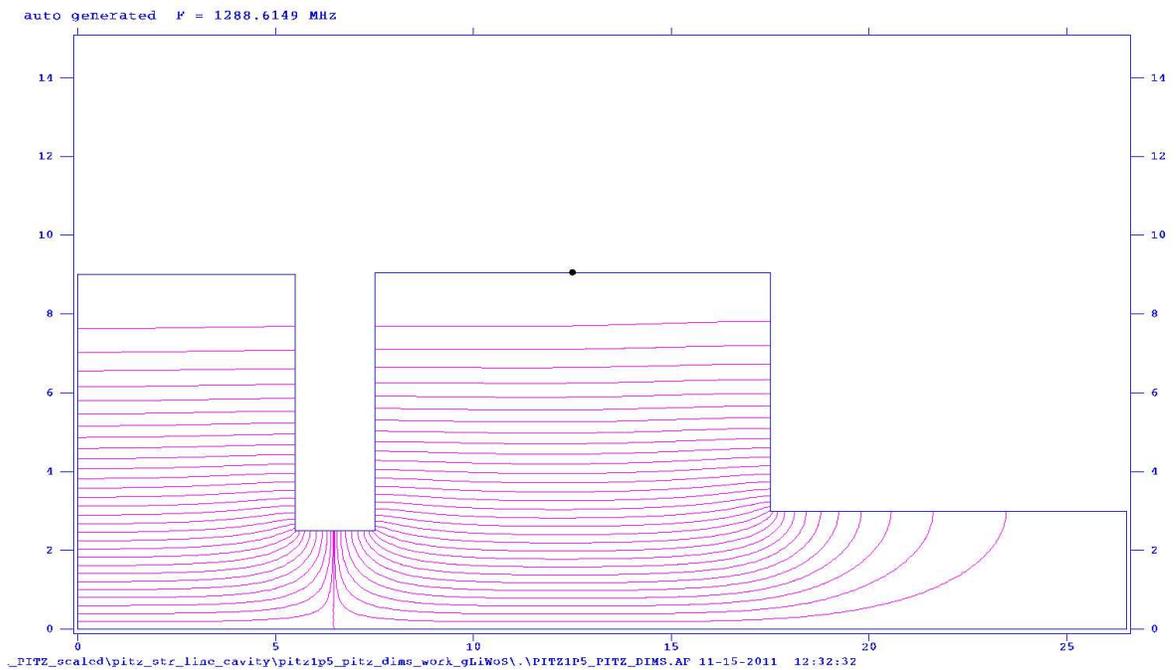


FIG. 20: Straight line cavity geometry using PITZ curvilinear dimensions. Axes units are cm.

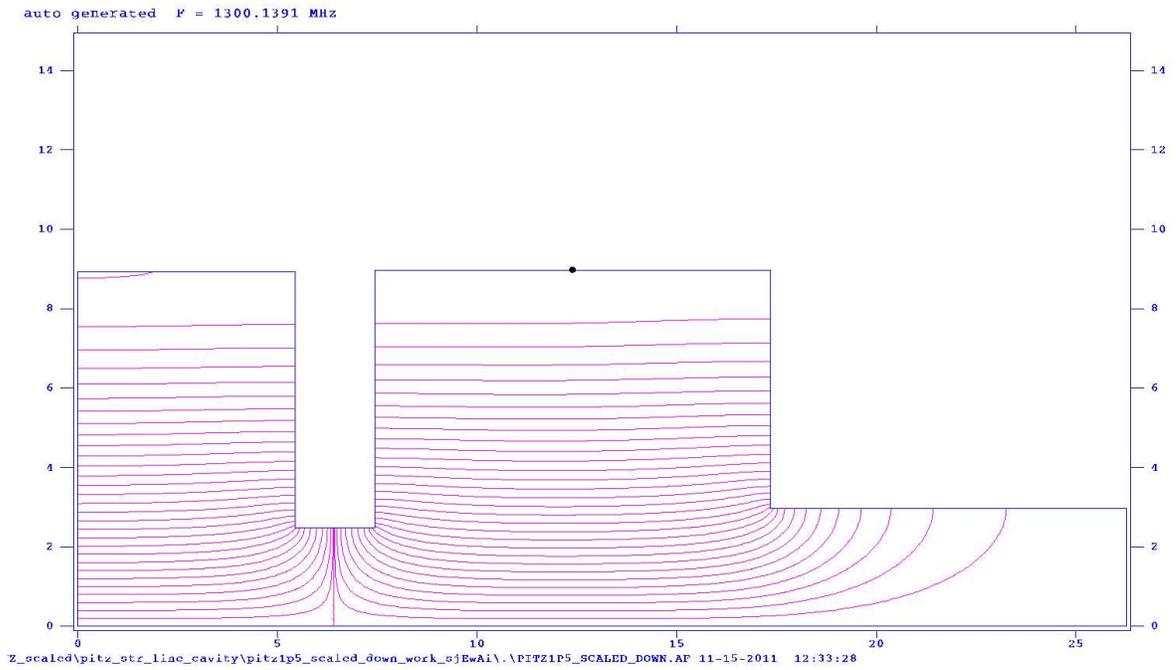


FIG. 21: Straight line geometry scaled to the PITZ frequency. Axes units are cm.

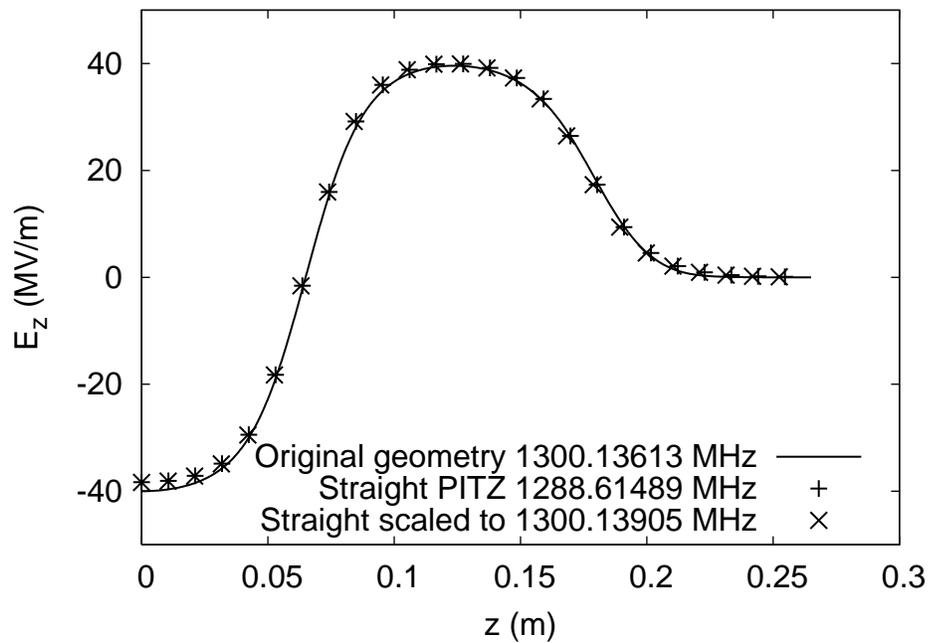


FIG. 22: On-axis field profiles for the three cavity geometries used in the parameter scans.

TABLE 4: Dimensions for the three study geometries

<b>Dimension (cm)</b>	<b>PITZ curvilinear geometry [63]</b>	<b>Straight line geometry with PITZ dimensions</b>	<b>Straight line geometry scaled to PITZ frequency</b>
<b>Frequency (MHz)</b>	<b>1300.1361</b>	<b>1288.6149</b>	<b>1300.1391</b>
Cell 1 radius	9.0148	9.0148	8.9349
Cell 1 length	5.5	5.5	5.4513
Iris radius	2.5 (smallest)	2.5	2.4779
Iris length	2	2	1.9823
Cell 2 radius	9.0488	9.0488	8.9686
Cell 2 length	10	10	9.9114
Exit tube and coupler radius	3 at exit of Cell 2 1.675 at tube entrance	3	2.9734
Exit tube and coupler length	9	9	8.9203
Total length	26.5	26.5	26.2653

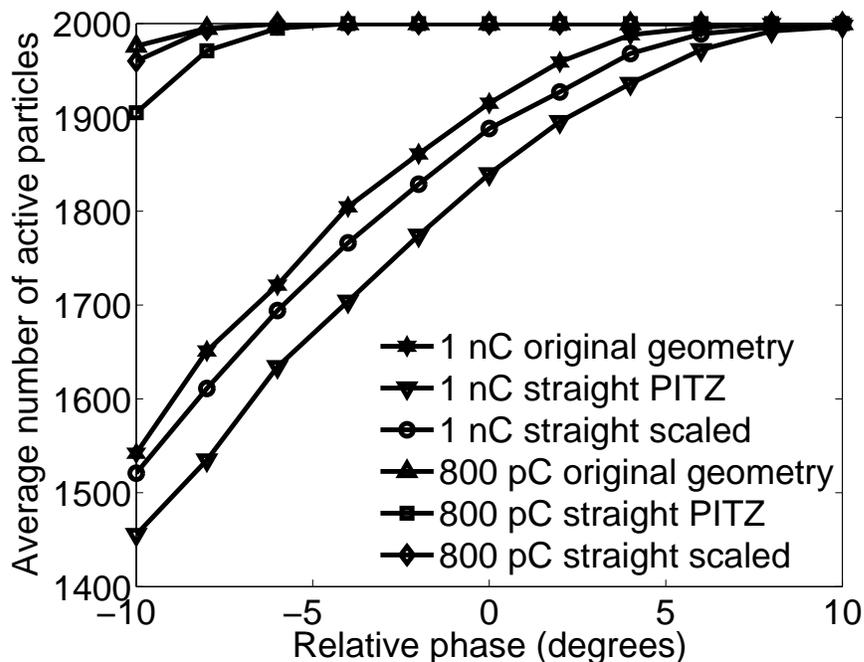


FIG. 23: Average number of active particles at the end of each simulation for each combination of particle distribution and cavity geometry.

distribution performs better in terms of particle loss. Complementary to reporting particle loss mechanisms, ASTRA also reports the number of active particles remaining at the end of each simulation. As part of the parameter scans, the number of active particles is recorded. Neither distribution is lossless. The loss pattern shows a strong dependence on RF phase and a weak dependence on solenoid setting. This is reflected in Figure 23 where the average number of active particles across all solenoid settings is shown as a function of RF phase. For phases greater than  $-4^\circ$ , the simulations for the 800 pC distribution are lossless whereas the 1 nC distribution has losses for most of the negative phases in the scan. This is notable because these are the phases where RF guns typically run. The assumption that lossless transmission simulation results are more reliable than those with losses justifies the choice to lower the bunch charge from 1 nC to 800 pC in this research.

The parameter scans in Figures 24, 25, and 26 are consistent with each other and previously published results. The PITZ work only provides a transverse emittance contour plot for the parameter scan [7], and the transverse emittance contours here

match the PITZ result to the same level that [10] does. The actual transverse emittance values are different for each bunch charge distribution, but more importantly, across geometry descriptions for a given bunch charge distribution, the locations of the minimum with respect to the solenoid and RF phase settings are in agreement. As in [10], the beam size contour plots are provided to show that the location of the minimum emittance in each parameter scan coincides with the minimum spot size region as expected. These two observations confirm that the model is reasonable.

Considering the parameter scan results relative to the changes made in each set guides approaches to use in the optimization to follow. The changes in the bunch distribution do not significantly alter the pattern of the contours. Lowering the bunch charge does lead to a direct improvement in the transverse emittance in all cases. This suggests that reducing the bunch charge to obtain lossless, and therefore more reliable, simulations in the optimization is acceptable, and that the net effect of doing so lowers the transverse emittance. Also, whether the cavity geometry is made with curved surfaces and rounded corners or straight lines and hard edge corners does not affect the contours. Therefore, one might expect that straight line geometries, which are intrinsically simpler to optimize, provide useful information about the general optimization problem. In particular, the contour values for the straight line geometry scaled to the PITZ frequency fall between the curved geometry and the straight line cavity using PITZ dimensions. This suggests that the scaled geometry is a good reference to use in the optimization.

Finally, because the PITZ RF gun has no longitudinal emittance requirement, there is no reference set of longitudinal emittance contours for comparison. The longitudinal emittance is a candidate optimization objective function. The longitudinal emittance contours are provided to establish a reference that can be used to interpret the progress of an optimization using the longitudinal emittance.

## 4.2 FIELD MORPHING

The field morphing technique is used to find the minimum transverse emittance and beam size under conditions similar to the parameter scan experiment. Primarily, this exercise establishes that the optimization system works. It also validates the proposed approach to optimize the RF gun field profile by varying it in response to the beam dynamics. Third, it provides initial insights into what to expect from the geometry optimization system when applied to a similar problem.

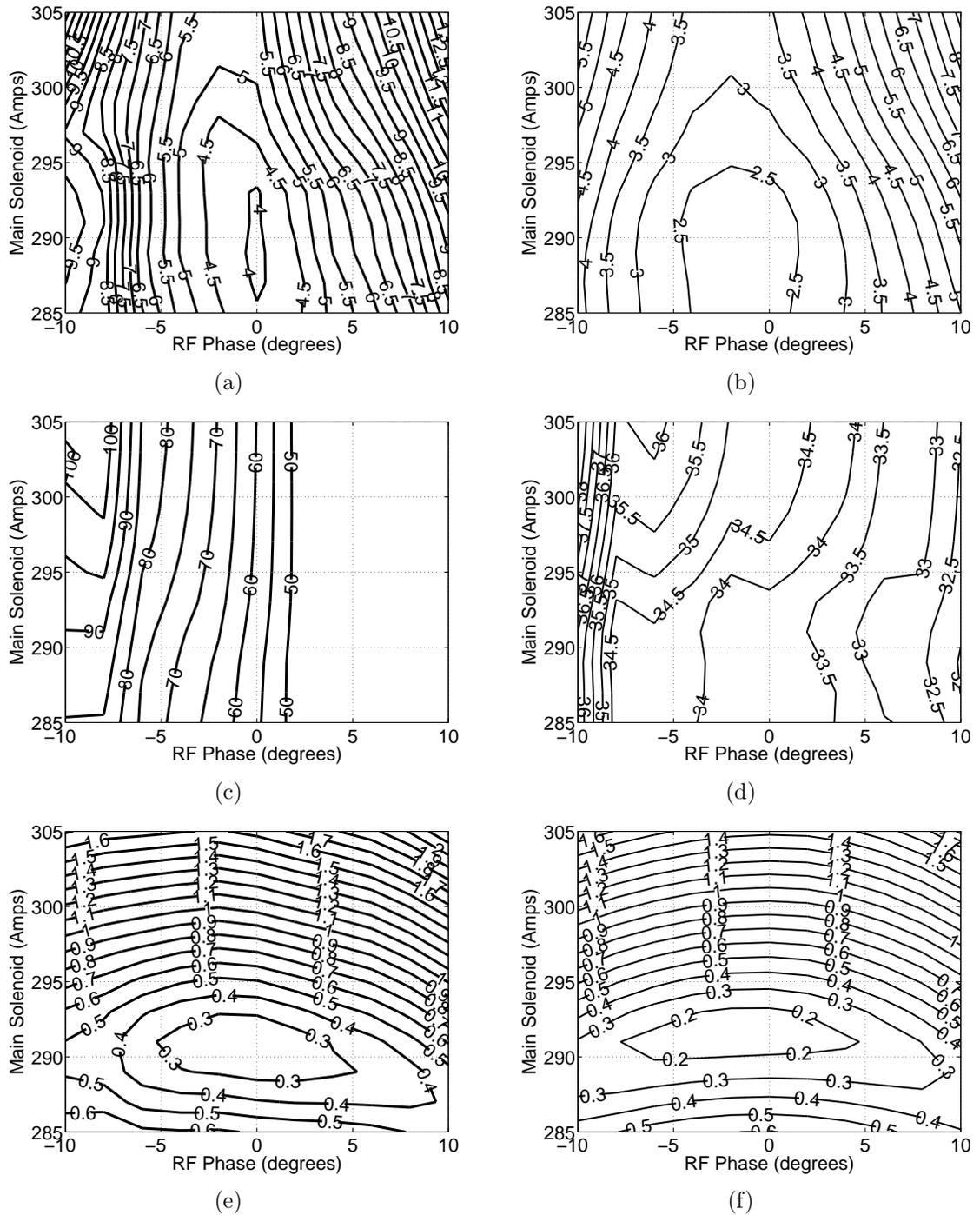


FIG. 24: Parameter scan results for the PITZ curvilinear geometry: (a) normalized transverse emittance for 1 nC; (b) normalized transverse emittance for 800 pC; (c) normalized longitudinal emittance for 1 nC; (d) normalized longitudinal emittance for 800 pC; (e) beam size for 1 nC; (f) beam size for 800 pC.

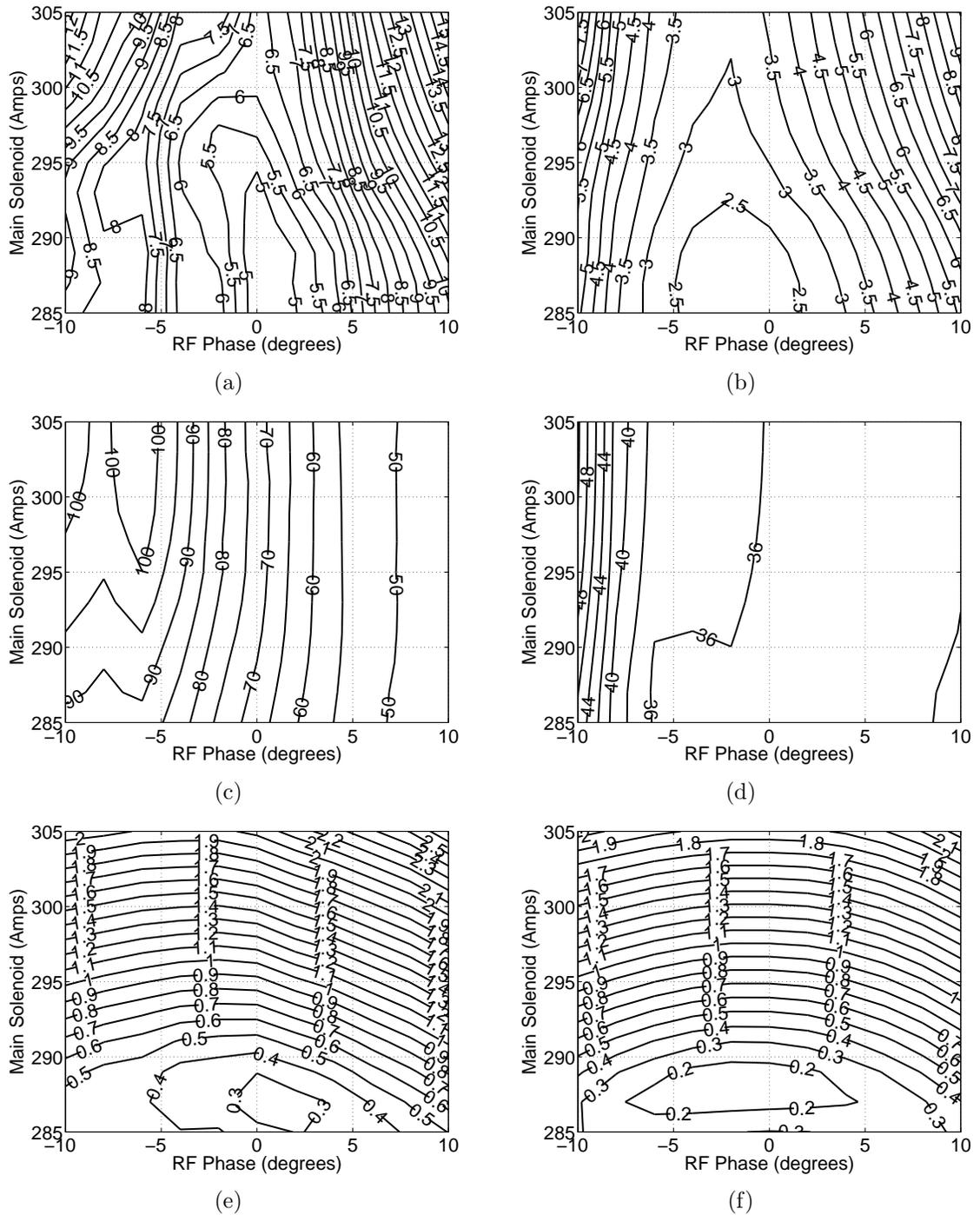


FIG. 25: Parameter scan results for the straight line geometry: (a) normalized transverse emittance for 1 nC; (b) normalized transverse emittance for 800 pC; (c) normalized longitudinal emittance for 1 nC; (d) normalized longitudinal emittance for 800 pC; (e) beam size for 1 nC; (f) beam size for 800 pC.

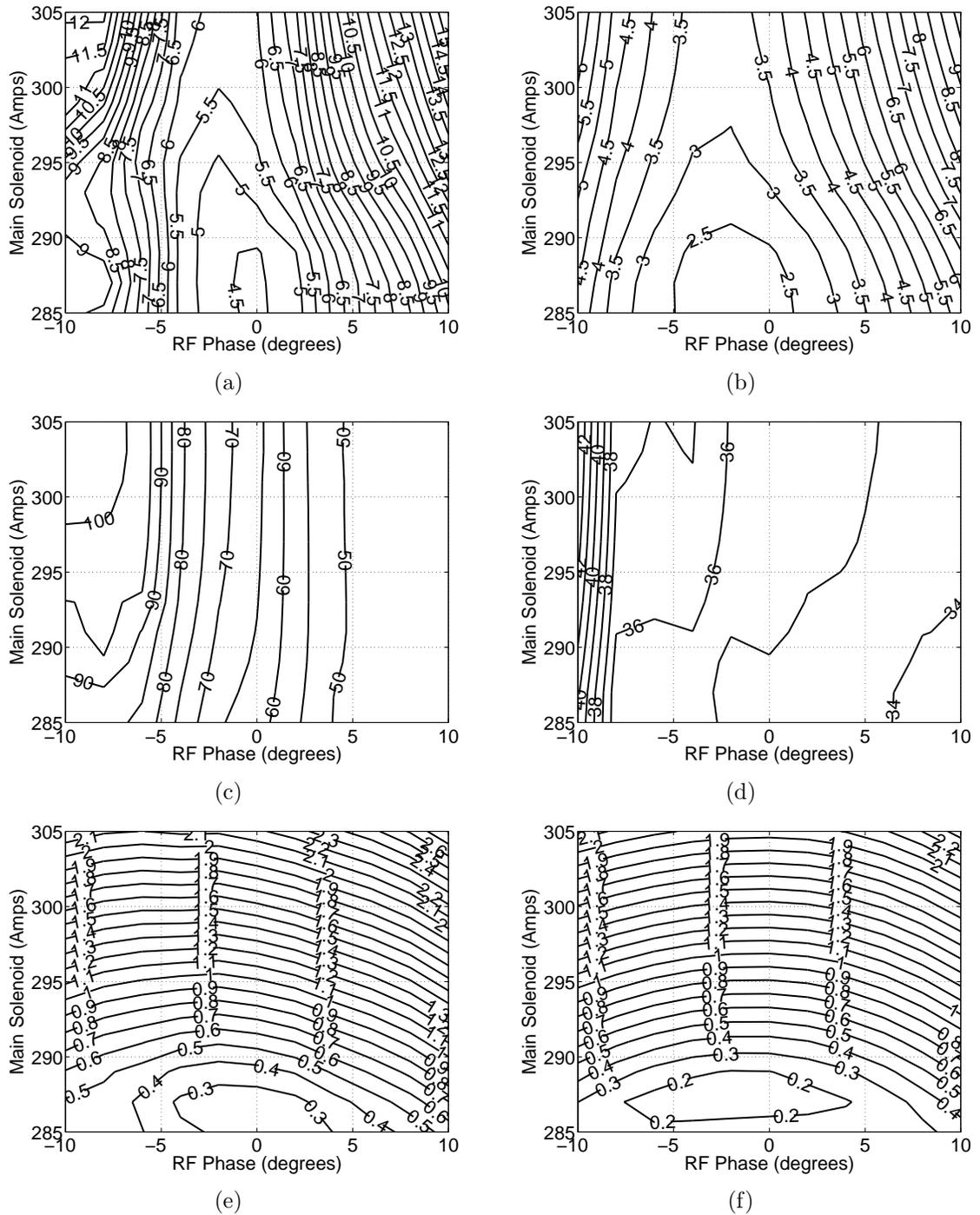


FIG. 26: Parameter scan results for the scaled straight line geometry: (a) normalized transverse emittance for 1 nC; (b) normalized transverse emittance for 800 pC; (c) normalized longitudinal emittance for 1 nC; (d) normalized longitudinal emittance for 800 pC; (e) beam size for 1 nC; (f) beam size for 800 pC.

The problem set up is the same as the RF phase and solenoid settings scan. The layout of the beam line and the field profile for the main solenoid are carried forward. The field profile for the RF gun though is no longer fixed since the optimization generates it. The gradient is set to 40 MV/m, and the 800 pC particle distribution is used. The optimization is configured to reject simulations with particle losses. The cavity frequency used in the ASTRA simulations is the frequency of the generated field, and the peak RF gradient is not rescaled to guarantee the peak gradient is fixed in a relative location between the cells. The number of individuals per population is 96, and the maximum number of generations is 40.

The objectives of the optimization are to minimize the transverse emittance and beam size. Technically, there are four objectives since ASTRA reports these quantities for the horizontal and vertical planes [22]. The beam and the fields in this problem are cylindrically symmetric, and that means the beam characteristics in the horizontal and vertical planes match in the particle distribution at all points along the beam line within statistical limits.

The main constraint is that  $\min [f_{morphing}(z)]$  must be positive. This is to ensure that  $f_{morphing}(z)$  does not introduce unwanted zero crossings. Additional constraints are that the beam size and emittance must also be positive. These quantities by definition are positive, so these constraints guard against unexpected invalid simulation results.

The decision variables are the first seven pairs of Fourier coefficients of  $f_{morphing}(z)$ ,  $a_1 - a_7$  and  $b_1 - b_7$ ; the relative RF phase of the gun; and the main solenoid strength. The range for the main solenoid strength is the same as in the parameter scan, and the relative RF phase range is opened up to  $\pm 15^\circ$ . The Fourier coefficients are allowed to vary between 0 and 0.5. The units for the resulting field profiles' amplitudes are not specified since ASTRA normalizes the profiles so the peak magnitude is 1 before scaling to the desired gradient setting in MV/m [22].

Figure 27 shows a sample of the non-dominated fronts from the 40 generations. Recall that the non-dominated solutions in a population provide an estimate of the Pareto-optimal front. They meet all of the constraints and have the best objective values found so far. This figure shows that the estimate of the Pareto-optimal front is progressively moving toward smaller and smaller beam sizes and emittances. Admittedly, the final ranges of emittances and beam sizes are unacceptably large, so these solutions are not attractive from an accelerator design standpoint. Also, the front

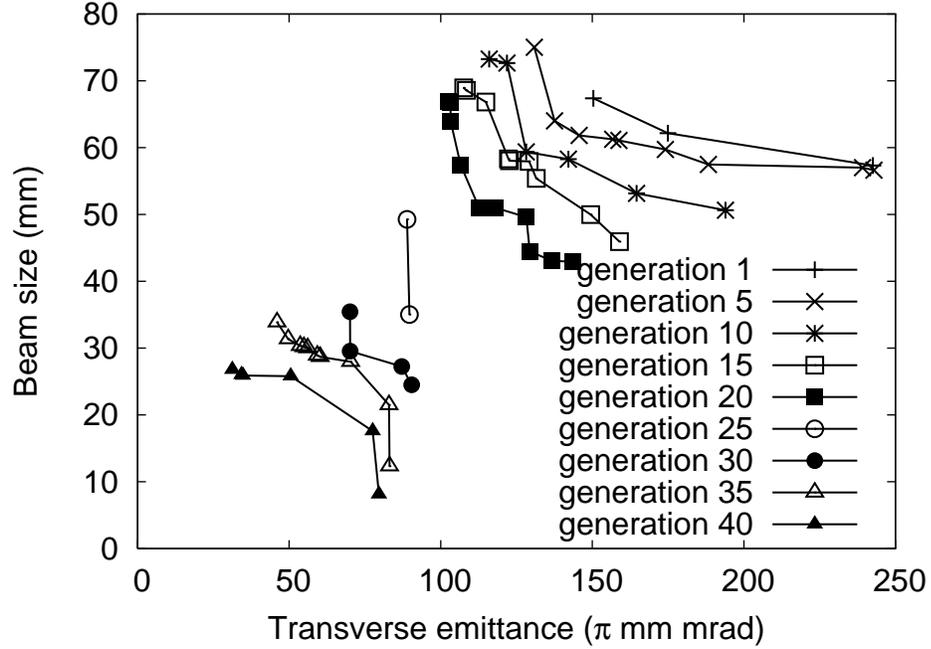


FIG. 27: Field morphing non-dominated individuals for several generations.

size is very small compared to the number of individuals in the population pointing to a need for refinement of the optimization problem parameters. Still, the moving front shows that the optimization system works and that the proposed approach is viable.

Consider now the generated field profiles from the fronts of the first and last generations in Figures 28 and 29. There is a similarity in the field profiles produced. From the outset, the optimization processing shows a preference for unbalanced field profiles to obtain small emittances. To date, cavities, whether for guns or accelerating elements in linacs, are designed to have balanced or nearly balanced field profiles [65].

One way to characterize the balanced or unbalanced nature of the field profile is to use field flatness [66], a percentage defined as

$$field\ flatness = 100 \frac{|E_{peak}|_{\max} - |E_{peak}|_{\min}}{\frac{1}{n_{cells}} \left( \sum_{i=1}^{n_{cells}} |E_{peak}|_i \right)}$$

where  $|E_{peak}|_{\max}$  and  $|E_{peak}|_{\min}$  are the maximum and minimum peak field amplitudes across the cells,  $|E_{peak}|_i$  is the peak of the  $i$ -th cell, and  $n_{cells}$  is the number of cells.

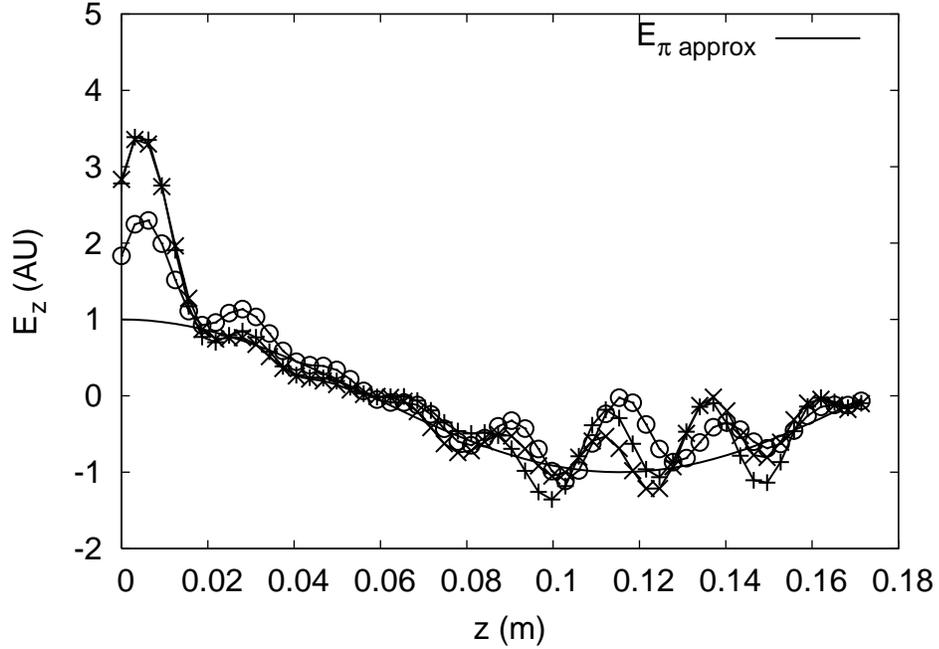


FIG. 28:  $E_z$  vs.  $z$  profiles for front in first generation. The source sine,  $E_{\pi_{approx}}$ , is provided for reference.

Under this definition, a flat or balanced field then has 0 % field flatness. For the purposes of this definition, a 1.5 cell cavity has two cells, and its  $\pi$  mode has 2 peak amplitudes. This field flatness definition can be further refined to indicate the relative ordering of the peak extremes. If in the  $z$  coordinate, the maximum peak value is to the left of (has a smaller  $z$  coordinate than) the minimum peak value, the signed field flatness is

$$\text{signed field flatness} = -1(\text{field flatness})$$

If, on the other hand, the minimum peak value is to the left of the maximum peak value, the signed field flatness and field flatness are equal.

The signed field flatness values for all of the profiles in these figures are negative, meaning the larger peak amplitude is in the first cell. This is consistent with the benefit of RF guns where rapid acceleration of the particles leads to smaller emittance growth [67]. The average signed field flatness for the fields in the front of the last generation is -91 %. The field profiles fall into two groups. The average signed field

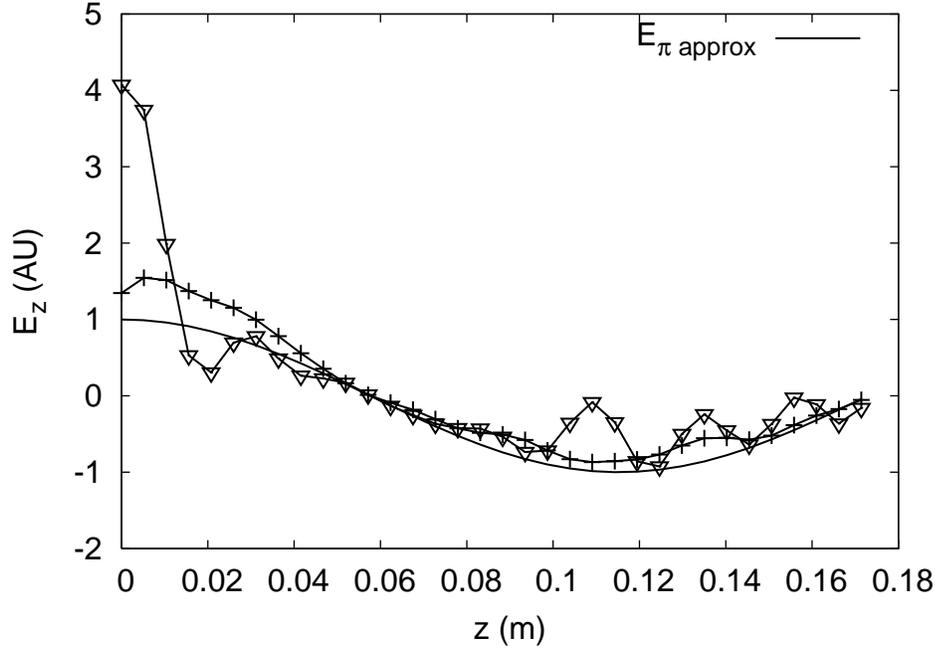


FIG. 29: Representative  $E_z$  vs.  $z$  profiles for front in last generation. The source sine,  $E_{\pi_{approx}}$ , is provided for reference.

flatness of the four smoother profiles is -56 %, and the average of the other two is -123 %. For the first group, the peak in the first cell is almost twice the peak amplitude in the second cell, and in the latter case, the ratio is 4 to 1. These results are far from nearly flat, in contrast to the PITZ case where the flatness is 10 % or less [68].

Figure 30 shows the components of the field morphing process for the field profile in the last front that produces transverse emittance  $34.733 \pi$  mm mrad and spot size 25.899 mm. The approximation to the  $\pi$  mode,  $E_{\pi_{approx}}(z)$ , the morphing function,  $f_{morphing}(z)$ , and its  $a_n$  and  $b_n$  terms are all shown. Summing the  $a_n$  and  $b_n$  terms with the offset 1 gives  $f_{morphing}(z)$ . The curve for  $f_{morphing}(z)$  is well above zero as required by the constraint. The resulting field profile,  $E_z(z)$ , is also shown.

Initial attempts to optimize the transverse emittance for this problem using this approach are described in [11]. The set up for those optimizations is slightly different from the one described here. For those, the problem definition included an approximate description of the dimensions of the beam line enclosure. This defines a set of apertures in the beam line that the beam must avoid to transport to the

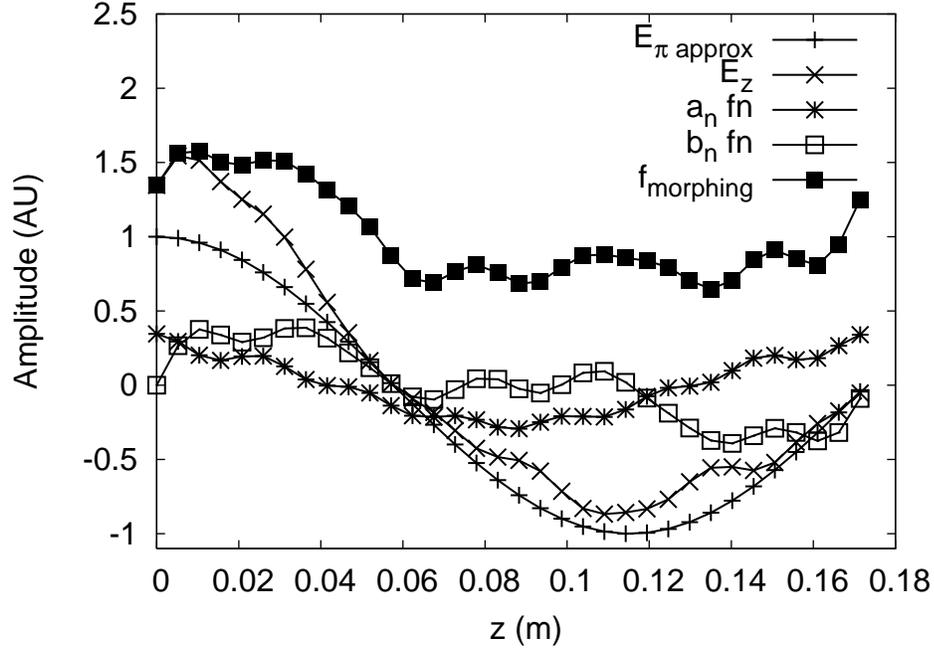


FIG. 30: Details for  $E_z$  vs.  $z$  profile that gives transverse emittance  $34.733 \pi$  mm mrad and spot size 25.899 mm

end of the beam line. A related difference is that two particle loss mechanisms were allowed, particles less than  $z_{min}$  and interception on apertures, but no attempt was made to minimize the losses. Also, the 1.65 nC particle distribution from [10] was reused. The RF phase and solenoid settings were fixed to the values corresponding to the minimum emittance found in [10]. A final difference is the phases used for the RF were not relative to the crest phase. Unfortunately, these phases do not translate between field maps even similar ones, and using these phases can lead to invalid simulation results that otherwise might have been valid using relative phases. Despite all of these differences, the optimizations point to unbalanced field profiles as this more robust optimization configuration does.

From this field morphing exercise come three conclusions. The first is that the proposal to change the field profile of the gun cavity as part of the beam dynamics optimization works and makes sense to do. The second is that field morphing while producing non-physical fields can yield compelling results that merit further study. Lastly, specifically for RF gun design, it points to the possibility that gun designs

TABLE 5: Decision variables

Variable	Units	Lower bound	Upper bound
relative RF phase	degrees	-10	15
main solenoid strength	Tesla	-0.180	-0.1
tube iris radius	cm	2.4529	2.5029
tube iris length	cm	1.9073	2.0073
cell 1 radius	cm	8.9249	8.9449
cell 1 length	cm	5.3763	5.4763
cell 2 radius	cm	8.9586	8.9786
cell 2 length	cm	9.88646	9.9864

with unbalanced field profiles lead to better emittances.

### 4.3 CAVITY GEOMETRY MORPHING

Finally, the cavity morphing optimization is applied to a variation of the parameter scan experiment. In addition to minimizing the transverse emittance and beam size, the longitudinal beam emittance is minimized. With this addition, the goal of this optimization is to increase the brightness of the source. Recall from (2) that brightness is inversely proportional to the product of the transverse emittances and the longitudinal emittance. This is not part of the PITZ RF gun design or its requirements. This is an exercise to see if the design can be improved to increase its brightness.

The baseline cavity geometry for this optimization is the straight line cavity geometry scaled to the PITZ frequency. From the parameter scans presented, the emittance product,  $\varepsilon_{n,x}\varepsilon_{n,z}$ , for the 800 pC bunch charge for this geometry is  $76.24 \pi^2 \text{ mm}^2 \text{ mrad keV}$ . This calculation uses the point with the minimum transverse emittance in the contour plot to determine this factor. The longitudinal emittance decreases as the relative RF phase increases but at the expense of the transverse emittance. The parameter scan indicates that the brightness can be improved only marginally by adjusting the RF phase and main solenoid strength since the longitudinal emittance does not change drastically over the entire parameter scan. If an improvement is to be made, a different set of parameters needs to be considered.

TABLE 6: Linear relationship variables

<b>Variable</b>	<b>Tracked variable</b>	<b>slope</b>	<b>Offset</b>
cell 1 neck width	cell 1 length	1	0
cell 1 iris exit wall radius	tube iris radius	1	0
cell 2 neck width	cell 2 length	1	0
cell 2 iris entrance wall radius	tube iris radius	1	0

In this optimization, the number of individuals is 96, and the maximum number of generations is 10. As stated above, the objectives are the same as for the field morphing optimization except for the addition of longitudinal emittance. The decision variables and bounds are listed in Table 5. The upper bounds for the main solenoid and RF phase are increased over the field morphing optimization settings. According to [12], the frequency of the cavity is very sensitive to the cell radii, so their bounds have been set to 0.02 cm windows around the scaled straight geometry radii. The limits on the other dimensions are not so restrictive. This optimization uses linear relationships to match some cavity dimensions to dimensions designated as decision variables, and those are listed in Table 6.

The constraints related to beam characteristics are the same as for the field morphing optimization. Similar to the field morphing optimization, there are constraints related to the cavity morphing process. The frequency and field flatness of a cavity depend on the cell radii of the cavity [12]. Changing the cell radii can drastically change the resonance frequency of the geometry. Instead of tuning individual geometries to a desired frequency, constraints are used to guide the optimization to cell dimensions that lead to desirable frequencies. In this case, the desired frequency is 1300 MHz, and in the absence of equality constraints, two constraints are used to place upper and lower bounds on the acceptable frequencies. These are 1300.5 MHz and 1299.5 MHz, respectively. Likewise, the range of acceptable signed field flatnesses is controlled with two constraints. The bounds are  $\pm 101\%$ . These limits are chosen to allow for a large range of flatnesses while at the same time limiting them to reasonable values. Even at 100 %, the difference in amplitudes between the two cells is quite large.

Fronts are shown in Figures 31, 32, and 33. Bear in mind that the optimization search space is nominally 3D, as opposed to 2D, in the field morphing case. This

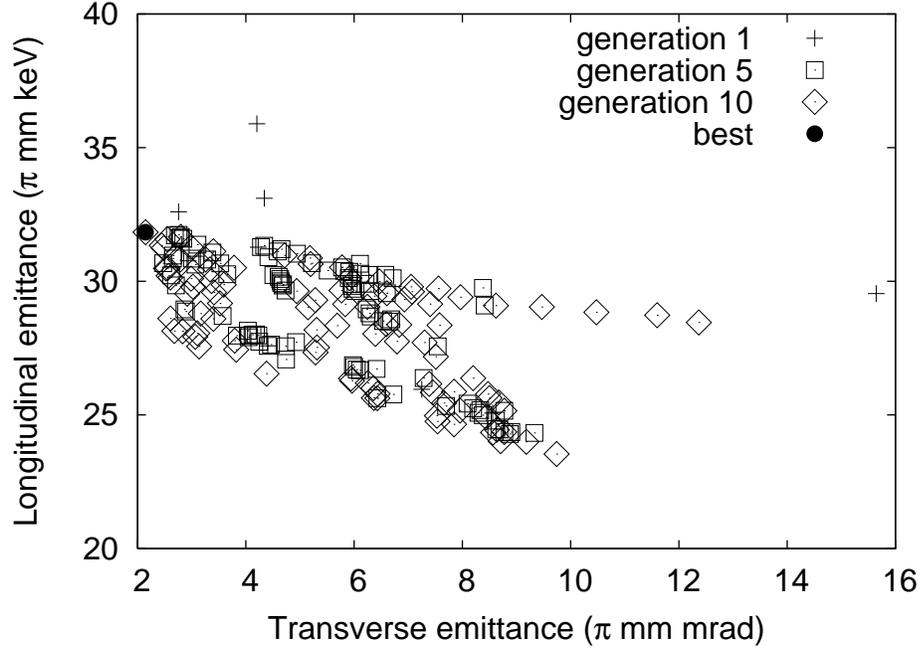


FIG. 31: Cavity geometry morphing fronts for transverse and longitudinal emittances

means that the search space plots are 3D projections onto 2D planes. This obscures the fronts in the plots to some extent. It may appear that later generations are gravitating toward apparently inferior solutions when actually the optimization is working to minimize the third objective. This may lead to poorer results in one or more of the other objectives.

From Figure 31, the best combination of transverse emittance and longitudinal emittance is approximately  $2 \pi$  mm mrad and  $32 \pi$  mm keV. Fortunately, according to the Figures 32 and 33, the beam size is small too for this combination. The optimization does not appear to be able to lower the transverse emittance below  $2 \pi$  mm mrad. It does lower the longitudinal emittance to less than  $24 \pi$  mm keV but as expected with a Pareto-optimal front at the expense of transverse emittance and beam size. The actual best values are transverse emittance  $2.1467 \pi$  mm mrad, longitudinal emittance  $31.834 \pi$  mm keV, and beam size  $0.16649$  mm. This leads to a brightness emittance factor,  $\varepsilon_{n,x}\varepsilon_{n,z}$ , of  $68.34 \pi^2 \text{ mm}^2 \text{ mrad keV}$ , a 12 % improvement.

Figures 34 and 35 show that the constraints are working. These plots show the

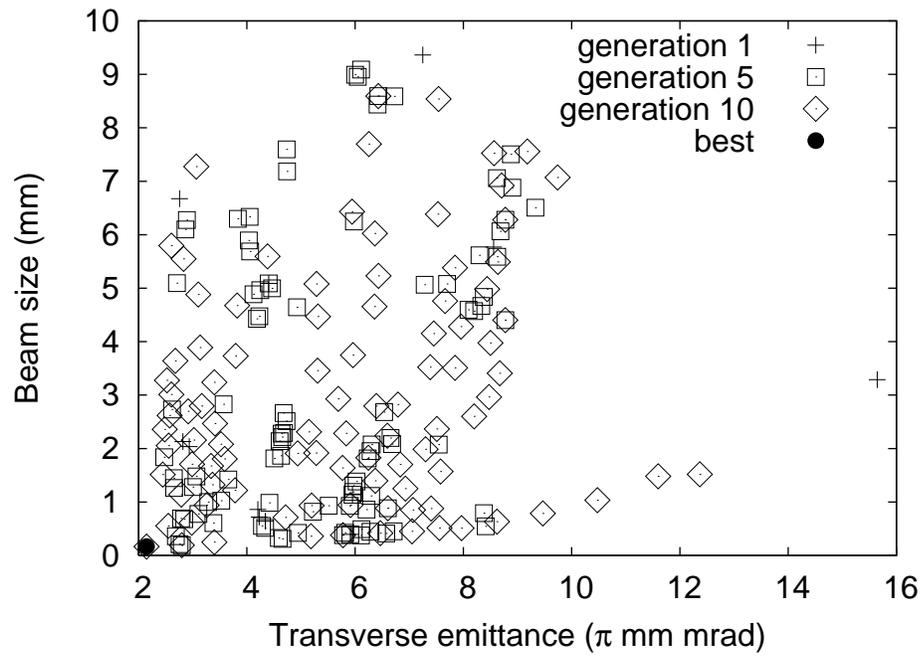


FIG. 32: Cavity geometry morphing fronts for transverse emittance and beam size

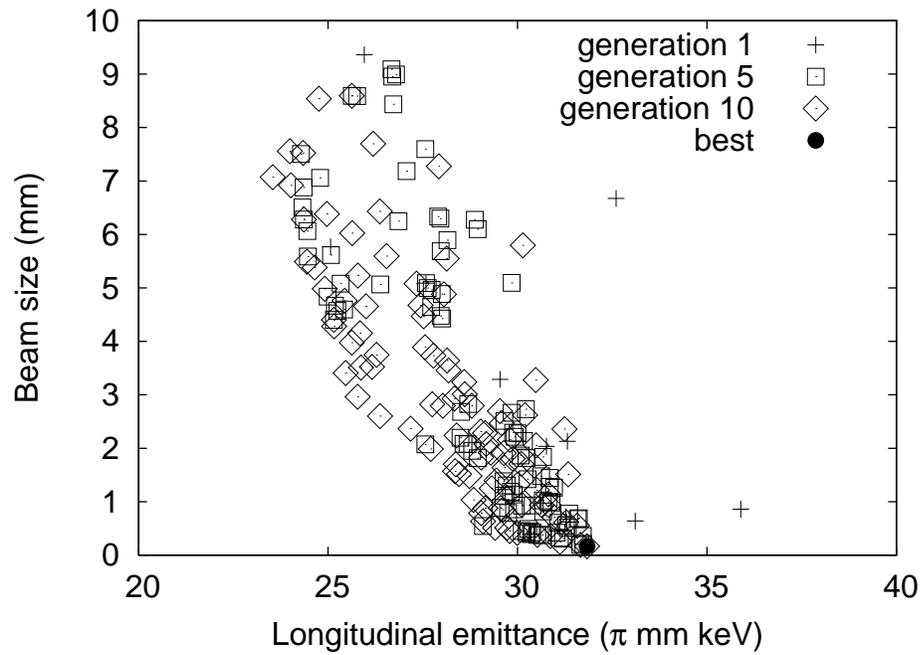


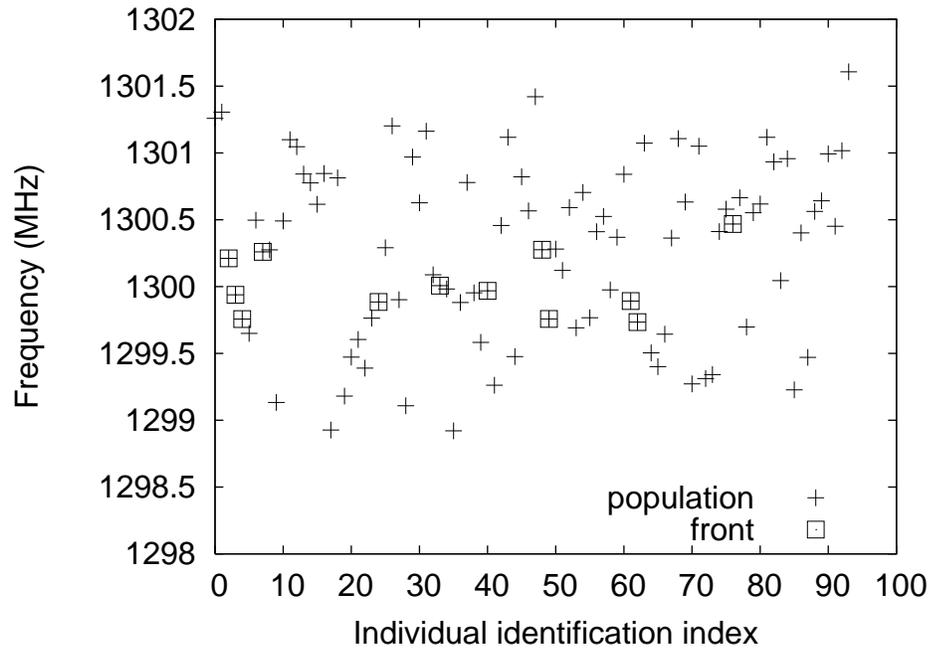
FIG. 33: Cavity geometry morphing fronts for longitudinal emittance and beam size

TABLE 7: Geometry dimensions comparison

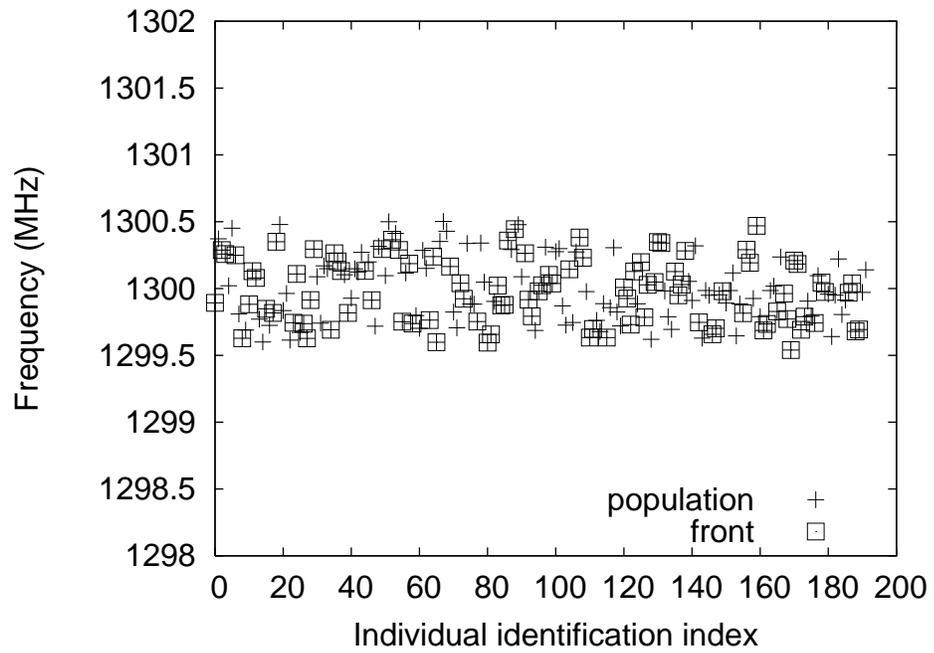
<b>Dimension (cm)</b>	<b>Straight line geometry scaled to PITZ frequency</b>	<b>High brightness straight line geometry</b>
<b>Frequency (MHz)</b>	<b>1300.1391</b>	<b>1300.10216</b>
Cell 1 radius	8.9349	8.93332
Cell 1 length	5.4513	5.38151
Iris radius	2.4779	2.48267
Iris length	1.9823	1.91288
Cell 2 radius	8.9686	8.97212
Cell 2 length	9.9114	9.97716
Exit tube and coupler radius (not varied)	2.9734	2.9734
Exit tube and coupler length (not varied)	8.9203	8.9203
Total length	26.2653	26.19185

first and last populations of the optimization and the members of the front, the non-dominated individuals. Note that the first population is randomly generated, and it is half the size of subsequent generations. The initial population consists of only new individuals; there is no archive to augment its population as there is for later generations. For both sets of constraints, in the first generation, there are individuals outside of the constraint limits as expected for a randomly generated population, but the individuals in the front are within the limits. By the last generation, almost all individuals in the population lie within the constraint limits. Also, for the signed field flatness, the front values tend to be negative even in the first generation. This conclusion is consistent with the finding of the field morphing exercise. The signed field flatness and frequency of the low brightness emittance factor case are -31.14 % and 1300.10216 MHz. The field profile for this case is shown in Figure 36. Its geometry is shown in Figure 37 and its geometry parameters are listed in Table 7.

These results demonstrate that the cavity geometry morphing optimization works. Further, they also show that this method can be used to improve an RF gun design

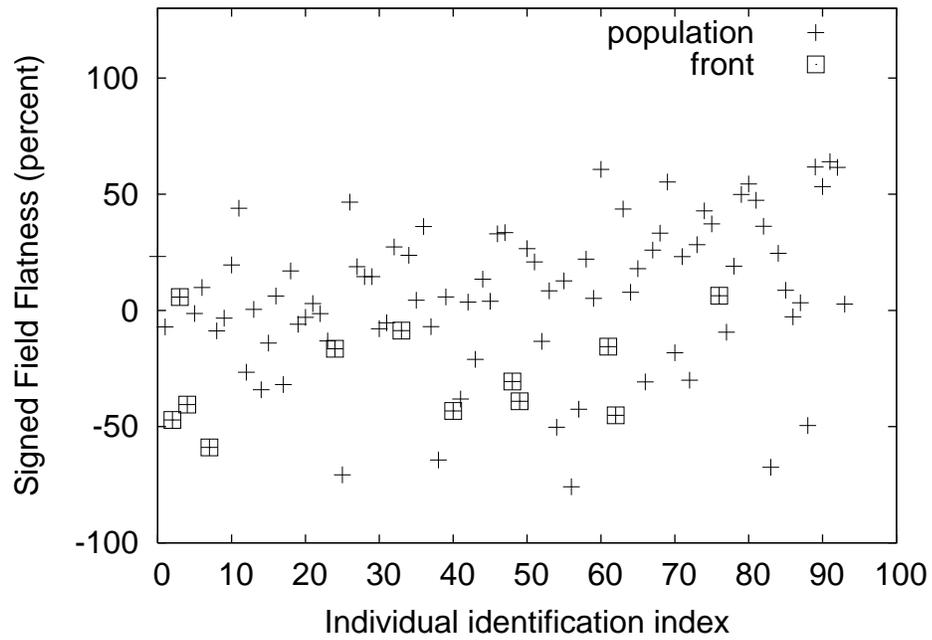


(a)

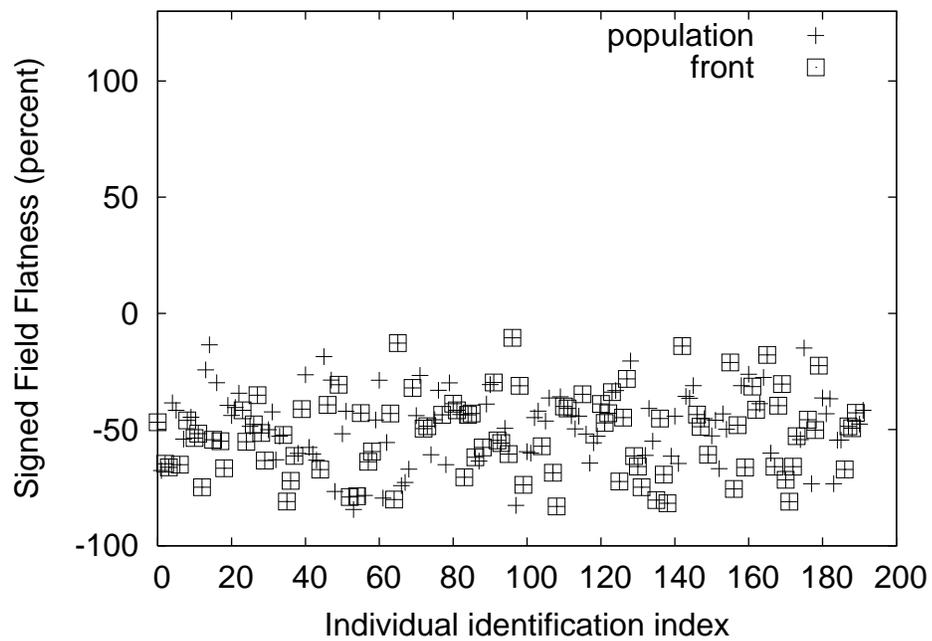


(b)

FIG. 34: Frequency for the first and last populations with members of the fronts marked: (a) first generation; (b) last generation.



(a)



(b)

FIG. 35: Signed flatness for the first and last populations with members of the fronts marked: (a) first generation; (b) last generation.

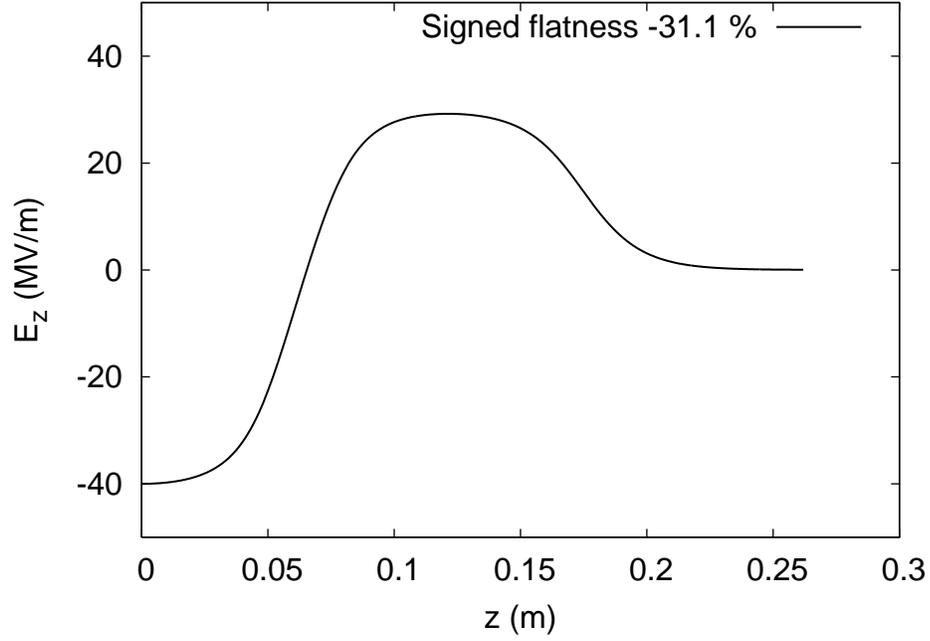


FIG. 36: Field profile for cavity geometry yielding transverse and longitudinal emittances  $2.1467 \pi$  mm mrad and  $31.834 \pi$  mm keV, respectively.

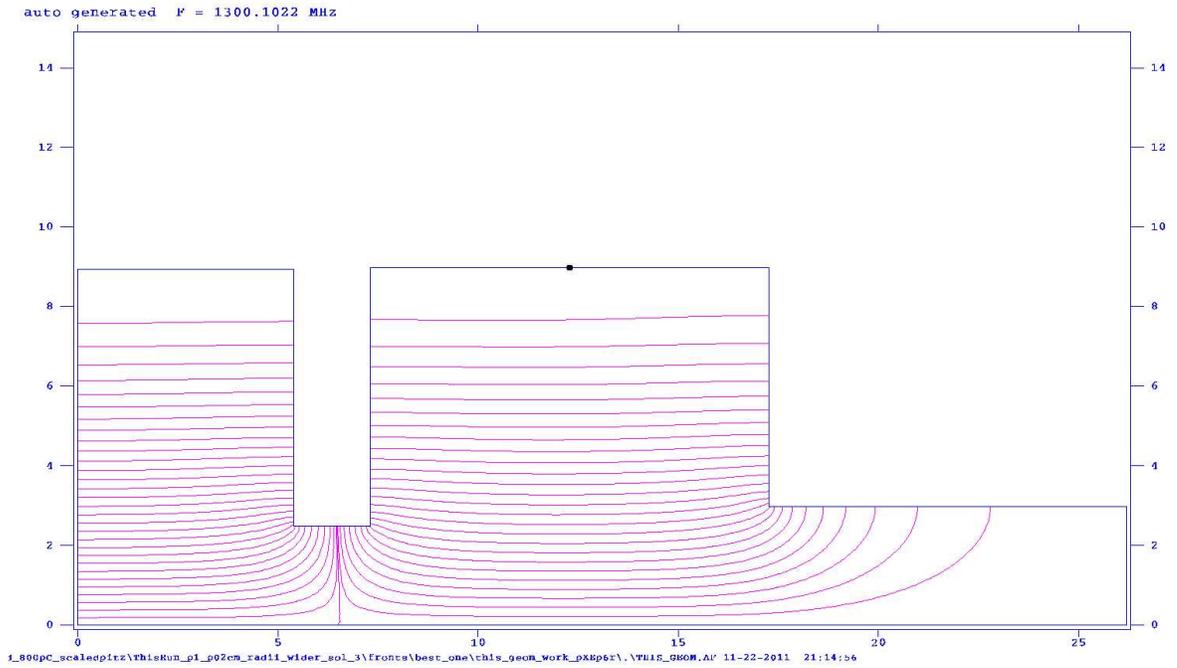


FIG. 37: Geometry for selected cavity geometry. Axes units are cm.

to produce a brighter beam. The previously mentioned field morphing method is not consistent with any reasonable geometric boundary conditions. That method suggests that skewing the field profile in the gun so that the peak amplitude is higher in the first cell leads to better emittance. The cavity morphing method adheres to boundary conditions by design, and the results from the cavity morphing method reinforce the field morphing conclusion. An RF gun made with the reported geometry will perform better from a brightness standpoint.

## CHAPTER 5

### SUMMARY AND CONCLUSION

RF guns are integral to the success of present and future accelerator based light sources. It is important for the designs of these devices to be optimized to produce the best quality beam as the requirement for brightness increases with each new light source. Automation of the injector design process is useful because it enables the injector designer to consider more designs more quickly. It also gives the designer the ability to consider more design parameters to identify perhaps subtle or unorthodox changes for improved performance. This conclusion summarizes the work performed in this research and its findings in support of automating the injector design process for RF guns. It also contains suggestions for improvements to the automated design system to make its results more physically realizable and the system easier to use in general. Finally, future research directions based on this work are listed.

This research has achieved two goals. The first is to develop a software tool that allows injector designers to optimize the field profile of an RF gun and the injector design in response to the performance characteristics of the beam dynamics. The second is to apply the system to a state of the art RF gun to improve its performance.

This research builds on an injector design automation tool, APISA, based on GAs. APISA was developed at Cornell and is in turn based on PISA from the ETH in Switzerland. GAs use a population-based approach to search the objective space for solutions to optimization problems with conflicting objectives and constraints. GAs are especially well suited for injector optimization because they do not use or require derivative information or analytical functional forms for the objectives or constraints. It is often the case with injector performance that the interrelationship between variables, objectives, and constraints is nonlinear or unknown. For that reason, APISA uses the beam dynamics simulation program ASTRA to model the injector and determine its performance characteristics. To extend APISA for use with RF guns, this research adds the ability to modify the field profile of the RF gun as part of the optimization. Previously, in APISA the field profiles were fixed.

Two methods for varying the field profile for the RF gun are provided. The first method, called field morphing, ignores physical boundary conditions. It assumes a functional form for the field profile to approximate the shape of a  $TM_{010}$  accelerating

$\pi$  mode of a multi-cell RF cavity. This approximate field profile can be modified then by a parameterized morphing function in response to the beam dynamics in the system. Despite having possibly non-physical boundary conditions, optimizations using this method can highlight desirable field characteristics to have in the field produced by a physical cavity geometry.

The second more realistic method, called geometry morphing, addresses the boundary condition deficiency of the first method. Because the field produced in an RF cavity is solely a function of the geometry of the cavity, this approach uses field profiles produced by an electromagnetic field solver for geometries of the RF gun that have been modified by the optimization. The dimensions of the RF gun cavity can be decision variables in the optimization that are changed in response to the beam dynamics performance. For each modified geometry description, the optimization system invokes the field solver to find the field profile to use in the beam dynamics simulation. A present limitation of this system is that it uses straight line approximations for the cavity geometries. As with the field morphing method, this method can identify desirable field profile characteristics and the types of cavity dimension changes needed to produce them.

Both methods have been applied to the state of the art PITZ 1.5 cell RF gun. In both instances, the optimizations indicated that improved emittance performance is possible with unbalanced field profiles. To date, RF gun designs have balanced field profiles. This conclusion is in line with accepted practice where the field amplitude peaks at the cathode in the half cell, but the results from the two methods go further in saying that the peak field should be much higher at the cathode than it is in the full cell. The cavity morphing method shows that an RF gun can be modified to produce a brighter beam if designed to produce these significantly unbalanced field profiles. It should be noted that no requirement on extracted beam energy is placed on the optimizations.

There are several possible improvements for the system. They fall into three categories. The first applies to the field morphing method. The second applies to the geometry description, and the third applies to the optimization system itself. Each will be described separately below.

Presently, the field morphing method can only morph the assumed form of the  $\pi$  mode approximation. The method may be more useful and have more real world applications if it morphed the field profile from a physical cavity. Additionally, the

field profile morphing method should be able to modify user provided field profiles from a variety of cavity geometries. These changes would extend the utility of the field morphing capability to other cavity geometries. Additionally, the peak field rescaling capability for cavity morphing should be implemented for field morphing.

The geometry description developed for this research is very flexible and could be extended to describe more detailed cavity geometries. For example, the geometry description could be improved to include rounded corners and curved surfaces to better reflect elliptical or re-entrant cavity geometries. Also, the addition of an axisymmetric field coupler element would allow the coupler geometry to be changed as part of the optimization and lead to better field representations in the coupler region even if held fixed. The cavity geometry naturally defines a set of apertures, or constrictions in the beam enclosure due to the irises in the cavity, and these apertures can affect particle transmission. The aperture information is not available from the existing system. It would be useful for the geometry description translation process to produce the size and location of beam line apertures to include in the beam dynamics simulation to account for this possible loss mechanism in the optimization. Finally, the geometry description assumes that the cavity origin,  $(r = 0, z = 0)$ , is located at the base of the first (most upstream) vertical wall. While this is perfect for RF guns where the center of the cathode is at  $(r = 0, z = 0)$ , it is not suitable for other cavity geometries where it is preferable to place the  $(r = 0, z = 0)$  location at the geometric center of the cavity. Making the origin user configurable would allow the same geometry description format to be used if the optimization system is extended to modify other cavities in the beam line in addition to the RF gun or in lieu of it.

The optimization system is very flexible and powerful, but it can be improved. First, the particle distribution creation system could be expanded. A useful addition to the existing particle distribution creation system is to allow the user to set distribution parameters to default or fixed values without using decision variables. The method used for setting defaults for the field morphing coefficients can serve as a model. Another suggestion is to allow the optimization system to use the particle distribution tool provided by the beam dynamics simulation program. Second, the methods for setting variables in the optimization without affecting the decision variable count should be expanded. It is now possible to establish a linear relationship between a decision variable and another variable in the optimization. Consideration should be given to nonlinear relationships. Third, the constraint system should be

expanded. It would be useful to be able to define constraints in terms of other variables in the system as opposed to fixed values. This would provide a way to order or prioritize constraints. For example, it might be useful to ensure that one constraint value is always less than another constraint value. Also, support for strict equality and weak inequality constraints could be added. The present workaround to provide an equality constraint is to define two bounding strict inequality constraints.

Two clear ways to improve the reliability of the system are outlined here. First, the system would benefit from a better way to identify and deal with failed or stuck program executions. Sometimes possible decision variable combinations are unfairly marked unsuitable simply because the simulation failed to complete in the allotted time. Increasing the time for each process is a work around but leads to unnecessarily long optimization execution times. The addition of diagnostics to identify stuck processes and the ability to optionally restart them would reduce the frequency of this problem. Second, incorporating a Windows based program in a high performance computing linux based environment presents its own challenges and contributes to the fragility of the system. Finding linux based alternatives would reduce the complexity of the system and increase its reliability.

In terms of usability, there are two recommendations to make the system easier to use. The first relates to the data produced by the system. The system produces a lot of very useful data, but there are few if any tools to organize and interpret the results. A system that uses the configuration information in the system to automatically aggregate and distill the data by generation, non-dominated front, decision variables, constraints, and objectives would greatly help in interpreting the data and bring to light the predictive nature of the evolution process. The second relates to the fragmented nature of the optimization configuration. Because configuration information is spread across several files in different locations, the initial set up of an optimization is fairly error prone. Centralizing the configuration information can address that problem.

Finally, this conclusion comes to the future directions for this research. Of a more immediate nature, for the PITZ gun design, the effect of adding the bucking solenoid to the system and varying the gradient of the gun can be studied. Also, imposing more constraints and objectives based on cavity and field characteristics may lead to additional cavity design recommendations. Using the existing cavity geometry morphing system, it is possible to study the effect of inclining the walls of

the gun cell toward each other. Also, the effectiveness of re-entrant cavity shapes for RF guns can also be considered with the existing system. The results of these studies could be further strengthened with the addition of curved cavity geometry shapes. Another outstanding question with respect to RF gun design is the optimal frequency. Presently, the frequency of the gun used in an injector design is determined by existing cavity designs and the underlying RF infrastructure. Free of these operational limitations, this optimization system can be used to see if there is a better operational frequency. Lastly, the field morphing method can be used to find an optimal number of cells for a gun design.

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## APPENDIX A

### ASTRA OVERVIEW

#### A.1 INTRODUCTION

ASTRA is a beam dynamics code used to model injectors in the accelerator community. It is mainly used to simulate cylindrically symmetric systems but has 3D capabilities [22]. This discussion describes the overall approach ASTRA uses for modeling charged particle beams with space charge forces in accelerator beam lines. All formulas and physical quantities in this discussion are expressed in SI (MKS) units. The ASTRA suite of programs are listed with descriptions in Table 8.

#### A.2 PHYSICAL SYSTEM TO SIMULATE

ASTRA numerically describes the interactions between a collection of charged particles with electromagnetic fields that exist outside the bunch (external fields) and those that originate from the close proximity of the charged particles in the bunch (internal self fields). In general, the Newton-Lorentz force equation [69],

$$\mathbf{F} = m \frac{d\mathbf{v}}{dt} = q (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \quad (5)$$

describes how a charged particle responds to electric and magnetic fields. The electric and magnetic fields, both internal and external, can be found using Maxwell's equations [47],

$$\nabla \cdot \mathbf{D} = \rho, \quad (6)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (7)$$

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}, \quad (8)$$

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0, \quad (9)$$

where, for charged particles in vacuum [70],  $\mathbf{D} = \varepsilon_0 \mathbf{E}$  is the electric displacement,  $\varepsilon_0$  is the electric permittivity of free space,  $\mathbf{E}$  is the electric field,  $\rho$  is the charge density,  $\mathbf{B} = \mu_0 \mathbf{H}$  is the magnetic induction,  $\mu_0$  is the magnetic permeability of free space,  $\mathbf{H}$  is the magnetic field, and  $\mathbf{J}$  is the current density or displacement current [47]. Because charged particle beams are typically accelerated to relativistic

TABLE 8: ASTRA programs and descriptions [22]

<b>Program</b>	<b>Description</b>
generator	Creates particle distributions from several different probability density functions based on user provided settings. These particle distributions establish the initial state of the particle bunch in terms of relative positions in space, time, momentum, and charge.
Astra	Beam dynamics simulation program. Its inputs are particle distributions, beam line descriptions, and field maps.
postpro	Graphics program to plot phase space related quantities
lineplot	Graphics program to plot calculated beam characteristics as a function of position along the beam line or scanned quantities for parameter scans.
fieldplot	Graphics program to plot field profiles for external and space charge fields.

energies, ASTRA incorporates aspects of special relativity in its calculations. For ease of discussion, the classical non-relativistic case is presented unless an idea or concept from special relativity is used or needed explicitly.

External electromagnetic fields are used to control the path, expanse, and energy of the particles [71,72]. External electric fields accelerate the particles when the field is directed along the beam path. These fields can be fixed for DC guns or time varying as produced in RF resonant cavities. The remaining external fields are magnetic and constitute the beam transport system [71,72]. The beam transport system is mainly responsible for containing the beam envelope which describes the extremes of all the possible paths that the particles in the bunch can follow along the beam line [71,72]. The beam transport system consists of various types of magnets including solenoids, dipoles, and quadrupoles [71,72]. Each magnet type serves a specific purpose in the beam transport system. Dipoles bend the beam in one plane. Solenoids focus or defocus the beam in all planes. Each solenoid's action depends on its length relative to the Larmor or cyclotron frequency [71,73],

$$\omega_L = \frac{q\mathbf{B}}{m}.$$

Quadrupoles act in two planes simultaneously focusing in one and defocusing in the other.

The internal fields are the particle self fields that give rise to space charge forces [70]. These forces push particles away from each other degrading the bunch and its quality, and this is unacceptable in many accelerator applications. Gravity and the earth's field are part of the physical system of a particle accelerator, but they are not explicitly accounted for in the simulation system. In general, the earth's field is not included in the model because the effect can be easily calculated and counterbalanced in the beam transport system design. Also, gravity is neglected because its effect is small compared to the forces that result from the electromagnetic field strengths used in the accelerators [14].

### A.3 PARTICLE BASED SIMULATION

A naïve approach to computing the trajectory of the particles in a charged particle bunch is to compute each individual particle trajectory. To find a single particle trajectory, the external and internal forces acting on the particle must be calculated. The self fields arise from the other particles in the bunch, and the interaction between the one particle and the remaining particles must be calculated. This process must then be repeated for each particle in the bunch. Because the number of particles is so large, computing all pair-wise interactions in a charged particle bunch is unreasonable. Instead, ASTRA uses macro-particles to describe the particle bunch [42, 69, 74]. Here, one simulation particle represents several particles in the physical bunch, and the macro-particle's properties reflect those of the individual particles it represents [42, 69, 74]. For charged particle beams, the collection of macro-particles maintains the charge to mass ratio of the physical beam [42, 69].

Once the number of macro-particles to represent the system is chosen, the physical particle distribution is partitioned into a spatial grid [42, 69, 74]. Most particle bunches in accelerators can be enclosed by a cylinder [25] that can be divided into thin rings populated with point-like particles [22]. ASTRA uses this ring based particle mesh approach. The grids extend just beyond the boundary of the bunch [22] and do not extend to the physical boundaries of the vacuum enclosure [69, 74].

Because the macro-particles are distributed across a grid and each macro-particle represents several physical particles, the movement or redistribution of individual

particles as a result of the forces acting on them has to be accounted for in the macro-particle model [42, 69]. ASTRA uses a ring based Particle in Cell (PIC) method [42, 69, 74] with cubic spline interpolation to determine the charge density for each grid cell for its cylindrically symmetric computations [22].

#### A.4 EXTERNAL FIELDS

ASTRA imports field calculation results computed by an electromagnetic field solver code [22] such as Poisson Superfish [24], Microwave Studio [75], or Opera3d [76]. It also uses internal numerical models for dipole and quadrupole elements [22]. When using fields calculated outside the simulation code, the fields can be described with three dimensional maps for which the system performs linear interpolations in three dimensions to find the necessary field values at a particle’s location [77]. For cylindrically symmetric systems only the electric or magnetic field amplitudes along the center axis,  $E_z(z, r = 0)$  or  $B_z(z, r = 0)$ , are required [22]. In this case, the other electric and magnetic field components for the RF cavity electric fields can be found using a subset of Maxwell’s equations [77],

$$\begin{aligned}\nabla \cdot \mathbf{E} &= 0, \\ \nabla \times \mathbf{B} &= \frac{1}{c^2} \frac{dE}{dt}.\end{aligned}$$

A similar technique can be used for the magnetic fields for the solenoids by solving  $\nabla \times \mathbf{B} = 0$  since  $\mathbf{J} = \mathbf{0}$  at  $r = 0$  (which is outside the area occupied by the current carrying magnet coils) [72]. For the electric fields that represent RF cavities, the time variation of the electric field amplitude is modeled with a sinusoid with a phase shift ( $\cos(\omega t + \varphi)$ ) [22]. ASTRA has analytic expressions with configurable parameters for dipoles and quadrupoles [22].

#### A.5 INTERNAL FIELDS

The Debye length [70],

$$\lambda_D = \left( \frac{\varepsilon_0 k_B T}{q^2 n} \right)^{\frac{1}{2}},$$

where  $k_B$  is Boltzmann’s constant,  $T$  is the temperature of the collection of particles in Kelvin, and  $n$  is the particle density, determines whether or not the self field or space charge of the electrons is significant [69, 70, 78]. For electron beams, if  $\lambda_D$  is smaller than the inter-particle spacing,  $\ell_p$ , then an electron’s self field is “shielded”

from the other electrons in the system and collisions between particles have to be considered [69, 70, 78]. Also as long as  $\lambda_D$  is much larger than  $\ell_p$ , the self field forces can be derived from smooth functions satisfying Poisson's equation

$$\nabla^2\varphi = -\frac{\rho}{\epsilon_o}, \quad (10)$$

and treated for other particles as external forces [70].

The size of  $\lambda_D$  relative to the bunch radius,  $r_{bunch}$ , is still more significant [70]. If  $\lambda_D$  is much smaller than or comparable to  $r_{bunch}$ , each particle's self field is significant and must be included in the simulation process [70]. When  $\lambda_D$  is much smaller than  $r_{bunch}$ , the flow of the particles can be assumed to be laminar meaning the particle paths do not cross [70]. When  $\lambda_D$  is comparable to  $r_{bunch}$ , this last assumption is no longer valid. The thermal velocity distribution of the particles must be considered, and the self fields become nonlinear [70]. If  $\lambda_D$  is larger than  $r_{bunch}$ , then self fields can be ignored entirely [70]. For context, consider that, for Jefferson Lab's polarized source,  $\lambda_D$  is 12.5  $\mu\text{m}$  and  $\ell_p$  is 5.92  $\mu\text{m}$  under the simplifying assumption that the 0.3 pC bunch is a 180  $\mu\text{m}$  long cylinder with a 600  $\mu\text{m}$  radius [79, 80]. Clearly,  $\lambda_D$  is much larger than  $\ell_p$  and much less than  $r_{bunch}$ , so the smooth self field and laminar flow approximations apply. ASTRA is applicable to beams in this regime where particle paths do not cross, space charge forces cannot be ignored, but can be found using Poisson's equation.

### A.5.1 SIMPLIFYING SELF FIELD CALCULATIONS BY LORENTZ TRANSFORMATION TO BUNCH REST FRAME

Because charged particle beams in particle accelerators move from non-relativistic to relativistic energies in relatively short distances ranging from a few centimeters to several meters, it is reasonable to calculate the space charge forces between particles in a reference frame that moves with the beam (rest frame) instead of the laboratory (lab) frame. The main advantage of this method is that evaluating the self fields becomes an electrostatic problem because the particles are at rest, so there is relatively little current flow to generate magnetic fields [22]. Another is that the relativistic form of the equations applies in the classical limit of Galilean relativity, so the transition from non-relativistic to relativistic energies is handled automatically [64].

To see how the self field calculation problem is simplified, consider the example of two Cartesian coordinate axes where one is fixed and the other, denoted with primes,

is attached to an electron moving at the speed of light in the positive  $x$  direction from Jackson [47]. The two sets of axes are coincident at  $t = t' = 0$ . The fields in the rest frame of the electron, observed from a point that is a distance  $b$  in the  $y$  direction from the origin of the lab frame are [47]

$$\begin{aligned} E'_x &= -\frac{qv t'}{4\pi\epsilon_0 r'^3}, \\ E'_y &= \frac{qb}{4\pi\epsilon_0 r'^3}, \\ E'_z &= B'_x = B'_y = B'_z = 0. \end{aligned}$$

Lorentz transforming back to the lab frame using [73]

$$\begin{aligned} E_x &= E'_x, \\ E_y &= \gamma [E'_y + v B'_x], \\ E_z &= \gamma [E'_z - v B'_y], \\ B_x &= B'_x, \\ B_y &= \gamma [B'_y - (v/c^2) E'_z], \\ B_z &= \gamma [B'_z + (v/c^2) E'_y], \\ \gamma &= [1 - (v/c)^2]^{-1/2}, \end{aligned}$$

and [73]

$$\begin{aligned} x &= \gamma [x' + vt'], \\ y &= y', \\ z &= z', \\ t &= \gamma [t' + (v/c^2) x'], \end{aligned}$$

reveals the magnetic field that is associated with the moving charge [47, 73]

$$\begin{aligned} E_x &= -\frac{\gamma qvt}{4\pi\epsilon_0 [(\gamma vt)^2 + b^2]^{3/2}}, \\ E_y &= \frac{\gamma qb}{4\pi\epsilon_0 [(\gamma vt)^2 + b^2]^{3/2}}, \\ E_z &= B_x = B_y = 0, \\ B_z &= \gamma \frac{v}{c^2} \frac{qb}{4\pi\epsilon_0 [(\gamma vt)^2 + b^2]^{3/2}} = \frac{\mu_0}{4\pi} \frac{\gamma qbv}{[(\gamma vt)^2 + b^2]^{3/2}}. \end{aligned}$$

Because under relativity the electric and magnetic fields are not independent, only one of the fields can be made to vanish in one of the two frames [47]. Even so, the ability to eliminate one field in one frame greatly simplifies the self field calculation.

A problem with this method is that ASTRA transforms the particle positions and velocities to the rest frame of the bunch using the average velocity of the bunch [22]. Not all of the particles in the bunch have this velocity; some particles move faster and some slower. This means that the magnetic fields do not completely vanish in this rest frame, and ASTRA is neglecting a possibly significant source of magnetic fields.

### A.5.2 SOLVING POISSON'S EQUATION

For electrostatic or nearly electrostatic ( $\rho$  varies slowly with time) problems,

$$\frac{\partial \mathbf{B}}{\partial t} = 0$$

(or approximately so). In this case, Maxwell's equations, (6) to (9) reduce to

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}, \quad (11)$$

$$\nabla \times \mathbf{E} = 0. \quad (12)$$

Now, a scalar potential,  $\varphi$ , satisfies (12) since

$$\nabla \times \nabla \varphi = 0,$$

so for

$$\mathbf{E} = -\nabla \varphi, \quad (13)$$

(11) and (12) can be combined to form Poisson's equation, (10) [47]. The process for finding  $\mathbf{E}$  is to find the potential,  $\varphi$ , from the charge density,  $\rho$ , using Poisson's equation and then find the electric field,  $\mathbf{E}$ , using (13).

One standard method for solving partial differential equations is to use Fourier series [81, 82]. Consider Poisson's equation for an  $a \times b$  rectangle in Cartesian coordinates

$$-\frac{\rho}{\varepsilon_0} = \frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} \quad (14)$$

with Dirichlet boundary conditions

$$\varphi(0, y) = \varphi(a, y) = \varphi(x, 0) = \varphi(x, b) = 0.$$

If  $\rho(x, y)$  and  $\varphi(x, y)$  are expressed as Fourier series [42, 83, 84]

$$\begin{aligned}\rho(x, y) &= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \alpha_{mn} \sin\left(\frac{m\pi x}{a}\right) \sin\left(\frac{n\pi y}{b}\right), \\ \varphi(x, y) &= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \beta_{mn} \sin\left(\frac{m\pi x}{a}\right) \sin\left(\frac{n\pi y}{b}\right),\end{aligned}$$

where  $\alpha_{mn}$  and  $\beta_{mn}$  are Fourier coefficients such that

$$\alpha_{mn} = \int_0^a d\xi \int_0^b \rho(\xi, \eta) \sin\frac{m\pi\xi}{a} \sin\frac{n\pi\eta}{b} d\eta$$

and  $\beta_{mn}$  depends on  $\alpha_{mn}$ , then (14) gives

$$\begin{aligned}\sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \alpha_{mn} \sin\left(\frac{m\pi x}{a}\right) \sin\left(\frac{n\pi y}{b}\right) \\ = \varepsilon_0 \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \beta_{mn} \left[ \left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2 \right] \sin\left(\frac{m\pi x}{a}\right) \sin\left(\frac{n\pi y}{b}\right).\end{aligned}$$

This leads to

$$\beta_{mn} = \frac{\alpha_{mn}}{\varepsilon_0 \left[ \left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2 \right]}$$

and, by (13), [42]

$$\begin{aligned}\mathbf{E} = - \left\{ \hat{i} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \beta_{mn} \frac{m\pi}{a} \cos\left(\frac{m\pi x}{a}\right) \sin\left(\frac{n\pi y}{b}\right) \right. \\ \left. + \hat{j} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \beta_{mn} \frac{n\pi}{b} \sin\left(\frac{m\pi x}{a}\right) \cos\left(\frac{n\pi y}{b}\right) \right\}.\end{aligned}$$

For cylindrically symmetric systems, the cylindrical form of Poisson's equation is used, and the  $a \times b$  rectangle is a representative planar section of a cylinder with radius  $a$  and length  $b$  [83]. The planar section is shown in Figure 38. The boundary conditions for the cylindrically symmetric system are slightly different [83]. Along  $r = a$ , the Dirichlet boundary condition still holds. Along  $r = 0$ , though, the boundary condition is Neumann, meaning the derivative of the normal is specified [81, 82], and for this case, it is zero. Finally, periodic boundary conditions are used at  $z = 0$  and  $z = b$ .

The numerical version for solving Poisson's equation using Fourier series is essentially the same except that it solves the finite difference form of Poisson's equation

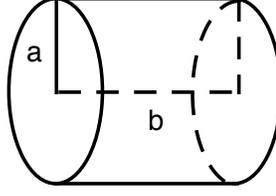


FIG. 38: Cylinder and planar section for Poisson's equation.

and takes advantage of Fast Fourier Transform techniques to compute the series solution for  $\rho$  from the charge distributed across the grid [42, 69, 83, 85]. The finite difference form of (14) is [42, 69, 74, 86, 87]

$$-\frac{\rho_{i,j}}{\varepsilon_0} = \frac{\varphi_{i+1,j} - 2\varphi_{i,j} + \varphi_{i-1,j}}{(\Delta x)^2} + \frac{\varphi_{i,j+1} - 2\varphi_{i,j} + \varphi_{i,j-1}}{(\Delta y)^2}.$$

The finite difference method of expressing differential equations is based on Maclaurin series expansions [86, 87]. The central difference based finite difference form of the first derivative in one dimension is [42, 87]

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

where  $h$  is the interval size between uniformly spaced  $x$  values. This expression is found from the difference of the two following Maclaurin series [42]

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(iv)}(x) + \dots \quad (15)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(iv)}(x) + \dots \quad (16)$$

The trivial derivation proceeds as

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{2h^3}{3!}f'''(x) + \dots$$

$$f(x+h) - f(x-h) = 2hf'(x) + O(h^3)$$

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + O(h^2).$$

The likewise  $O(h^2)$  second derivative used in Poisson's equation is found in a similar fashion by truncating the sums in (15) and (16) at the  $O(h^4)$  term and solving for  $f''(x)$  [42].

## A.6 SOLVING THE EQUATIONS: INTEGRATION

The final part of the simulation process after computing the individual fields and forces for each particle is to compute the particle trajectory. This involves computing the total force acting on each particle and then solving (5) numerically. The forces are treated as a sum of the forces due to external fields and forces from fields derived internally within the bunch [22, 70, 83]. ASTRA uses a fourth order Runge-Kutta method with adaptive step size to integrate the Lorentz force equation [22]. The fixed step Runge-Kutta method on which the adaptive step size version is based is described here.

Systems modeled with first order differential equations such as (5) can be integrated using the Runge-Kutta technique [42]. It is computationally quick, accurate, and self-starting. It calculates all quantities for a given instance of time in a single simulation time step [42]. The Runge-Kutta technique falls in the category of numerical methods that find a direct solution to first order differential equations with initial values (initial value problems) [42, 86, 87] of the form

$$\frac{dy}{dx} = f(x, y), \quad (17)$$

$$y(x_o) = y_o. \quad (18)$$

The general Runge-Kutta technique is an improvement on the Euler direct solution method [42, 86, 87]. The basis of the Euler method is that a point  $(x_1, \tilde{y}_1)$  on a curve's tangent at a nearby point  $(x_o, y_o)$  is a good approximation for the point  $(x_1, y_1)$  on the curve [42]. In terms of a truncated Maclaurin series development where  $h = x - x_o$ , the Euler method is derived from [42, 86, 87]

$$y(x) \approx y(x_o) + h \left. \frac{dy}{dx} \right|_{x_o} = y(x_o) + h y'(x_o). \quad (19)$$

By the system represented in (17) and (18), (19) becomes

$$y(x) \approx y(x_o) + h f(x_o, y(x_o)) = y_o + h f(x_o, y_o)$$

or, more generally, [42, 86, 87]

$$x_{n+1} = x_n + h,$$

$$y_{n+1} = y_n + h f(x_n, y_n).$$

The error for the Euler method is  $O(h)$  [42].

The Euler method can be improved with a better approximation for  $(x_1, y_1)$  derived from the average of the slopes at  $(x_o, y_o)$  and  $(x_1, y_1)$  [42] or

$$y_1 = y_o + \frac{h}{2}(y'_o + y'_1).$$

Here  $y'_o = f(x_o, y_o)$  is the same as before, but  $y'_1$  depends on  $y_1$ , an unknown. Using the simple Euler method to give an estimate for  $y_1$  [42],

$$\bar{y}_1 = y_o + hf(x_o, y_o),$$

leads to an estimate for  $y'_1$ ,

$$\bar{y}'_1 = f(x_1, \bar{y}_1).$$

Now,  $y_1$  is

$$y_1 = y_o + \frac{h}{2}\{f(x_o, y_o) + f(x_1, y_o + hf(x_o, y_o))\}.$$

The general scheme for the Euler predictor-corrector method with error  $O(h^2)$  is [42]

$$\begin{aligned} x_{n+1} &= x_n + h, \\ y_{n+1} &= y_n + \frac{1}{2}(k_1 + k_2), \\ k_1 &= hf(x_n, y_n), \\ k_2 &= hf(x_{n+1}, y_n + k_1). \end{aligned}$$

The Euler predictor-corrector method is an example of a second order Runge-Kutta method [42]. The most commonly used fourth order Runge-Kutta scheme is [87]

$$\begin{aligned} y_{n+1} &= y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4), \\ k_1 &= hf(x_n, y_n), \\ k_2 &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1\right), \\ k_3 &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_2\right), \\ k_4 &= hf(x_n + h, y_n + k_3). \end{aligned}$$

Fourth order Runge-Kutta methods have  $O(h^4)$  and require four evaluations of  $f(x, y)$ , but the increased accuracy offsets the computational expense [42].

## APPENDIX B

### POISSON SUPERFISH

#### B.1 INTRODUCTION

Poisson Superfish is an electromagnetic field solver from Los Alamos National Laboratory used in the accelerator community to calculate field information for magnets and cylindrically symmetric RF cavity elements [48]. It is a collection of programs that takes as input a geometry description of the structure of the magnet or the RF element and other relevant information such as boundary condition treatment, current flowing in magnet coil packs, and frequency for RF elements. From the geometry description, a grid is generated, and the fields are calculated on the grid. With the field and geometry information, various figures of merit and physical quantities of interest to accelerator designers are calculated [48]. This appendix provides a listing of the main Poisson Superfish programs in Table 9, and the methods used in Poisson Superfish to compute the fields for RF cavities.

What follows is a reorganized and annotated restatement of the derivations and information found in the theory summary of the document Poisson Superfish (LA-UR-96-1834 Revised December 10, 2005). This describes the equations that Poisson Superfish solves to calculate the field and the resonance frequency for a cavity. The numerical techniques used to compute solutions to these equations are not discussed.

#### B.2 DERIVATION OF GENERALIZED HELMHOLTZ EQUATION

To find the field of a mode, Maxwell's equations are simplified into two generalized Helmholtz equations, one for transverse magnetic (TM) modes and the other for transverse electric (TE) modes. Accelerator designers are typically more interested in TM modes because these are accelerating modes, so Poisson Superfish solves the TM mode version to find the cavity field. With an appropriate problem configuration, though, Poisson Superfish can solve for the TE mode. This section outlines the derivation of these generalized Helmholtz equations [48].

TABLE 9: Main Poisson Superfish programs [48]

Program	Description
automesh	Generates triangular mesh for problem geometry description
poisson	Solves Poisson's equation for magneto-static problems using successive over relaxation
pandira	Solves Poisson's equation for magneto-static problems using direct matrix inversion
fish	Solves wave equation/Helmholtz equation for cavity structures
sfo	Calculates various physical quantities and figures of merit for poisson, pandira, and fish solutions
wsfplot	Plots geometry, triangular mesh, and field contours for poisson, pandira, and fish solutions
sf7	Field interpolator
tblplot	Plots output from sf7
autofish	Runs automesh, fish, sfo, and wsfplot as one program

Maxwell's equations take the general form

$$\begin{aligned}
\nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t}, \\
\nabla \cdot \mathbf{D} &= \rho, \\
\nabla \times \mathbf{H} &= \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}, \\
\nabla \cdot \mathbf{B} &= 0,
\end{aligned}$$

where  $\mathbf{E}$  is the electric field,  $\mathbf{B}$  is the magnetic induction,  $\mathbf{D} = \varepsilon \mathbf{E}$  is the electric displacement,  $\varepsilon$  is the electric permittivity,  $\rho$  is the charge density,  $\mathbf{H} = \mathbf{B}/\mu$  is the magnetic field intensity,  $\mu$  is the magnetic permeability, and  $\mathbf{J}$  is the current density [47]. Because an accelerating cavity is a vacuum or dielectric filled space enclosed in a perfectly conducting surface, there is no charge density ( $\rho = 0$ ) or electric current density ( $\mathbf{J} = 0$ ) to create electric or magnetic fields in the cavity, so Poisson Superfish recasts Maxwell's equations in terms of two nonphysical quantities that mirror the functionality of the charge and current densities. These are magnetic

charge density,  $\sigma$ , and magnetic current density,  $\mathbf{K}$ . These new quantities then act as excitation sources for electric and magnetic fields in the cavity. The resulting set of equations that Poisson Superfish attempts to solve is

$$\nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t} + \mathbf{K}, \quad (20)$$

$$\nabla \cdot \mathbf{E} = 0, \quad (21)$$

$$\nabla \times \mathbf{H} = \varepsilon \frac{\partial \mathbf{E}}{\partial t}, \quad (22)$$

$$\nabla \cdot \mathbf{H} = \frac{\sigma}{\mu}. \quad (23)$$

Since  $\sigma$  and  $\mathbf{K}$  do not exist in reality, they should not be present in the final solutions to these equations. As the solutions approach resonance,  $\mathbf{K}$  diminishes to zero as required. Incidentally, these nonphysical quantities are the reason that a drive point location is needed in the geometry description. Poisson Superfish needs to have a source location for these quantities.

For three dimensional geometries such as RF cavities, Poisson Superfish takes advantage of the generally cylindrically symmetric nature of these devices and restricts itself to purely cylindrically symmetric problems. This implies that there is no azimuthal,  $\varphi$ , dependence in the fields (i.e.,  $\partial(\cdot)/\partial\varphi = 0$ ,  $\mathbf{E} = \mathbf{E}(r, z, t)$ , and  $\mathbf{B} = \mathbf{B}(r, z, t)$ ). (20) to (23) take the following forms with component expressions provided for reference. (20) becomes

$$\begin{aligned} \left(-\frac{\partial E_\varphi}{\partial z}\right) \hat{\mathbf{r}} + \left(\frac{\partial E_r}{\partial z} - \frac{\partial E_z}{\partial r}\right) \hat{\boldsymbol{\varphi}} + \frac{1}{r} \left(\frac{\partial(rE_\varphi)}{\partial r}\right) \hat{\mathbf{z}} \\ = -\mu \frac{\partial}{\partial t} (H_r \hat{\mathbf{r}} + H_\varphi \hat{\boldsymbol{\varphi}} + H_z \hat{\mathbf{z}}) + (K_r \hat{\mathbf{r}} + K_\varphi \hat{\boldsymbol{\varphi}} + K_z \hat{\mathbf{z}}), \end{aligned}$$

and in component form

$$-\frac{\partial E_\varphi}{\partial z} = -\mu \frac{\partial H_r}{\partial t} + K_r, \quad (24)$$

$$\frac{\partial E_r}{\partial z} - \frac{\partial E_z}{\partial r} = -\mu \frac{\partial H_\varphi}{\partial t} + K_\varphi, \quad (25)$$

$$\frac{1}{r} \left(\frac{\partial(rE_\varphi)}{\partial r}\right) = -\mu \frac{\partial H_z}{\partial t} + K_z. \quad (26)$$

(21) is

$$\frac{1}{r} \frac{\partial(rE_r)}{\partial r} + \frac{\partial E_z}{\partial z} = 0. \quad (27)$$

(22) becomes

$$\left(-\frac{\partial H_\varphi}{\partial z}\right) \hat{\mathbf{r}} + \left(\frac{\partial H_r}{\partial z} - \frac{\partial H_z}{\partial r}\right) \hat{\boldsymbol{\varphi}} + \frac{1}{r} \left(\frac{\partial(rH_\varphi)}{\partial r}\right) \hat{\mathbf{z}} = \varepsilon \frac{\partial}{\partial t} (E_r \hat{\mathbf{r}} + E_\varphi \hat{\boldsymbol{\varphi}} + E_z \hat{\mathbf{z}}),$$

and is written in component form as

$$-\frac{\partial H_\varphi}{\partial z} = \varepsilon \frac{\partial E_r}{\partial t}, \quad (28)$$

$$\frac{\partial H_r}{\partial z} - \frac{\partial H_z}{\partial r} = \varepsilon \frac{\partial E_\varphi}{\partial t}, \quad (29)$$

$$\frac{1}{r} \left( \frac{\partial (r H_\varphi)}{\partial r} \right) = \varepsilon \frac{\partial E_z}{\partial t}. \quad (30)$$

Finally, (23) is

$$\frac{1}{r} \frac{\partial (r H_r)}{\partial r} + \frac{\partial H_z}{\partial z} = \frac{\sigma}{\mu}. \quad (31)$$

These equations are combined to form the two Helmholtz equations and an analogy to the charge conservation equation. One Helmholtz equation in terms of  $E_\varphi$  is used to find TE modes, and the other in terms of  $H_\varphi$  is for TM modes.

The first step in deriving the  $E_\varphi$  equation is to combine (24), (26) and (29) to form one equation in terms of  $E_\varphi$ ,  $K_r$ , and  $K_z$

$$-\frac{\partial}{\partial r} \left[ \frac{1}{r} \frac{\partial (r E_\varphi)}{\partial r} \right] - \frac{\partial^2 E_\varphi}{\partial z^2} + \mu \varepsilon \frac{\partial^2 E_\varphi}{\partial t^2} = \frac{\partial K_r}{\partial z} - \frac{\partial K_z}{\partial r}. \quad (32)$$

This equation comes about after taking the partial derivative of (24) with respect to  $z$

$$\begin{aligned} \frac{\partial}{\partial z} \left( -\frac{\partial E_\varphi}{\partial z} \right) &= \frac{\partial}{\partial z} \left( -\mu \frac{\partial H_r}{\partial t} + K_r \right) \\ \frac{\partial}{\partial z} \left( -\frac{\partial E_\varphi}{\partial z} + \mu \frac{\partial H_r}{\partial t} \right) &= \frac{\partial K_r}{\partial z} \end{aligned}$$

to get

$$-\frac{\partial^2 E_\varphi}{\partial z^2} + \mu \frac{\partial^2 H_r}{\partial z \partial t} = \frac{\partial K_r}{\partial z}. \quad (33)$$

Similarly, for (26) the partial derivative with respect to  $r$  results in

$$\frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial (r E_\varphi)}{\partial r} \right) + \mu \frac{\partial^2 H_z}{\partial r \partial t} = \frac{\partial K_z}{\partial r}. \quad (34)$$

Next, subtracting (34) from (33) leads to

$$-\frac{\partial^2 E_\varphi}{\partial z^2} + \mu \frac{\partial^2 H_r}{\partial z \partial t} - \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial (r E_\varphi)}{\partial r} \right) - \mu \frac{\partial^2 H_z}{\partial r \partial t} = \frac{\partial K_r}{\partial z} - \frac{\partial K_z}{\partial r}.$$

Now, assuming separable and continuous functions (i.e., mixed partial derivatives commute) and using (29) to rewrite the  $H_r$  and  $H_z$  terms as an  $E_\varphi$  term, the result is (32). Note that the right hand side of (32) is the  $\varphi$  component of  $\nabla \times \mathbf{K}$  and can

be written as  $[\nabla \times \mathbf{K}]_\varphi$ . Likewise, (25), (28) and (30) can be combined to form one equation in terms of  $H_\varphi$  and  $K_r$

$$-\frac{\partial}{\partial r} \left[ \frac{1}{r} \frac{\partial (rH_\varphi)}{\partial r} \right] - \frac{\partial^2 H_\varphi}{\partial z^2} + \mu\varepsilon \frac{\partial^2 H_\varphi}{\partial t^2} = \varepsilon \frac{\partial K_\varphi}{\partial t}. \quad (35)$$

These equations can be simplified to be purely spatially dependent. Assuming that the time varying portion of  $\mathbf{K}$  is oscillatory,  $\mathbf{K}$  can be written as

$$\mathbf{K}(r, z, t) = \overline{\mathbf{K}}(r, z) \sin \omega t \quad (36)$$

where  $\omega = 2\pi f$  and  $f$  is the resonance frequency in Hertz. By the time dependence of  $E_\varphi$  in (32) and  $H_\varphi$  in (35), then  $E_\varphi$  and  $H_\varphi$  are

$$\begin{aligned} E_\varphi(r, z, t) &= \overline{E}_\varphi(r, z) \sin \omega t, \\ H_\varphi(r, z, t) &= \overline{H}_\varphi(r, z) \cos \omega t. \end{aligned} \quad (37)$$

In order to use the identical code to solve for TE and TM modes,  $H_\varphi$  is rescaled to have the same units as  $E_\varphi$  as follows

$$H_\varphi(r, z, t) = \sqrt{\frac{\varepsilon}{\mu}} \overline{H}_\varphi(r, z) \cos \omega t. \quad (38)$$

With the time behavior for  $E_\varphi$  and  $H_\varphi$  determined, the time dependence can be removed from (32) and (35) since each term has a common  $\sin \omega t$  factor after substituting in for  $E_\varphi$  and  $H_\varphi$ . Further, noting that for a cylindrically symmetric problem in cylindrical coordinates

$$\nabla^2 f = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial f}{\partial r} \right) + \frac{\partial^2 f}{\partial z^2}$$

the  $E_\varphi$  and  $H_\varphi$  derivative terms with respect to  $r$  and  $z$  can be combined, and the spatially dependent forms of (32) and (35) are

$$\nabla^2 \overline{E}_\varphi - \frac{1}{r^2} \overline{E}_\varphi + k^2 \overline{E}_\varphi = -[\nabla \times \overline{\mathbf{K}}]_\varphi \quad (39)$$

and

$$\nabla^2 \overline{H}_\varphi - \frac{1}{r^2} \overline{H}_\varphi + k^2 \overline{H}_\varphi = -k \sqrt{\frac{\varepsilon}{\mu}} \overline{K}_\varphi \quad (40)$$

where  $k = \sqrt{\mu\varepsilon}\omega$  is the eigenvalue. (39) and (40) are general forms of the Helmholtz equation. These are the equations that Poisson Superfish solves to find the fields.

Once solutions for  $\bar{E}_\varphi$  and  $\bar{H}_\varphi$ , and thereby  $E_\varphi$  and  $H_\varphi$ , are known,  $H_r$ ,  $H_z$ ,  $E_r$ , and  $E_z$  can be found by time integration of (24), (26), (28) and (30), respectively. The general forms of these solutions are

$$H_r = -\sqrt{\frac{\varepsilon}{\mu}} \frac{1}{k} \left( \frac{\partial \bar{E}_\varphi}{\partial z} + \bar{K}_r \right) \cos \omega t, \quad (41)$$

$$H_z = \sqrt{\frac{\varepsilon}{\mu}} \frac{1}{k} \left( \frac{1}{r} \frac{\partial (r \bar{E}_\varphi)}{\partial r} - \bar{K}_z \right) \cos \omega t, \quad (42)$$

$$E_r = -\frac{1}{k} \frac{\partial \bar{H}_\varphi}{\partial z} \sin \omega t, \quad (43)$$

$$E_z = \frac{1}{kr} \frac{\partial (r \bar{H}_\varphi)}{\partial r} \sin \omega t. \quad (44)$$

(43) and (44) satisfy (27). To satisfy (31) using (41) and (42), one develops a restriction for the magnetic charge and magnetic current densities akin to the electric charge continuity equation for the standard set of Maxwell's equations. This is the analogous magnet charge conservation

$$\nabla \cdot \bar{\mathbf{K}} \sin \omega t + \frac{\partial \sigma}{\partial t} = 0. \quad (45)$$

There is a sign difference though. Using (45) results in (31) giving  $-\sigma/\mu$  instead of  $\sigma/\mu$ .

### B.3 DERIVATION OF EQUATION FOR FINDING RESONANCE

Poisson Superfish uses a normalized quantity derived from the Poynting vector,  $\mathbf{S} = \mathbf{E} \times \mathbf{H}$ , to find the resonance frequency of a mode [88]. The normalized quantity in terms of the wave number,  $k = \omega/c = 2\pi f/c$  where  $f$  is the cavity frequency, is

$$D(k^2) = kc \frac{\int \sqrt{\frac{\varepsilon}{\mu}} \bar{\mathbf{H}} \cdot \bar{\mathbf{K}} dv}{\int \varepsilon \bar{H}^2 dv}. \quad (46)$$

To see how  $D(k^2)$  is useful in finding resonance, it is necessary to express it differently. In the process of deriving an alternative expression, (46) is also derived [48].

First, integrate the Poynting vector following the standard prescription of taking the divergence of  $\mathbf{S}$  and then applying the Divergence theorem to find an expression for the energy in the system. Using (20) and (22) from Maxwell's equations recast

in terms of  $\sigma$  and  $\mathbf{K}$  the divergence of  $\mathbf{S}$  is

$$\begin{aligned}
\nabla \cdot (\mathbf{E} \times \mathbf{H}) &= \mathbf{H} \cdot (\nabla \times \mathbf{E}) - \mathbf{E} \cdot (\nabla \times \mathbf{H}), \\
&= \mathbf{H} \cdot \left( -\mu \frac{\partial \mathbf{H}}{\partial t} + \mathbf{K} \right) - \mathbf{E} \cdot \left( \varepsilon \frac{\partial \mathbf{E}}{\partial t} \right), \\
&= -\mu \mathbf{H} \cdot \frac{\partial \mathbf{H}}{\partial t} + \mathbf{H} \cdot \mathbf{K} - \varepsilon \mathbf{E} \cdot \frac{\partial \mathbf{E}}{\partial t}, \\
&= \mathbf{H} \cdot \mathbf{K} - \left( \mu \mathbf{H} \cdot \frac{\partial \mathbf{H}}{\partial t} + \varepsilon \mathbf{E} \cdot \frac{\partial \mathbf{E}}{\partial t} \right), \\
&= \mathbf{H} \cdot \mathbf{K} - \frac{1}{2} \left( \varepsilon \frac{\partial E^2}{\partial t} + \mu \frac{\partial H^2}{\partial t} \right), \\
\nabla \cdot (\mathbf{E} \times \mathbf{H}) &= \mathbf{H} \cdot \mathbf{K} - \frac{1}{2} \frac{\partial}{\partial t} (\varepsilon E^2 + \mu H^2).
\end{aligned}$$

Note for  $\mathbf{E}$  and in like fashion for  $\mathbf{H}$  that

$$\frac{\partial}{\partial t} \left( \frac{\varepsilon E^2}{2} \right) = \frac{\varepsilon}{2} \frac{\partial}{\partial t} (\mathbf{E} \cdot \mathbf{E}) = \frac{\varepsilon}{2} 2\mathbf{E} \cdot \frac{\partial \mathbf{E}}{\partial t} = \varepsilon \mathbf{E} \cdot \frac{\partial \mathbf{E}}{\partial t}.$$

Integrating  $\nabla \cdot (\mathbf{E} \times \mathbf{H})$  over the volume of the closed surface  $a$  gives

$$\int \nabla \cdot (\mathbf{E} \times \mathbf{H}) dv = \int \mathbf{H} \cdot \mathbf{K} - \frac{1}{2} \frac{\partial}{\partial t} (\varepsilon E^2 + \mu H^2) dv.$$

The Divergence theorem changes the volume integral on the left hand side into a surface integral so

$$\oint (\mathbf{E} \times \mathbf{H}) \cdot d\mathbf{a} = \int \mathbf{H} \cdot \mathbf{K} dv - \frac{1}{2} \int \frac{\partial}{\partial t} (\varepsilon E^2 + \mu H^2) dv.$$

Rearranging terms and moving the time derivative outside the integral gives

$$\oint (\mathbf{E} \times \mathbf{H}) \cdot d\mathbf{a} + \frac{1}{2} \frac{\partial}{\partial t} \int \varepsilon E^2 + \mu H^2 dv = \int \mathbf{H} \cdot \mathbf{K} dv, \quad (47)$$

the Poynting theorem for cavity fields. This equation describes how energy changes inside the cavity and transfers in and out of it on the left side of the equation as a result of the rate of work done on the cavity field by the magnetic current,  $\mathbf{K}$ , on the right side.

Because the cavity surface  $a$  is closed, all energy stays within surface  $a$ . This means the first term in (47), describing energy entering and leaving the cavity through the boundary surface  $a$ , is zero. This leaves

$$\frac{1}{2} \frac{\partial}{\partial t} \int \varepsilon E^2 + \mu H^2 dv = \int \mathbf{H} \cdot \mathbf{K} dv. \quad (48)$$

The left side represents the time dependent change in energy in the fields in the cavity. Assuming the previously stated spatial and time dependence for  $\mathbf{K}$ ,  $\mathbf{E}$ , and  $\mathbf{H}$ , (36) to (38), gives

$$\mathbf{H} \cdot \mathbf{K} = \sqrt{\frac{\varepsilon}{\mu}} \bar{\mathbf{H}} \cdot \bar{\mathbf{K}} \sin \omega t \cos \omega t, \quad (49)$$

$$E^2 = \mathbf{E} \cdot \mathbf{E} = \bar{E}^2 \sin^2 \omega t, \quad (50)$$

$$H^2 = \mathbf{H} \cdot \mathbf{H} = \frac{\varepsilon}{\mu} \bar{H}^2 \cos^2 \omega t. \quad (51)$$

Now, using (49) in the right hand side of (48) gives

$$\int \mathbf{H} \cdot \mathbf{K} dv = \sin \omega t \cos \omega t \int \sqrt{\frac{\varepsilon}{\mu}} \bar{\mathbf{H}} \cdot \bar{\mathbf{K}} dv.$$

Using (50) and (51) in the left hand side of (48) gives

$$\frac{1}{2} \frac{\partial}{\partial t} \int \varepsilon E^2 + \mu H^2 dv = \omega \sin \omega t \cos \omega t \int \varepsilon (\bar{E}^2 - \bar{H}^2) dv.$$

Substituting these into (48) gives

$$\int \sqrt{\frac{\varepsilon}{\mu}} \bar{\mathbf{H}} \cdot \bar{\mathbf{K}} dv = \omega \int \varepsilon (\bar{E}^2 - \bar{H}^2) dv.$$

This can be used to construct  $D(k^2)$  and its alternative expression as follows

$$\begin{aligned} \int \sqrt{\frac{\varepsilon}{\mu}} \bar{\mathbf{H}} \cdot \bar{\mathbf{K}} dv &= \omega \int \varepsilon (\bar{E}^2 - \bar{H}^2) dv, \\ \omega \frac{\int \sqrt{\frac{\varepsilon}{\mu}} \bar{\mathbf{H}} \cdot \bar{\mathbf{K}} dv}{\int \varepsilon \bar{H}^2 dv} &= \omega^2 \frac{\int \varepsilon (\bar{E}^2 - \bar{H}^2) dv}{\int \varepsilon \bar{H}^2 dv}, \\ kc \frac{\int \sqrt{\frac{\varepsilon}{\mu}} \bar{\mathbf{H}} \cdot \bar{\mathbf{K}} dv}{\int \varepsilon \bar{H}^2 dv} &= (kc)^2 \frac{\int \varepsilon \bar{E}^2 dv}{\int \varepsilon \bar{H}^2 dv} - (kc)^2 \frac{\int \varepsilon \bar{H}^2 dv}{\int \varepsilon \bar{H}^2 dv}. \end{aligned}$$

Note the left hand side in the last line is (46).

$$D(k^2) = (kc)^2 \frac{\int \varepsilon \bar{E}^2 dv}{\int \varepsilon \bar{H}^2 dv} - (kc)^2.$$

From this formulation of  $D(k^2)$ , it is clear that on resonance, when the energy stored in the electric and magnetic fields is equal, the ratio of integrals is one and,

therefore,  $D(k^2)$  is zero. Finding the zeros of  $D(k^2)$  is the first step in determining the resonance frequency.

Unfortunately, not all zeros of  $D(k^2)$  correspond to structure resonances. The derivative of  $D(k^2)$  with respect to  $(kc)^2$  is used to identify true resonances. This derivative is

$$D'(k^2) = \frac{D(k^2)}{2(kc)^2} - \frac{1}{2} \frac{\int \varepsilon (\overline{E}^2 + \overline{H}^2) dv}{\int \varepsilon \overline{H}^2 dv}. \quad (52)$$

It evaluates to -1 when  $D(k^2)$  is zero and the energy stored in the electric and magnetic fields is equal,  $\overline{E} = \overline{H}$ , which is true on resonance. This means the second step for finding the resonance frequency is to check that  $D'(k^2)$  is -1 for the resonance in question.

The derivative for  $D(k^2)$  in (52) is found using the following steps. Rewriting (46) as a product in terms of  $(kc)^2$

$$D(k^2) = \sqrt{(kc)^2} \left( \int \sqrt{\frac{\varepsilon}{\mu}} \overline{\mathbf{H}} \cdot \overline{\mathbf{K}} dv \right) \left( \int \varepsilon \overline{H}^2 dv \right)^{-1},$$

and applying the chain and product rules gives three terms. The first term in the derivative is simply

$$\frac{\int \sqrt{\frac{\varepsilon}{\mu}} \overline{\mathbf{H}} \cdot \overline{\mathbf{K}} dv}{\int \varepsilon \overline{H}^2 dv} \frac{d}{d(kc)^2} \sqrt{(kc)^2} = \frac{1}{2kc} \frac{\int \sqrt{\frac{\varepsilon}{\mu}} \overline{\mathbf{H}} \cdot \overline{\mathbf{K}} dv}{\int \varepsilon \overline{H}^2 dv} = \frac{D(k^2)}{2(kc)^2},$$

the first term of in (52). The general expression for the second term in the derivative with  $\omega = kc$  is

$$\begin{aligned} \frac{kc}{\int \varepsilon \overline{H}^2 dv} \frac{d}{d(kc)^2} \left( \int \sqrt{\frac{\varepsilon}{\mu}} \overline{\mathbf{H}} \cdot \overline{\mathbf{K}} dv \right) &= \frac{kc}{\int \varepsilon \overline{H}^2 dv} \int \sqrt{\frac{\varepsilon}{\mu}} \frac{d}{d(kc)^2} (\overline{\mathbf{H}} \cdot \overline{\mathbf{K}}) dv, \\ &= \frac{\omega}{\int \varepsilon \overline{H}^2 dv} \int \sqrt{\frac{\varepsilon}{\mu}} \left[ \frac{d\overline{\mathbf{H}}}{d(kc)^2} \cdot \overline{\mathbf{K}} + \overline{\mathbf{H}} \cdot \frac{d\overline{\mathbf{K}}}{d(kc)^2} \right] dv, \\ &= \frac{\omega}{\int \varepsilon \overline{H}^2 dv} \int \sqrt{\frac{\varepsilon}{\mu}} \left[ \overline{\mathbf{H}}' \cdot \overline{\mathbf{K}} + \overline{\mathbf{H}} \cdot \overline{\mathbf{K}}' \right] dv. \end{aligned}$$

If, as  $\omega = kc$  nears resonance,  $\overline{\mathbf{K}}$  is changed slowly to keep  $\overline{H}^2$  constant, then  $\overline{\mathbf{H}}'$  and  $(\overline{H}^2)'$  are zero, and

$$\frac{kc}{\int \varepsilon \overline{H}^2 dv} \frac{d}{d(kc)^2} \left( \int \sqrt{\frac{\varepsilon}{\mu}} \overline{\mathbf{H}} \cdot \overline{\mathbf{K}} dv \right) = \frac{\omega}{\int \varepsilon \overline{H}^2 dv} \int \sqrt{\frac{\varepsilon}{\mu}} \overline{\mathbf{H}} \cdot \overline{\mathbf{K}}' dv.$$

This simplifies to the second term in (52) as will be shown subsequently. The third term is

$$\begin{aligned} kc \int \sqrt{\frac{\varepsilon}{\mu}} \bar{\mathbf{H}} \cdot \bar{\mathbf{K}} dv \frac{d}{d(kc)^2} \left( \int \varepsilon \bar{H}^2 dv \right)^{-1} \\ = -kc \frac{\int \sqrt{\frac{\varepsilon}{\mu}} \bar{\mathbf{H}} \cdot \bar{\mathbf{K}} dv}{\left( \int \varepsilon \bar{H}^2 dv \right)^2} \int \frac{d}{d(kc)^2} \left( \varepsilon \bar{H}^2 \right) dv = 0 \end{aligned}$$

because  $(H^2)' = 0$ . Combining all three terms gives

$$D'(k^2) = \frac{D(k^2)}{2(kc)^2} + \omega \frac{\int \sqrt{\frac{\varepsilon}{\mu}} \bar{\mathbf{H}} \cdot \bar{\mathbf{K}}' dv}{\int \varepsilon \bar{H}^2 dv}. \quad (53)$$

To convert (53) to the form in (52), use

$$\nabla \cdot (\bar{\mathbf{E}} \times \bar{\mathbf{H}}' - \bar{\mathbf{E}}' \times \bar{\mathbf{H}}) = \nabla \cdot (\bar{\mathbf{E}} \times \bar{\mathbf{H}}') - \nabla \cdot (\bar{\mathbf{E}}' \times \bar{\mathbf{H}}) \quad (54)$$

to derive an expression for the numerator of the second term. The left hand side expands to

$$\bar{\mathbf{H}}' \cdot (\nabla \times \bar{\mathbf{E}}) - \bar{\mathbf{E}} \cdot (\nabla \times \bar{\mathbf{H}}') - \bar{\mathbf{H}} \cdot (\nabla \times \bar{\mathbf{E}}') + \bar{\mathbf{E}}' \cdot (\nabla \times \bar{\mathbf{H}}). \quad (55)$$

Two of the curl terms are known from (20) and (22)

$$\begin{aligned} \nabla \times \bar{\mathbf{E}} &= \bar{\mathbf{K}} + \sqrt{\varepsilon\mu\omega} \bar{\mathbf{H}}, \\ \nabla \times \bar{\mathbf{H}} &= \sqrt{\varepsilon\mu\omega} \bar{\mathbf{E}}. \end{aligned}$$

Their associated derivatives with respect to  $(kc)^2$  are

$$\begin{aligned} \nabla \times \bar{\mathbf{E}}' &= \bar{\mathbf{K}}' + \sqrt{\varepsilon\mu} \left( \frac{\bar{\mathbf{H}}}{2\omega} + \omega \bar{\mathbf{H}}' \right), \\ \nabla \times \bar{\mathbf{H}}' &= \sqrt{\varepsilon\mu} \left( \frac{\bar{\mathbf{E}}}{2\omega} + \omega \bar{\mathbf{E}}' \right). \end{aligned}$$

Using these in (54) and (55) gives

$$\nabla \cdot (\bar{\mathbf{E}} \times \bar{\mathbf{H}}' - \bar{\mathbf{E}}' \times \bar{\mathbf{H}}) = \bar{\mathbf{H}}' \cdot \bar{\mathbf{K}} - \bar{\mathbf{H}} \cdot \bar{\mathbf{K}}' - \frac{\sqrt{\varepsilon\mu}}{2\omega} (\bar{E}^2 + \bar{H}^2).$$

Integrating and applying the Divergence theorem to the left hand side leads to

$$\int \nabla \cdot (\bar{\mathbf{E}} \times \bar{\mathbf{H}}' - \bar{\mathbf{E}}' \times \bar{\mathbf{H}}) dv = \oint (\bar{\mathbf{E}} \times \bar{\mathbf{H}}' - \bar{\mathbf{E}}' \times \bar{\mathbf{H}}) \cdot d\mathbf{a}.$$

With an appropriate choice of boundary conditions, the right hand side vanishes, leaving

$$\int \nabla \cdot (\bar{\mathbf{E}} \times \bar{\mathbf{H}}' - \bar{\mathbf{E}}' \times \bar{\mathbf{H}}) dv = 0$$

$$\int \bar{\mathbf{H}}' \cdot \bar{\mathbf{K}} - \bar{\mathbf{H}} \cdot \bar{\mathbf{K}}' - \frac{\sqrt{\varepsilon\mu}}{2\omega} (\bar{E}^2 + \bar{H}^2) dv = 0.$$

Multiplying through by  $-\sqrt{\varepsilon/\mu}$  gives

$$\int \sqrt{\frac{\varepsilon}{\mu}} \left[ \bar{\mathbf{H}} \cdot \bar{\mathbf{K}}' - \bar{\mathbf{H}}' \cdot \bar{\mathbf{K}} + \frac{\sqrt{\varepsilon\mu}}{2\omega} (\bar{E}^2 + \bar{H}^2) \right] dv = 0$$

$$\int \sqrt{\frac{\varepsilon}{\mu}} (\bar{\mathbf{H}} \cdot \bar{\mathbf{K}}' - \bar{\mathbf{H}}' \cdot \bar{\mathbf{K}}) dv = \frac{-1}{2\omega} \int \varepsilon (\bar{E}^2 + \bar{H}^2) dv.$$

For  $\bar{\mathbf{H}}' = 0$ , we have an expression for the numerator integral in (53)

$$\int \sqrt{\frac{\varepsilon}{\mu}} \bar{\mathbf{H}} \cdot \bar{\mathbf{K}}' dv = \frac{-1}{2\omega} \int \varepsilon (\bar{E}^2 + \bar{H}^2) dv$$

and substituting it in to (53) gives (52).

## APPENDIX C

### APISA USER'S GUIDE

#### C.1 INTRODUCTION

The purpose of this appendix is to describe how to run and configure the optimization software. It follows the same order as 3.2 and 3.3. PISA will be discussed first, followed by APISA from Cornell, and finally, the additions to support this research. This is intended to serve as a user's guide for all of these programs and features.

#### C.2 PISA CONFIGURATION AND OPERATION

Recall that PISA is a system for easily mating MOOPs with EAs and GAs. Using two state machines, it separates the mating pool and archive selection from the problem model evaluation and individual creation. The state machines are referred to as the **selector** and the **variator**. Each state machine has a parameter file, and there is a set of files used for communication. This section describes the PISA files and how to run the system [21, 38, 41].

The **selector** state machine parameter file is specific to the EA, and since SPEA2 is used here, only its parameter file will be discussed. The default PISA SPEA2 parameter file contains

```
seed          11
tournament    2
```

The **seed** parameter is the seed for the random number generator. The **tournament** parameter specifies how many individuals participate in each tournament during tournament selection for the mating pool. In this example, two individuals are randomly picked to participate in each tournament. As stated previously, the SPEA2 algorithm also takes into account the distance (Euclidean norm) between individuals using the  $k$ -th nearest neighbor. In PISA for simplicity  $k$  is set to 1.

The **variator** configuration file contains more parameters since it sets up the problem to solve and controls more aspects of the optimization. It sets the maximum number of generations to produce and the name of the benchmark problem to run. An example PISA **variator** parameter file is

<code>problem</code>	KUR
<code>seed</code>	142
<code>number_decision_variables</code>	2
<code>maxgen</code>	100
<code>outputfile</code>	<code>dtlz_output.txt</code>
<code>individual_mutation_probability</code>	1
<code>individual_recombination_probability</code>	1
<code>variable_mutation_probability</code>	1
<code>variable_swap_probability</code>	0.5
<code>variable_recombination_probability</code>	1
<code>eta_mutation</code>	20
<code>eta_recombination</code>	15

The problems defined in the `variator` are named according to the authors who suggested them [89,90]. The `problem` parameter sets the problem to optimize. The `seed` parameter seeds the random number used in creating offspring individuals from individuals in the mating pool. The `number_decision_variables` parameter sets how many decision variables to use for the selected problem. The maximum number of generations to produce is set with the `maxgen` parameter. The file named in `outputfile` is where the results of the optimization are written. Specifically, this is the information for the latest set of archive individuals identified by the `selector` state machine. The information includes the decision variable settings and objective values.

The remaining parameters in the `variator` configuration file pertain to generating offspring. The parameters, `individual_recombination_probability` and `individual_mutation_probability`, are threshold probabilities for the recombination and mutations respectively. In order for the process to occur, a uniformly generated number between 0 and 1 must be less than or equal to the threshold. In this example, the threshold probabilities are both one, so both processes are allowed for all individuals. The two recombination methods, uniform crossover and SBX, also have threshold parameters. The `variable_swap_probability` parameter applies to uniform crossover while `variable_recombination_probability` applies to SBX. For individuals that undergo recombination, for this example, uniform crossover is applied to roughly 50 % of those individuals, and SBX is always applied. The

`eta_recombination` parameter is the  $\eta_{SBX}$  factor in the probability density function used in the SBX algorithm. Similarly, the `variable_mutation_probability` and `eta_mutation` parameters govern the polynomial mutation process, and `eta_mutation` is the  $\eta_{pm}$  parameter for its probability density function.

Six files are used for communication between the state machines. They share a common prefix chosen by the user and are designated by suffixes, `arc`, `cfg`, `ini`, `sel`, `sta`, and `var`. The `cfg` file is provided by the user and is used by both the `selector` and `variator`. The remaining files are generated by the state machines.

The `cfg` file defines characteristics of the population, `alpha`, `mu`, `lambda`, and `dim`. The default PISA `cfg` file contains

```
alpha      10
mu         10
lambda     10
dim        2
```

`alpha` is the number of individuals to generate for the initial population. `mu` is the number of individuals to use as parents, and `lambda` is the number of children or offspring to produce. For SPEA2, `mu` and `lambda` are equal. Lastly, `dim` is the number of objectives.

The `ini` and `var` files are similar. They are created by the `variator` for use by the `selector`. They both contain a list of the individual identifiers and objective information. The `ini` file provides data about the initial population, and the `var` file does the same for subsequent generations.

The `arc` and `sel` files are created by the `selector`. The `sel` file lists the individual identifiers for the mating pool, and the `arc` file lists the identifiers for the archive. These files are used by the `variator`. The `variator` uses the `arc` file information to prune individuals from the population.

Finally, the `sta` file is alternately written and read by both state machines. It is used to keep track of the current state of the state machine processes. To facilitate the easy interchange of `variators` and `selectors`, the PISA state machines have a common simple structure of numbered states. The `variator` uses even numbered states starting with zero while the `selector` uses odd numbered states. The `sta` file is the semaphore file mentioned previously. The state machines poll this file to coordinate processing. The active state machine, when it is finished, writes the next successive state number to the file. For example, after completing initialization, state

0, the `variator` state machine writes a 1 to the `sta` file. This signals the `selector` state machine to proceed to state 1.

To run the system, first the `variator` is started, and then the `selector` is started. The argument list for the `variator` and the `selector` is the same. The first argument is the program's parameter file, followed by a tag name for the optimization. This tag is the prefix name for the six communication files. The last argument is the polling interval in seconds. Here is an example calling sequence for a computer running the `c` shell on linux [54,59]

```
variator variator_parameter.txt TAG 0.2 >& variator.out &
selector selector_parameter.txt TAG 0.2 >& selector.out &
```

This starts a `variator` process in the background using the configuration information in `variator_parameter.txt` and `TAGcfg`. This process will check the `TAGsta` file once every 0.2 seconds. Any standard or error output is captured in `variator.out`. Similarly, the `selector` process is then started using `selector_parameter.txt` and `TAGcfg` with its output and errors logged in `selector.out`. The general purpose names `variator` and `selector` are used for the executables in this example, but the processes can be named differently.

### C.3 APISA SET UP

APISA [13] keeps the configuration system from PISA and builds on it. The changes to the files used to communicate to the `variator` and `selector` processes are described first. Next, the differences between the PISA and APISA `variator` and `selector` specific parameter files are covered, and finally, descriptions of configuration files added to the system complete the configuration file discussion.

Because the constraint value information is generated in the `variator` and used in the `selector`, both state machines need to know the number of constraints in a problem. For that reason, the number of constraints is added to the `cfg` file since both programs read it. An example `cfg` file setting up a problem expecting 6 constraints is

```
initial_population_size      8
parent_set_size              8
offspring_set_size           8
objectives                   2
```

## constraints

6

Note that in APISA the original variable names have been changed for readability. `alpha` has been renamed `initial_population_size`. `mu` is the same as `parent_set_size`. `lambda` is `offspring_set_size`. Finally, `dim` has become objectives.

In APISA, the `ini` and `var` files include values of the constraints in addition to the objectives. The `sel`, `arc`, and `sta` files are unchanged. APISA adds an output file to the common communication files to use for tracking the optimization. This new file is a history file (`his`) and is not required for the operation of either state machine to run. It is an information file created by the `variator` process. Since it is configured in the `variator` parameter file, it is discussed subsequently in the `variator` parameter file description.

The `selector` configuration file for SPEA2 has two additions, `k_neighbor` and `verbose` as shown

```
seed          11
tournament    2
k_neighbor    Sqrt
verbose       YES
```

The `k_neighbor` parameter makes it possible to set the  $k$  in the  $k$ -th nearest neighbor routine. It can be set to `Sqrt` to use the prescribed value in SPEA2 ( $\sqrt{N + \bar{N}}$ ) or to a positive integer. Debug information is written to the file `spea2_diag.log` when `verbose` is set to `YES`. This information includes the generation number and number of non-dominated individuals in the present archive.

The `variator` configuration file has a few additions. These are discussed next. An example file is

```
problem                ASTRA
astra_parameter_file    /full/path/to/ASTRA/cfg/ast_param
seed                    142
number_decision_variables 3
maxgen                  2
force_selection         NO
use_initial_decision_variables NO
use_initial_objectives  NO
```

<code>initial_data_file</code>	<code>/full/path/to/restart/file/initial.txt</code>
<code>outputfile</code>	<code>output.txt</code>
<code>individual_mutation_probability</code>	<code>1</code>
<code>individual_recombination_probability</code>	<code>1</code>
<code>variable_mutation_probability</code>	<code>1</code>
<code>variable_swap_probability</code>	<code>0.17</code>
<code>variable_recombination_probability</code>	<code>1</code>
<code>eta_mutation</code>	<code>20</code>
<code>eta_recombination</code>	<code>10</code>
<code>rotate_cw_objective12(deg)</code>	<code>0</code>
<code>append_last_generation</code>	<code>YES</code>

Although the parameter is not new, APISA adds a new **problem** type called **ASTRA**. This setting directs APISA to use ASTRA for problem evaluations. The related parameter addition is `astra_parameter_file`. The information in this tells the optimization where to find ASTRA-related set up information. The contents of this file are discussed below. ASTRA input files, their formats, and details of running ASTRA simulations are not discussed. The interested reader is referred to the ASTRA documentation [22].

Before proceeding with the discussion of the additions to the **variator** parameters, some minor changes related to file output are described first. Because APISA includes constraints, these values are included in the contents of the `outputfile` file. Similar to the `spea2_diag.log` file, diagnostic information for the **variator** is always written to `var_diag.log`; it does not have a `verbose` switch. The information written to the file includes the active nodes and the start time for each generation.

Three additions to the **variator** configuration file provide an optimization restart mechanism: `use_initial_decision_variables`, `use_initial_objectives`, and `initial_data_file`. When `use_initial_decision_variables` is set to **YES**, APISA will read decision variable settings from the file named in the `initial_data_file` file. This file contains one line per individual to add to the population, and each line contains the values for the decision variables, the objectives, and the constraints. If `use_initial_decision_variables` is set to **NO**, all individuals in the initial population are generated randomly, and warm restart is not used. The `use_initial_objectives` parameter is similar to the `use_initial_decision_variables` parameter, but it determines whether or not

the objective and constraint information is used from the file. If set to YES, the data in the file is used. If set to NO, the associated ASTRA simulations are run, and the objective and constraints values are determined from the ASTRA output files.

The `force_selection` parameter directs APISA to use results from previous generations that are still in the population (from the archive). This can reduce the number of individuals that need to be generated but can cause unexpected results [91]. This parameter should be used with care.

The `rotate_cw_objective12(deg)` parameter is specific to Cornell University's usage and is not generally useful. It assumes that the first two objectives for the optimization are related by a rotation. The angle specified is used in the rotation matrix to compute the rotated (or unrotated) values.

The `append_last_generation` parameter determines whether the `his` file mentioned previously in the communication file discussion contains a complete history (YES) or not (NO) for the optimization. If a complete history is generated, APISA appends the population information for each generation to the file. The population contains the archive and the new individuals created. The information provided is the same as in the `outputfile`, namely the values for the decision variables, objectives, and constraints. This allows one to see how the archive develops as the optimization progresses. If the parameter is set to NO, only the results for the last generation are provided as APISA overwrites the file each generation. In this case, the contents of the `his` file are the same as `outputfile`.

The file named in `astra_parameter_file` contains mainly administrative information such as path names for ASTRA and APISA files and maximum time allotments for job management. An example file contains

```

astra_binary           /full/path/to/ASTRA/executable/Astra
astra_input_file       /full/path/to/ASTRA/input/file/gun.in
available_nodes_file   /full/path/to/computer/list/nodes_list
night_nodes_file       NONE
max_jobs_node_file     NONE
check_nodes            YES
check_nodes_wait(sec)  30
maximum_time_per_job(min) 6000
maximum_jobs_per_node  1
keep_in_purgatory(sec) 60

```

```

niceness_level          0
use_unused_nodes_only  NO
users_usage_threshold  25.0
system_usage_threshold 25.0
node_inactive_wait(min) 15.0
generate_distributions  NO
append_results_file    /full/path/for/debug/data/RESULTS
distribution_directory  /full/path/for/new/distributions/dist
number_particles       1000
astra_output_names_file /full/path/to/ASTRA/out/data/ast_name
decision_variables_file /full/path/to/decision/cfg/decisions
objectives_file        /full/path/to/objective/cfg/objectives
constraints_file       /full/path/to/constraint/cfg/constraints

```

The file contents are described in terms of groups of related variables, and therefore will be discussed out of order relative to the example.

Beyond a linux or unix like operating system, APISA makes no assumptions about the file system or location of files. This makes APISA very configurable and means the user has to specify several file locations. The first two variables in the ASTRA set up file, `astra_binary` and `astra_input_file`, provide the location of the ASTRA program executable and the ASTRA input file to use as a template for each ASTRA run. For each individual, APISA makes a customized copy of the template file reflecting the individual's decision variable values to use as input to ASTRA. The individual ASTRA input files use the base name of the template file, `gun` in this case, followed by an individual identification number and a computer name. An example individual ASTRA input file name is `gun.000000008.computer1.in`.

The next set of ASTRA variables is located in the lower half of the file. These relate to the particle distribution. The `generate_distributions` variable indicates whether APISA should generate a particle distribution for each individual (YES) or use one particle distribution provided by the user for all individuals (NO). If the variable is set to YES, APISA will generate particle distributions containing the number of macro-particles specified with `number_particles` and put the files in the directory named in `distribution_directory`. Each distribution file is named according to its corresponding ASTRA input file but with a `.dis` file extension. For the example input file above, its generated distribution file is `gun.000000008.computer1.dis`.

APISA also changes the individual's ASTRA input file to include the name of the generated distribution file. If the distribution directory variable is set to `DEFAULT`, the distribution files are placed in the same directory as the template ASTRA input file. If the generate distributions parameter is set to `NO`, the values for the two other parameters are ignored, and ASTRA simply uses the particle distribution file named in the ASTRA template file. Although unused in this research, APISA's distribution capability is described briefly below in C.4 for completeness.

The last ASTRA related setting provides names and units to attach to data found in ASTRA emittance (`Xemit`, `Yemit`, and `Zemit`) data files since these output files contain only data tables without column headings [22]. These files contain beam characteristics calculated from the particle distribution at user designated points along the beam line. This name and unit information is contained in the file designated in `astra_output_names_file`. This file typically contains

```
z[m] t[ns] <x>[mm] s_x[mm] s_xp[mr] ex[mm-mr] <xyp>[mr]
z[m] t[ns] <y>[mm] s_y[mm] s_yp[mr] ey[mm-mr] <yyp>[mr]
z[m] t[ns] KE[MeV] s_z[mm] s_dE[keV] ez[mm-keV] <zde>[keV] .
```

The first and second lines are used for the data in the  $x$  and  $y$  emittance data files, respectively, and the third line is used for the  $z$  or longitudinal emittance output. The descriptions of these values and data files are in the ASTRA documentation [22]. Briefly, though, the first two columns in each line of these files contain the position in  $z$  and corresponding time for the recorded data. The remaining columns report the statistical moments of the particle distribution. For the  $x$  and  $y$  files, these translate, respectively, to the center position of the beam, rms beam size, rms angular size or divergence, normalized transverse emittance, and correlation term of the emittance. For the  $z$  file, these are the kinetic energy of beam, bunch length, energy spread, normalized longitudinal emittance, and energy correlation term or chirp.

The last three parameters in the configuration file specify the locations and names of the files providing the decision variables, objectives, and constraints for the optimization problem. These parameters are `decision_variables_file`, `objectives_file`, and `constraints_file`. Although it is a minor detour from the parameters in the `astra_parameter_file` file discussion, a description of each file immediately follows.

The decision variables file provides a list of ASTRA input file variables or initial particle distribution parameters, discussed in C.4, to change and the upper and lower

bounds for the generated values. An example decision variable file is

```
MaxB(1)  VARY                -0.179  -0.168
MaxB(2)  VARY  |->  MaxB(1)  0.5      1.0
MaxB(3)  VARY  |->  MaxB(1)  0         0
```

This three line example shows the two possible decision variable declarations. Each line designates a different solenoid field amplitude variable in the ASTRA input file to change. APISA uses the information in this file to generate values for these variables within the specified ranges for each individual in each generation. The first line indicates that the ASTRA input file variable `MaxB(1)` values are restricted to the range of -0.179 and -0.168 Tesla. The second line directs APISA to generate an offset for each individual between 0.5 and 1.0 Tesla and then sums it with that individual's `MaxB(1)` value to arrive at its value of `MaxB(2)`. The third line generates the value zero and sums it with the value of `MaxB(1)` to compute the value of `MaxB(3)`. This last line shows how to make two decision variables have the same value in Cornell's original version of APISA, and an alternative approach is presented in C.5.2. In this example while `MaxB(1)` differs between individuals, for each individual, `MaxB(3)` and `MaxB(1)` are always set to the same value.

The constraints file lists the ASTRA output and decision variables that are used as constraints in the optimization. As stated earlier, the constraints are limited to strict inequalities and are designated using the keywords `GREATER_THAN` and `LESS_THAN`. Each line in the file contains an output variable name followed by an inequality keyword and the upper or lower bound value. In the example below the horizontal beam size (`s_x`) must be greater than 1.0 mm, and the vertical beam size (`s_y`) must be less than 4.0 mm.

```
s_x  GREATER_THAN  1.0
s_y  LESS_THAN     4.0
```

The objectives file lists the objectives of the optimization, and because the system is designed to optimize a multi-objective system, the file must contain at least two objectives. An objective file entry contains an ASTRA output or decision variable followed by the keyword `MAXIMIZE` or `MINIMIZE`, depending on the optimization goal for the value. In this example the emittance in both the horizontal and vertical planes must be minimized.

```
ex MINIMIZE
ey MINIMIZE
```

Returning to the parameters in the `astra_parameter_file` file discussion, the remainder of the parameters in the ASTRA set up file either aid in debugging and tracking the progress of the optimization or are used to manage APISA in a parallel computing environment. The parallel computing controls are designed to allow APISA to run in any linux environment where there is a shared file system. That flexibility points to several configuration parameters and are discussed after the debug and tracking variables.

`append_results_file` can be used to track the optimization progress. This is different from the `outputfile` and `his` files described above. Its purpose is to create a record of all the various output values from ASTRA or computed from ASTRA results and the decision variable settings. The two previously discussed files provide values for the decision variables, objectives, and constraints, a considerably smaller set of values. If `append_results_file` is set to `NONE`, no file is created. If it is set otherwise, its value is used as the name of the file to create. In the example above, the created file is named `RESULTS`. After the first individual finishes processing, APISA writes to the bottom of the specified file the time that the optimization started along with the names of the decision and ASTRA output parameters. Then as each individual (including the first) finishes processing, APISA appends the decision variable and ASTRA output values to the file.

Another variable that can be used to monitor APISA intermediate results is `keep_in_purgatory(sec)`. APISA by default cleans up as it proceeds removing generated files once they are no longer needed. This reduces file system clutter as the process runs but can hamper debugging as ASTRA output files that a user may want to inspect disappear very soon after the ASTRA simulation stops. Setting the `keep_in_purgatory(sec)` parameter instructs APISA to wait the specified number of seconds after the ASTRA simulation completes before removing the files. In this example, APISA waits 60 seconds before removing files.

The discussion moves now to the parallel processing controls. These parameters are repeated here

```
available_nodes_file
night_nodes_file
max_jobs_node_file
```

```

check_nodes
check_nodes_wait(sec)
maximum_time_per_job(min)
maximum_jobs_per_node
niceness_level
use_unused_nodes_only
users_usage_threshold
system_usage_threshold
node_inactive_wait(min)

```

APISA is designed to run the ASTRA jobs for each generation in parallel and has been adapted to run in traditional and nontraditional parallel computing environments. It can run interactive jobs with user defined lower priorities on linux computers that share a file system. This second path can be used to create an informal parallel processing computing environment (such as an office environment), and several variables in the ASTRA set up file are available to tune running APISA concurrently on computers supporting interactive users.

As mentioned previously, for problems using a large number of individuals, it is best to run APISA on a cluster computer in order for them to finish processing in a reasonable length of time. The Portable Batch System (PBS) [92] for the cluster computer is used to request a group of computers to use and to start the `variator` and `selector` processes. Internally, APISA launches interactive shells on the individual nodes to run the ASTRA simulations. The list of nodes provided by the PBS is put in a file as part of the PBS job processing. That filename is used in the parameter discussed next.

The `available_nodes_file` contains a list of the computer nodes available for APISA to use and is required for all parallel computing environments. A node corresponds to a computer core. If a computer has a single quad core processor, and APISA is allowed to use all four cores, then the computer's name should appear four times in the node list file. APISA assigns to each node the model evaluation for an individual, but it relies on the linux operating system to balance the execution of the simulations among the available processors when multiple jobs are assigned to the same multi-processor computer.

The `check_nodes` and `check_nodes_wait(sec)` variables are used together to determine if a node is alive and therefore usable. If `check_nodes` is set to `YES`, when

APISA starts running, it will login into each computer in the `available_nodes_file` list and create an empty temporary file used only during the check nodes test. The `check_nodes_wait(sec)` variable determines how long APISA will wait before checking that the temporary file exists. If the file exists, APISA removes the file and marks the node usable. The time specified in `check_nodes_wait(sec)` is also used in other parts of the APISA processing for intermediate delays. If `check_nodes` is set to `NO`, APISA assumes the nodes are alive and ready for use.

The `maximum_time_per_job(min)` parameter specifies the maximum amount of wall clock time that APISA should allow for an individual's ASTRA simulation to complete. This parameter is used to decide if an ASTRA job is hung up. If a simulation has not completed within that time, APISA kills it, so the parameter should be set to ensure that the longest possible viable ASTRA simulation completes in time. If the longest simulation takes 30 minutes, then this parameter should be set to 31 minutes at a minimum.

The remaining parameters configure APISA processing to work in an environment that supports interactive users with minimal impact on those users. The first way to minimize APISA's impact on interactive users is to run ASTRA simulations at a lower priority than the default. When running in an ad hoc or informal parallel computing environment, APISA launches an interactive shell on the computer for each individual to run its ASTRA simulation. To lower the priority of the ASTRA simulations, APISA runs the simulations using the linux `nice` command. The value provided in `nice_level` is the niceness argument for the `nice` command. Another way to minimize interference with interactive users is to limit the number of jobs that APISA can run on each computer. The parameter `maximum_jobs_per_node` sets a default number of ASTRA simulations that can be run concurrently on a node where a node is a computer core. The file named in `max_jobs_node_file` can be used to provide a list of computers with individual job limits (`<computer_name> <number_of_jobs>`) to override the default value on a computer by computer basis. If the file name is `NONE`, then no overrides are needed, and the default is applied to all nodes.

A straightforward way to minimize the impact on interactive users is to run APISA when the interactive users are not using them, and this most likely occurs at night and on the weekends. The `night_nodes_file` parameter is the name of the file containing a list of computers that may be used without restriction during

these times. The `night_nodes_file` list of computers must appear in the master list of computers found in the `available_nodes_file` list. If the file name in `night_nodes_file` is something other than `NONE`, APISA checks the current time of day and day of the week for the after hours condition, and for computers in the night nodes list, APISA will send jobs to those computers during off-hours but not otherwise.

APISA can also be directed to monitor the usage of computers to see if they can support running ASTRA simulations. The last four parameters, `use_unused_nodes_only`, `users_usage_threshold`, `system_usage_threshold`, and `node_inactive_wait(min)`, work together to set up this mode of operation. The first parameter is set to `YES` or `NO`. When set to `NO`, APISA may use computers listed in the `available_nodes_file` list without restrictions. When set to `YES`, APISA uses the thresholds and time provided in the other three variables to determine if a computer is unused. If the user and system usage values as determined from the linux command `mpstat` are below the thresholds and remain below the thresholds for the specified amount of time, then APISA uses the computer until the user and system usages increase above the threshold. If these increases happen during an ASTRA simulation, the simulation process is killed.

#### C.4 DISTRIBUTION GENERATION IN APISA

As stated previously, it is possible to have APISA generate initial particle distributions to use in its ASTRA runs [13]. ASTRA provides a tool to generate initial particle distributions, but APISA does not use it. It can use ASTRA generated distributions as a fixed element of the optimization. If the user wants to vary the initial particle distribution as part of the optimization, APISA generates its own subject to parameters provided by the user as decision variables. The distributions that APISA generates are radially symmetric (cylinders) and simulate particles emitted from a photocathode. The settings for these distribution characteristics default to zero.

Some features of the particle distribution are not configurable. The angular distribution ( $\theta$ ) for the particle radial position is uniformly distributed over the range 0 to  $2\pi$ . A particle's transverse position is calculated in polar coordinates and then converted to Cartesian coordinates. The longitudinal position ( $z$ ) and momentum ( $p_z$ ) are uniformly zero, corresponding to all particles being emitted from the cathode surface located at  $z = 0$ .

The transverse momentum distributions ( $p_x, p_y$ ) are determined by the Maxwell-Boltzmann distribution to simulate thermal electrons. The general expression for this distribution is

$$f(p_x, p_y, p_z) = \frac{\exp\left(-\frac{p_x^2 + p_y^2 + p_z^2}{2mkT}\right)}{\sqrt[3]{2\pi mkT}}. \quad (56)$$

The configuration parameter is the distribution thermal energy in meV (DIST\_kT).

A so-called double-peak super-gaussian distribution is used to define the particle distribution time and radial profiles. The time distribution corresponds to time emitted from the photocathode. The parameters to define the distribution characteristics are

DIST\_XYtail  
 DIST\_XYdip  
 DIST\_XYellips  
 DIST\_Ttail  
 DIST\_Tdip  
 DIST\_Tellips  
 DIST\_Tslope

These control parameters can vary between 0 and 1. The tail variables, DIST\_XYtail for the transverse distribution and DIST\_Ttail for the time distribution, describe the size and shape of the distribution tails relative to its extent. Zero creates a distribution with no tails, and one leads to Gaussian shaped tails. Figure 39(a) provides illustrative examples. The dip variables, DIST\_XYdip and DIST\_Tdip, control the overlap between the two peaks in the double peak distribution. Zero gives a flattop, and the two peaks are merged to form one broad flattop profile. One means there are two distinct peaks as shown in Figure 39(b). The ellipse parameters, DIST\_XYellips and DIST\_Tellips, refer to the curvature of the flattop region. For zero, there is no curvature (top hat), while one leads to an ellipse. This progression is clear in Figure 39(c).

The distribution in time has an additional control for slope, DIST\_Tslope. This parameter changes the relative heights of the peaks in the double peak distribution. It skews the distribution relative to the first peak. If the slope is zero, the two peaks are of equal height or as in Figure 39(d) where there is only one flattop peak, a flat line. For a slope of one, the first peak is increased, and the second peak is greatly

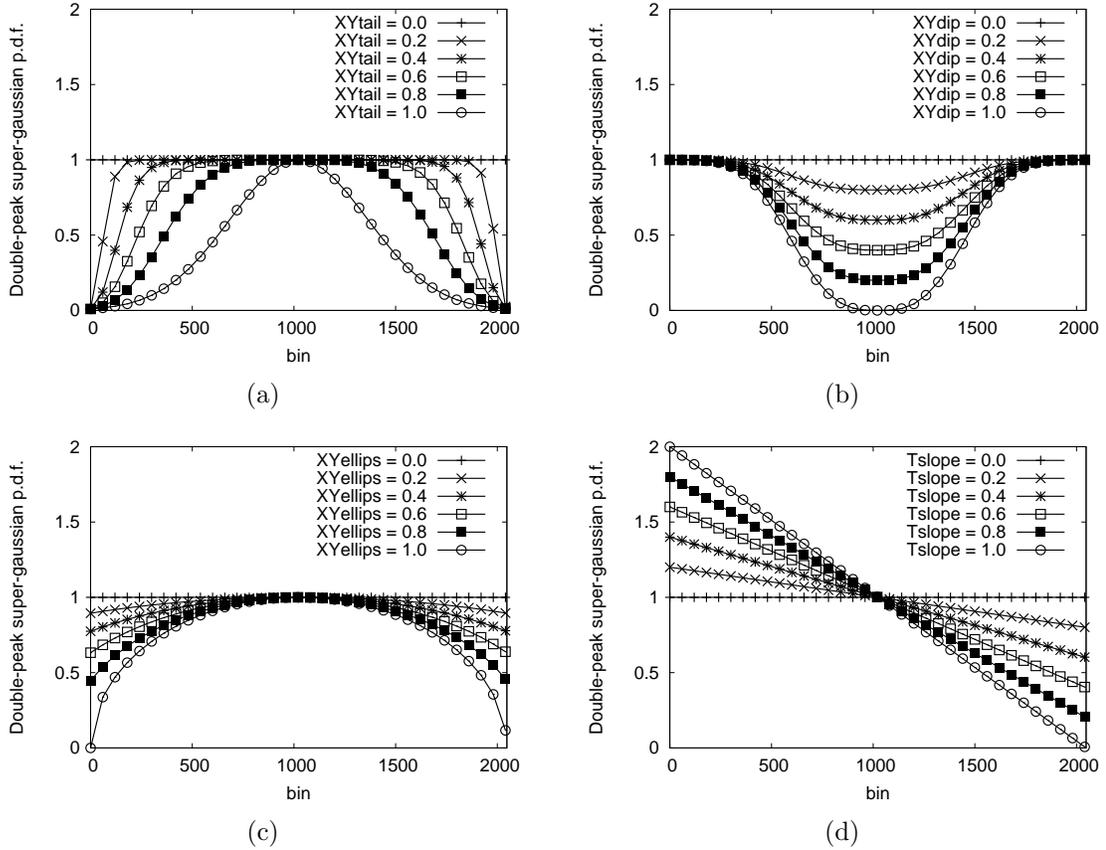


FIG. 39: Probability density functions used by APISA to generate particle distributions [13]. The parameters are (tail, dip, ellips, slope) and default to (0, 0, 0, 0). Only the parameter in the legend of each plot is varied: (a) tail; (b) dip; (c) ellips; (d) slope (for time only). Although the position variables are used for tail, dip, and ellips, they are identical to the time versions.

diminished. For the single flattop distribution in Figure 39(d), the slope parameter changes the tilt of the flattop.

## C.5 APISA UPGRADE: RF CAVITY FIELD GENERATION

The general configuration file changes to support the addition of these two field generation methods are described first. The geometry description used in cavity morphing is described next. In the course of describing the cavity geometry description, examples of the linear relationship method for setting variables in the decision file are given. Finally, the arguments for the programs written for this research, `ps_tuner`

and `xvfb_manager`, complete this appendix.

The communication, `variator`, and `selector` configuration files are unchanged from the original APISA files. The diagnostic file, `spea2_diag.log`, additionally includes the values for the objectives and constraints evaluations for the non-dominated individuals in the archive. The problem type in the `variator` parameter file remains ASTRA since the field generation methods are optional.

The main changes are to the ASTRA set up file. There are eleven additions. An example of the new ASTRA set up file is

```

astra_binary           /full/path/to/ASTRA/executable/Astra
astra_input_file       /full/path/to/ASTRA/input/file/gun.in
available_nodes_file   /full/path/to/computer/list/nodes_list
remote_shell_mode      ssh
night_nodes_file       NONE
max_jobs_node_file     NONE
check_nodes            YES
check_nodes_wait(sec)  30
maximum_time_per_job(min) 6000
maximum_jobs_per_node  1
keep_in_purgatory(sec) 60
niceness_level         0
use_unused_nodes_only  NO
users_usage_threshold  25.0
system_usage_threshold 25.0
node_inactive_wait(min) 15.0
generate_distributions NO
append_results_file    /full/path/for/debug/data/RESULTS
distribution_directory /full/path/for/new/distributions/dist
number_particles       1000
particle_loss_output_names_file /full/path/for/loss/names
passive_particle_loss_ok NO
backward_traveling_particle_ok NO
particle_loss_before_zmin_ok YES
cathode_field_particle_loss_ok NO
aperture_particle_loss_ok YES

```

```

generate_efield_profile          YES
efield_generation_method        MORPH_EFIELD
efield_profile_directory /full/path/for/new/profiles/fields
efield_config_file             /full/path/to/field/cfg/efld_config
astra_output_names_file /full/path/to/ASTRA/out/data/ast_name
decision_variables_file /full/path/to/decision/cfg/decisions
objectives_file                /full/path/to/objective/cfg/objectives
constraints_file                /full/path/to/constraint/cfg/constraints

```

Four additions, `generate_efield_profile`, `efield_generation_method`, `efield_profile_directory`, and `efield_config_file`, relate to field generation. The `generate_efield_profile` and `efield_profile_directory` parallel those for the particle distribution option in the original APISA. The first parameter takes a YES/NO value indicating whether or not APISA creates field profiles for each individual, and the second names where APISA writes the field profiles. The field profiles generated are named the same way the ASTRA input and generated particle distribution files are named (e.g. `gun.000000008.computer1.fld`). If APISA is creating field profiles, the `efield_generation_method` parameter tells APISA which field creation method to use. The `MORPH_EFIELD` value directs APISA to use field morphing, and the `MORPH_GEOMETRY` value directs APISA to use geometry morphing. Another file is created for each individual that has a `.info` extension (`gun.000000008.computer1.fld.info`), and the information written to the file depends on the method chosen. The fourth parameter, `efield_config_file`, contains configuration information relevant to the field creation method. The specifics of this file and the contents of the `.info` file will be discussed later in C.5.1 and C.5.2.

There are five parameters in the ASTRA set up file to indicate which, if any, particle loss mechanisms the optimization will allow. The parameters are `passive_particle_loss_ok`, `backward_traveling_particle_ok`, `particle_loss_before_zmin_ok`, `cathode_field_particle_loss_ok`, and `aperture_particle_loss_ok`. For each parameter that is set to YES, the optimization uses ASTRA simulation results with the allowed loss mechanisms; otherwise, the ASTRA simulation results are marked invalid. Similar to the `astra_output_names_file` variable, the `particle_loss_output_names_file` parameter provides names for the particle loss variables, so they can be used in the optimization. Here is a listing of the contents of an example file

`passive_particle_losses`  
`backward_traveling_particles`  
`particles_lost_before_zmin`  
`particles_lost_due_to_cathode_field`  
`aperture_losses`

These are included in the information written to the `append_results_file` file.

A minor addition is related to running interactive shells on linux computers. There are two ways to login into a computer remotely: Remote Shell (`rsh`) and Secure Shell (`ssh`). For computer security reasons, Secure Shell is preferred but is not always supported. The `remote_shell_mode` parameter allows the user to choose which shell tool to use when running APISA using interactive logins.

Next, the configuration and output related to each method is discussed after the common parameters are described, followed by individual discussions of the field creation specific parameters.

The common parameters are shown in Table 10. For either method, the file named in `efield_config_file` must contain `cavity_id` and `EFIELD_cav<cid>npts` where `<cid>` is replaced with the setting in `cavity_id`. The field profiles are on-axis profiles,  $E_z(r = 0, z)$  versus  $z$  in meters. The `cavity_id` parameter must appear first in the file since its value is used to read all other field variables in the file. The `EFIELD_cav<cid>npts` is also required. However, `EFIELD_cav<cid>update_ASTRA_freq` is optional. If it is left unspecified, the frequency in ASTRA input files is updated.

### C.5.1 FIELD MORPHING

The input parameters for the field morphing method are based on the formula for the morphing function,  $f_{morphing}(z)$ , the number of cells,  $n_{cells}$ , and the source frequency,  $f_{source}$ . The equation for  $f_{morphing}(z)$  is repeated here for reference.

$$f_{morphing}(z) = 1 + \sum_{n=1}^{15} a_n \cos\left(2\pi n \frac{z}{L_{cavity}}\right) + \sum_{n=1}^{15} b_n \sin\left(2\pi n \frac{z}{L_{cavity}}\right)$$

The input parameters for the field morphing method are listed in Table 11. It is assumed that gun cells are constructed of full cells and optionally preceded by a fractional cell. For example, if `EFIELD_cav<cid>ncells` has the value 1.5, then  $E_{\pi_{approx}}(z)$  is a partial sine wave that extends from  $45^\circ$  to  $180^\circ$ . The parameters in

TABLE 10: Common field generation input parameters

Parameter	Purpose	Value
cavity_id	Cavity identification number. It is the same as the index used in the <b>CAVITY</b> section of the ASTRA input file. The value of this parameter is used in the name of subsequent parameters.	positive integer
EFIELD_cav<cid>_npts	The number of points to produce for the field profile for cavity <cid>.	positive integer
EFIELD_cav<cid>_update_ASTRA_freq	Indicates whether or not for cavity <cid>, APISA should update the ASTRA input file to use the calculated frequency ( <b>YES</b> ) or let it be fixed ( <b>NO</b> )	<b>YES</b> (default) or <b>NO</b>

TABLE 11: Field morphing input parameters

Parameter	Equation Component	Value
EFIELD_MORPH_cav<cid>_A<1-15>	$a_n$	real number
EFIELD_MORPH_cav<cid>_B<1-15>	$b_n$	real number
EFIELD_cav<cid>_ncells	$n_{cells}$	positive real number
EFIELD_MORPH_cav<cid>_source_freq	$f_{source}$ in Hertz	positive real number

Tables 10 and 11 may appear in the file named in `efield_config_file` or a decision variable file (but not both). An example field configuration file is

```

cavity_id                1
EFIELD_cav1_ncells      1.5
EFIELD_MORPH_cav1_source_freq 1300e6
EFIELD_cav1_npts        1000
EFIELD_MORPH_cav1_A1    0.5
EFIELD_MORPH_cav1_B2    0.35

```

In this example, APISA creates 1000 point field profiles for ASTRA cavity number one. The field profile approximates the  $\pi$  mode of a one and a half cell structure using  $f_{source}$  equal to 1300 MHz. The two coefficients,  $a_1$  and  $b_2$ , of  $f_{morphing}(z)$  are fixed at 0.5 and 0.35, respectively. A sample decision variable file using parameters from the table is

```

EFIELD_MORPH_cav1_A2  VARY  0  0.25
EFIELD_MORPH_cav1_A3  VARY  0  0.75
EFIELD_MORPH_cav1_B3  VARY  0  0.50
EFIELD_MORPH_cav1_B4  VARY  0  0.30

```

Used in conjunction with the field configuration file, the Fourier coefficients listed as decision variables,  $a_2$ ,  $a_3$ ,  $b_3$ , and  $b_4$ , are varied in the optimization as specified while  $a_1$  and  $b_2$  are fixed to the values listed in the field configuration file. The rest of the coefficients,  $a_4$  through  $a_{15}$ ,  $b_1$ , and  $b_5$  through  $b_{15}$ , are set to zero.

TABLE 12: All field profile characteristics provided by the field morphing method

Parameter name (prefix EFIELD_MORPH_cav<cid>_)	Method of Calculation
AN_SUM	$\sum_{n=1}^{15} a_n$
ANFN_MAX	$\max \left[ \sum_{n=1}^{15} a_n \cos \left( 2\pi n \frac{z}{L_{\text{cavity}}} \right) \right]$
ANFN_MIN	$\min \left[ \sum_{n=1}^{15} a_n \cos \left( 2\pi n \frac{z}{L_{\text{cavity}}} \right) \right]$
BN_SUM	$\sum_{n=1}^{15} b_n$
BNFN_MAX	$\max \left[ \sum_{n=1}^{15} b_n \sin \left( 2\pi n \frac{z}{L_{\text{cavity}}} \right) \right]$
BNFN_MIN	$\min \left[ \sum_{n=1}^{15} b_n \sin \left( 2\pi n \frac{z}{L_{\text{cavity}}} \right) \right]$
EFIELD_MAX	$\max [E_z(z)]$
EFIELD_MIN	$\min [E_z(z)]$
EFIELD_FREQ_GHZ	Frequency of $E_z(z)$ determined via Fast Fourier Transform
F_COEFF_SUM	$\sum_{n=1}^{15} a_n + \sum_{n=1}^{15} b_n$
MORPHINGFN_MAX	$\max [f_{\text{morphing}}(z)]$
MORPHINGFN_MIN	$\min [f_{\text{morphing}}(z)]$

Characteristics of the resulting Fourier series function and the field profile generated are provided to the optimization and can be used in constraints or objectives files. These are written to the `.info` file and included in the output to the `append_results_file` file. Table 12 lists the available parameters. A constraint to ensure that the morphing function is above the  $z = 0$  axis as mentioned in 3.3.1 for cavity 1 is

```
EFIELD_MORPH_cav1_MORPHINGFN_MIN GREATER_THAN 0.0
```

In addition to the `.info` file, a diagnostic gnuplot [93] command file is created for each individual with the `.gpl` extension. The Fourier coefficients used to create the field profile are included in the comments of the command file for reference.

The file also contains the data and gnuplot commands to plot  $E_{\pi_{approx}}(z)$ ,  $E_z(z)$ , the  $a_n$  dependent term in  $f_{morphing}(z)$ , the  $b_n$  dependent term in  $f_{morphing}(z)$ , and  $f_{morphing}(z)$ . Unless a version of the `variator` executable is run that does not remove intermediate files, these diagnostic gnuplot files are not available after APISA finishes processing.

### C.5.2 GEOMETRY MORPHING

The cavity geometry morphing field configuration file contains more administrative information like the ASTRA set up file than the field morphing version. This is because cavity morphing follows the ASTRA processing model. It modifies a cavity geometry file and then passes it to a program to produce the field profile. In field morphing, each field profile is computed on the fly directly by APISA before launching the ASTRA simulation. Rather than list the parameters in a table, they are discussed individually. An example file is

```
cavity_id                1
EFIELD_cav1_npts        1000
EFIELD_GEOMETRY_cav1_description    /path/to/cav_desc.txt
EFIELD_GEOMETRY_field_variables_list  /path/to/PS/outvars.txt
EFIELD_GEOMETRY_helper_program_directory /path/to/PS/programs
EFIELD_cav1_update_ASTRA_freq        YES
EFIELD_GEOMETRY_cav1_history_file    /path/to/GeomHistory
EFIELD_GEOMETRY_cav1_rescale_MaxE    YES
EFIELD_GEOMETRY_cav1_rescale_peak_number 1
```

The generalized cavity description that APISA is to use as a template is named in `EFIELD_GEOMETRY_cav1_description`. The name of the file containing the expected list of output variables from the Poisson Superfish processing is given in `EFIELD_GEOMETRY_field_variables_list`. A sample subset listing contains

```
FIELDFLATNESS
FREQ
PiMode
SIGNED_FIELDFLATNESS
```

These are described in the `ps_tuner` discussion below and appear in the `append_results_file` output. APISA needs to know where `ps_tuner`, the program

to run Poisson Superfish, and `xvfb_manager` are located. The directory location for these programs is provided in `EFIELD_GEOMETRY_helper_program_directory`. The `EFIELD_GEOMETRY_cav1_history_file` parameter gives the filename where APISA records the geometry descriptions that lead to  $\pi$  modes. If it is set to `NONE`, the geometries are not recorded. `EFIELD_GEOMETRY_cav1_rescale_MaxE` and `EFIELD_GEOMETRY_cav1_rescale_peak_number` are related. The first indicates whether or not the `MaxE(1)` parameter in the ASTRA input file should be rescaled to guarantee that a particular peak in the generated field profile has the intended value of `MaxE(1)`. If it is set to `NO`, then `MaxE(1)` is not rescaled. If it is set to `YES`, `MaxE(1)` is rescaled so that the peak number (counting from 1) noted in `EFIELD_GEOMETRY_cav1_rescale_peak_number` is scaled to the value of `MaxE(1)` in the ASTRA input file. This value of `MaxE(1)` may be fixed or a newly generated value if `MaxE(1)` is a decision variable.

### Generalized geometry description

The geometry description file is discussed next. The geometry description breaks a cavity into a series of beam tubes and cells. These building blocks and their components are shown in Figure 40. There are additional elements for the search frequency and drive point location. Each building block is described with examples. A list of permissible and default units follows. Finally, naming for cavity components in decision variables is discussed including example uses of the linear relationship method for setting variables.

The cell element name is `pillbox_cell`. Each cell section starts with a `pillbox_cell` keyword and ends with `pillbox_cell end`. Between these are the components and their settings. An example pillbox cell with an exit iris is shown in Table 13. This creates a pillbox cavity with a 9 cm radius that can be used as a gun cell. The cell is 5.5 cm in length from entrance to exit. The entrance wall extends to the symmetry axis. The exit wall stops 2.5 cm above the symmetry axis creating the exit iris for the cell. The pillbox cavity can be changed to a re-entrant cell with entrance and exit tubes. This is shown in Table 14. Adding the entrance iris offset causes an entrance beam tube to be added. Nonzero wall angles tilt the walls, in this case, toward each other. Making the neck width smaller than the main cell width makes the opening to the beam tube smaller than the main cell width. The neck and cell offsets move the base of the main cell away from the symmetry axis. All of

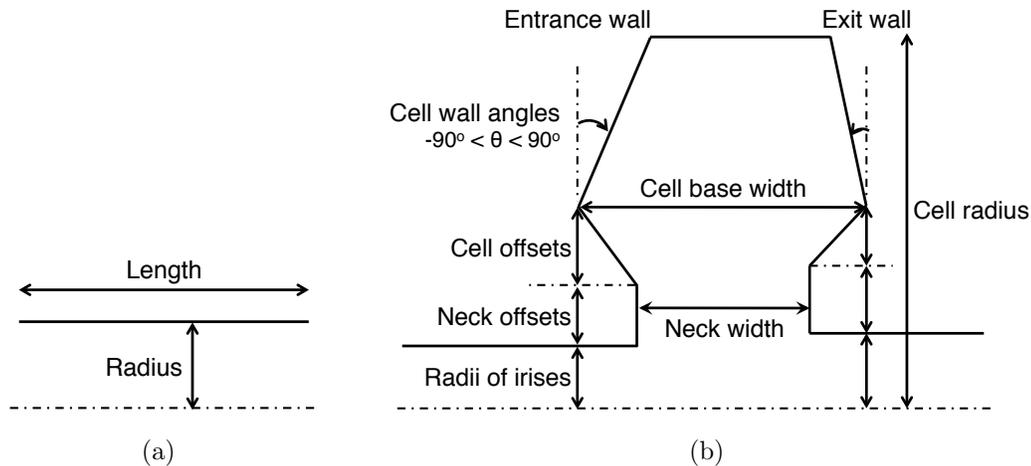


FIG. 40: Cavity and beam tube layout for geometry description [12]: (a) beam tube or iris; (b) cell (Figure 9 reproduced for convenience). The beam enters each element from the left. The axis across the bottom is the axis of rotation and typically corresponds to the beam axis. The components of the cell on the left side are called entrance quantities. The exit quantities are on the right.

the changes here are mirror symmetric, but they do not have to be. The entrance values do not have to match the exit values (or only differ by a sign). They can be set independently.

There is a separate beam tube element called the `tube_iris`. Its block is structured the same way, but it only has two components. An example file for a one cell pillbox cavity with a downstream beam tube is in Table 15.

The elements have units associated with them. The accepted units for length and their abbreviations are inches (`in`), millimeters (`mm`), centimeters (`cm`). If a length unit is omitted, the default, centimeters, is assumed. For frequency, the permissible units are hertz (`Hz`), kilohertz (`kHz`), megahertz (`MHz`), and gigahertz (`GHz`). The default is megahertz. For angles, `degrees` and `radians` are accepted, and the default is degrees. All units are converted to the default units, and the Poisson Superfish file generated uses the default units. Here is the example in Table 15 expanded to use the `frequency` and optional drive point location elements

```
frequency 1300 MHz
major_element_for_drive_point 2
pillbox_cell
  cell_radius 9 cm
```

TABLE 13: Pillbox geometry example

<pre>pillbox_cell   cell_radius 9 cm   iris_entrance_wall_radius 0 cm   iris_exit_wall_radius 2.5 cm   cell_base_width 5.5 cm   cell_base_entrance_wall_angle 0 degrees   cell_base_entrance_wall_offset 0 cm   cell_base_exit_wall_angle 0 degrees   cell_base_exit_wall_offset 0 cm   neck_width 5.5 cm   neck_entrance_wall_offset 0 cm   neck_exit_wall_offset 0 cm pillbox_cell end</pre>	
--	---

TABLE 14: Re-entrant cavity geometry example based on pillbox example

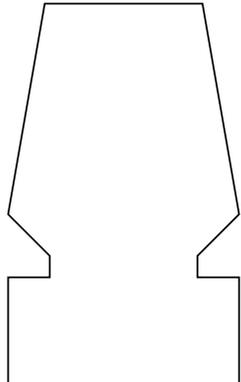
<pre>pillbox_cell   cell_radius 9 cm   iris_entrance_wall_radius 2.5 cm   iris_exit_wall_radius 2.5 cm   cell_base_width 5.5 cm   cell_base_entrance_wall_angle 10 degrees   cell_base_entrance_wall_offset 1 cm   cell_base_exit_wall_angle -10 degrees   cell_base_exit_wall_offset 1 cm   neck_width 3.5 cm   neck_entrance_wall_offset 0.5 cm   neck_exit_wall_offset 0.5 cm pillbox_cell end</pre>	
---	---

TABLE 15: One cell cavity with exit beam tube

<pre> pillbox_cell   cell_radius 9 cm   iris_entrance_wall_radius 0 cm   iris_exit_wall_radius 2.5 cm   cell_base_width 5.5 cm   cell_base_entrance_wall_angle 0 degrees   cell_base_entrance_wall_offset 0 cm   cell_base_exit_wall_angle 0 degrees   cell_base_exit_wall_offset 0 cm   neck_width 5.5 cm   neck_entrance_wall_offset 0 cm   neck_exit_wall_offset 0 cm pillbox_cell end tube_iris   length 2 cm   radius 2.5 cm tube_iris end </pre>	
--	--

```

iris_entrance_wall_radius 0 cm
iris_exit_wall_radius 2.5 cm
cell_base_width 5.5 cm
cell_base_entrance_wall_angle 0 degrees
cell_base_entrance_wall_offset 0 cm
cell_base_exit_wall_angle 0 degrees
cell_base_exit_wall_offset 0 cm
neck_width 5.5 cm
neck_entrance_wall_offset 0 cm
neck_exit_wall_offset 0 cm
pillbox_cell end
tube_iris
  length 2 cm
  radius 2.5 cm
tube_iris end

```

The elements in the file are counted starting from 0, so `frequency` is element 0. In this example, the drive point will be first placed in the major element `pillbox_cell`

during the  $\pi$  mode search, and that is element number 2 in the file. A major element is a `pillbox_cell` or a `tube_iris`.

Some name mangling is needed to use a parameter in the cavity geometry file as a decision variable in the optimization. To uniquely identify which parameter in the cavity geometry file is to be changed, the decision variable name includes the cavity identification number, the cavity element location, and the dimension. An example decision file based on the example in Table 15 is

```
cav1-tube_iris1-radius VARY 1.5 5
cav1-pillbox_cell1-iris_exit_wall_radius LINEAR
    cav1-tube_iris1-radius SLOPE 1 OFFSET 0
```

The first variable name points to the `radius` feature in the first `tube_iris` element in the cavity description file for cavity one. Further it directs APISA to vary this dimension between 1.5 and 5 cm. The second line points to the `iris_exit_wall_radius` feature of the first `pillbox_cell` element in the cavity one description file. Note that the line break in the second entry is not permitted in decision, constraint, and objective files. This example shows how a variable can be made linearly related to another one and how the optimizer can set neighboring elements as described in 3.3.2.

To create a symmetric re-entrant cell as mentioned in 3.3.3, if the optimization is varying the `cell_base_entrance_wall_angle` in Table 14, then the `cell_base_exit_wall_angle` can be made to track the first using

```
cav1-pillbox_cell1-cell_base_entrance_wall_angle VARY 10 -10
cav1-pillbox_cell1-cell_base_exit_wall_angle
    LINEAR cav1-pillbox_cell1-cell_base_entrance_wall_angle
    SLOPE -1 OFFSET 0
```

The entrance wall angle is varied between  $-10^\circ$  and  $10^\circ$ , and the exit angle is set to track it but with the opposite sign. If the entrance wall tilts outward (negative angle), so will the exit wall with the corresponding positive angle.

The linear relationship can be used to implement the APISA example in C.3 where one `MaxB` is made equal to another. Using the linear relationship, it can be written as

```
MaxB(1) VARY -0.179 -0.168
MaxB(2) VARY |-> MaxB(1) 0.5 1.0
MaxB(3) LINEAR MaxB(1) SLOPE 0 OFFSET 0
```

Here, the decision variable count is two instead of three.

### **ps\_tuner program**

For cavity field generation, APISA calls the `ps_tuner` program. It handles all Poisson Superfish related processing from producing Poisson Superfish geometry files for the building block geometry description to running the Poisson Superfish programs to find the  $\pi$  mode field profile. It uses one input file from the user and if running under Wine another from the `xvfb_manager` program. `ps_tuner` produces four output files. The arguments for the program are described after the output files, and the input files are described last.

Each output file is named according to the geometry file that `ps_tuner` is converting. Filename suffixes are used to differentiate the files. The first output file is the field profile for the  $\pi$  mode `ps_tuner` finds or a zero profile if no  $\pi$  mode is found. The second file is the `.info` file. It contains information extracted or derived from the Poisson Superfish output files. A representative subset of this information is in Table 16. The third file is the `.peaks` file. This provides the normalized peak amplitudes in the field profile. `MaxE` rescaling uses this information. The last file is `_new.cfg` and is a record of the building block description that produced the  $\pi$  mode. The main differences between the new config file and the original description are the units of the elements, the search frequency, and the drive point location. The `ps_tuner` program works with the default units named previously, and the new configuration file reflects that.

The `ps_tuner` program has several arguments shown in Table 17. A typical calling sequence is

```
ps_tuner -a -p 45 -c cav_desc.txt
```

This directs `ps_tuner` to run Poisson Superfish under Wine and to use the Xvfb process associated with process identification 45. It takes the geometry description `cav_desc.txt` and produces output files `cav_desc.fld` for the field profile, `cav_desc.fld.info` for the associated field characteristics, `cav_desc.fld.peaks` for the normalized peak amplitudes for field profile, and `cav_desc_new.cfg` for the final geometry description.

TABLE 16: Sample `ps_tuner` provided information

Output name	Description
FIELDFLATNESS	Using $n_{cells}$ determined from the geometry description, un-normalized peak information for the field profile for $ E_{peak} _{\max}$ , $ E_{peak} _{\min}$ , and $ E_{peak} _i$ , <i>field flatness</i> = $100 \frac{ E_{peak} _{\max} -  E_{peak} _{\min}}{\frac{1}{n_{cells}} \left( \sum_{i=1}^{n_{cells}}  E_{peak} _i \right)}$
FREQ	Resonance frequency for the geometry calculated by the Poisson Superfish program fish
PiMode	Indicates if <code>ps_tuner</code> found a $\pi$ mode (1) or not (0).
SIGNED_FIELDFLATNESS	Same as FIELDFLATNESS except the sign is derived from the relative position of the minimum and maximum peaks. If the maximum is to the left of the minimum, the sign is negative; otherwise, it is positive.

TABLE 17: `ps_tuner` arguments and descriptions

Argument	Name	Description
<code>-a</code>	add	Add the <code>.fld</code> extension to the field profile, info, and peaks file names
<code>-c filename</code>	configuration	Name of the general cavity description. The path name may be included. If it is not, the program looks for the file in the present working directory. It is assumed that the filename has an extension such as <code>.txt</code> or <code>.cfg</code> . The base name of the file (name minus any extension) is used as the base name for the output files.
<code>-d path</code>	directory	The full directory path to the location where <code>ps_tuner</code> should run and put results. If it is omitted, the program writes the output files to the present working directory.
<code>-e cygwin wine</code>	environment	The program runs under Wine on linux and Cygwin [94] in Windows. The default environment Wine is assumed. Running under Wine requires the <code>-p</code> flag.
<code>-i cid</code>	identification	The names of the output parameters written to the info file are prepended with <code>EFIELD_GEOMETRY_cav&lt;cid&gt;_.</code> Using this option allows the info file values to be used in objectives and constraints.
<code>-k</code>	clean	Do not clean up intermediate files and directories the program creates. This is overridden by APISA.
<code>-p pid</code>	pid	The process identification (pid) of the program that calls <code>ps_tuner</code> . This is only needed for running under Wine. It identifies which <code>xvfb_manager</code> information file should be checked for Xvfb display information.
<code>-t table_size</code>	table	The number of $(z, E_z(r=0, z))$ pairs to write out for the field profile.
<code>-v</code>	verbose	Print debug information

TABLE 18: `xvfb_manager` arguments and descriptions

Argument	Name	Description
<code>-k</code>	kill	Kill the Xvfb process associated with the process identification named in the <code>pid</code> argument. This cannot be used with the <code>-l</code> option.
<code>-l</code>	launch	Launch an Xvfb process for the process identification named in the <code>pid</code> argument as necessary. This cannot be used with the <code>-k</code> option.
<code>-p pid</code>	pid	The process identification number with which to associate the Xvfb process. This is required.

### `xvfb_manager` program

APISA uses the `xvfb_manager` program to manage the Xvfb processes that instances of `ps_tuner` need in order to run Poisson Superfish under Wine. Its purpose is to launch and kill Xvfb processes. It has no user provided input files and produces two specially named output files, a lock file and a data file. The arguments for the program are listed in Table 18. The `xvfb_manager` processing is discussed next followed by a description of the input files.

When the `xvfb_manager` program is directed to launch an Xvfb process, it first checks to see if the data file for the provided process identification exists in the current working directory. If the file exists, the program reads the display number from it. The program checks to see if there is a matching Xvfb process running for the user calling the program. If the correct Xvfb process is running, the program does nothing, but if the Xvfb process is not running, it starts it. In this mode, `xvfb_manager` acts as a restart mechanism. When there is no data file, the program cycles through display numbers searching for one that is available for the user calling the program. Once it finds an unused display number, it writes the number to the data file and launches the appropriate Xvfb process.

Processing for killing an Xvfb process is much simpler. The `xvfb_manager` program reads the data file to determine which Xvfb process to kill in the event that several Xvfb processes are running for a particular user. It kills the Xvfb process

with the designated display owned by the user calling the program. It then removes the data file and exits.

The output files are named `xvfb_manager_<pid>_<computer name>.info` for the data file and `xvfb_manager_<pid>_<computer name>.lck` for the lock file. The process identification, `<pid>`, is provided as an argument to `xvfb_manager`. The computer name is the name of the computer where `xvfb_manager` is running and is determined from the operating system. These files also serve as input files to the `xvfb_manager` program. The lock file exists only while `xvfb_manager` is running. Each instance of `xvfb_manager` checks if a lock file with the provided process identification exists in the current working directory before processing. If it does, the program does nothing and exits under the assumption that another instance of `xvfb_manager` is manipulating the Xvfb processing. If it does not find the file, it creates one, performs the required Xvfb processing, removes the lock file, and then exits. The data file contains the X Windows display number for the Xvfb process launched by an `xvfb_manager` program for the provided process identification.

Here are two examples of running the `xvfb_manager` program. They both refer to pid 45. The first example launches an Xvfb process

```
xvfb_manager -p 45 -l
```

The second one kills an Xvfb process

```
xvfb_manager -p 45 -k
```

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### RECENT PUBLICATIONS

1. M. Kramer, et. al., in *Physical Review Special Topics - Accelerator and Beams*, in preparation
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