Resource Management and Optimization Efficiency Issues in a Simulation Software Package

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***Abstract*—This work is a component of a larger project that attempts to map the primary factors impacting the software development process of simulation software. In this paper, we describe resource management and optimization efficiency repercussions stemming from the perfective maintenance approach as identified in the development of auxiliary functionality in an advanced Monte Carlo simulation tool that examines the addition of a diamond head attachment to a fiber optic in order to increase the efficiency of the fiber. We found that adding a diamond head did increase the efficiency of the fiber optic, but that modifications necessary to implement the additional functionality in the software required drastically greater computational resources.**

***Index Terms*—Optimization Efficiency; Perfective Maintenance; Monte Carlo Simulation.**

I. INTRODUCTION

The perfective maintenance of a software product constitutes the modification of the software to improve the effectiveness of the product by adding functionality, as well as improved performance and maintainability. In this paper, we describe the adjust approach for perfective maintenance as expressed in Three-Dimensional Fiber Optic Probe Spectroscopy simulation software (FOPS3D). This software is a complementary scientific software tool that simulates the effects on the absorbance level of the evanescent field of an optical fiber with a tapered thickness. In FOPS3D, we use the Monte Carlo approach by firing rays chosen randomly according to a specified distribution into an optical fiber. The number of collisions encountered within the unclad section are counted and averaged over the (large) number of rays fired into the fiber (histories) in order to yield the average relative absorbance.

In previous work [1][2], the first requirement of the investigation was the development of software that can simulate the effect of tapered fiber thickness on ray absorbance. The Fiber Evanescent Wave Spectroscopy (FEWS) software tool was designed with reference to this requirement. Progress in the research [3][4] required an examination of the effect of fiber bending on the absorbance level and thereby led to new demands for additional functionality permitting user manipulation of the spatial presentation of the tapered fiber. This added capability was a necessary component of research performed for improving the efficiency of the fiber. For this objective, the developer required a change from a combinatorial geometry to a computer graphics approach. A supplementary enhancement required by the developer, to examine the effects of the attachment of a diamond head to the optical fiber, led us to develop a new version of FOPS3D software that incorporated Diamond Head functionality in other words, a perfective maintenance to the FOPS3D software.

Simulation software development takes place within the domain of scientific software development. At the beginning of the article, we examined the main features of FOPS3D and how it generally relates to scientific simulation software. In this paper, we aim to isolate a particular concern, which is the transformation of a geometrical problem into a graphical one as presented through the model of an optical fiber. Geometry has two primary display options, one of which is combinatory geometry (CG) with predefined structures that we can use to describe a system.

Using CG as the geometric approach, poses many challenges, one of which is describing complex geometric systems. The most direct way to describe such a system is to use a graphical module to represent the system graphically and to scrutinize the results, as we did with the optical fiber. While, in terms of development, this is a more straightforward approach, it is more vulnerable to the intrinsic limitations in software and hardware. Therefore, the development of scientific software within the strictures of software engineering must take into account many factors, such as efficient use of computing power, software maintainability, Graphics Processing Unit (GPU) rendering capabilities, etc.

In Subsections A of Section II, we provide a detailed physical description of, and exact specifications for, the system being simulated. In Subsections II-B we cover the mathematical constants that were employed for the work. Subsection II-C covers the Monte Carlo approach to the simulation process. In Section III, we discuss the development of the perfective maintenance of the simulation. Finally, in Section IV, we discuss the lessons learned from the process and the course of future development.

II. PHYSICAL BACKGROUND

Previous work [5][6] found that there is a significant difference in the molecular structure of benign lesions spectra as compared with the spectra of malignant cancerous regions. For diagnostic purposes, this discovery led to the application of fiber evanescent wave spectroscopy (FEWS) based on the

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phenomenon of attenuated total reflection (Figure 1)) and to a development of a software simulation tool in order to simulate effects on the absorbance of the evanescent field of an optical fiber.

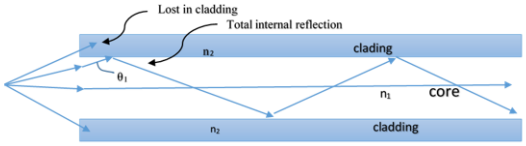

Figure. 1. Ray propagates when $n_1 < n_2$ and $angle > criticalangle$

A. Fiber System Description

The simulation system includes flexible optic fibers, a ray source emitter, and a diamond head in order to improve efficiency. The main properties of the fibers are fiber length, unclad section length, fiber radius, unclad part radius, and reflection coefficients. The simulated Infrared (IR) source emits rays into the fiber. The middle section, which is the region of interest, has its jacket and cladding removed. As shown in Fig. 2, the taper is conical, narrowing down to a thinner cylindrical midsection, with the index of refraction of the core n1, the liquid index of refraction n_2, and n_{cl} of the cladding.

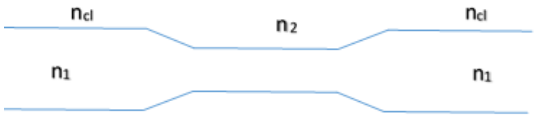

Figure. 2. Tapered midsection

The simulation system allows for user defined properties such as the radius of the simulated fiber, the radius of the unclad part of the fiber, its bending angle, and whether to add a diamond head. Next, the simulated IR source emits rays according to a radial distribution. This is simulated with Monte Carlo techniques. The light beam is propagated through the fiber and hits the fiber medium. The simulation history is defined by the hits of the IR beam in the unclad part that successfully travel through the fiber up to the light sensor. The unbiased mean value of hits is used for calculating the Fresnel transmission coefficient. In the simulation tool, the use of the diamond, increases the number of beam hits in the unclad part by reflecting a significant part of the beam back to the unclad section of the fiber. All of these manipulations can be performed in the simulation, as well as the capability to adjust the radius of the unclad part relative to the rest of the fibers radius. The specifications of the fiber with the diamond head were taken from an existing fiber with a diamond head (Figure 3).As constants in the simulation, we employed a diamond head that is 1 cm long and a fiber with a length of 10 cm.

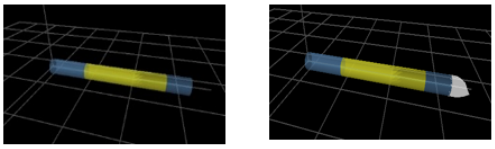

Figure. 3. a) Fiber without Diamond Head. (b) Fiber with Diamond Head.

B. Radiation Source and Absorbance Analysis

In order to describe and sample each incoming ray, we need the radial distance, r, and angle θ, relative to the z axis, when r is a Gaussian distribution for a beam waist as given by [7]:

$$I(r) = I_o e^{-8r^2/r_o^2} \tag{1}$$

where r_θ is the radius of the laser aperture and I_0 is the irradiance at the center of the aperture. In order for evanescent to propagate the incident angle must be less than the critical angle of the cladded section, the light will be totally reflected without attenuation. The angular distribution given by [8] is:

$$p(\theta) \propto \begin{cases} sin\theta/cos^2\theta, & \theta < \theta_{cl} \\ 0, & \theta_{cl} \end{cases} \tag{2}$$

According to the BeerLambert law, the transmitted power P(z) along a fiber is given by [9]:

$$P(z) = P_0 e^{-\gamma z} \tag{3}$$

where P_0 is the power at the input face of the fiber, and γ is the effective evanescent absorption coefficient (which varies for different orientations of the ray) which obey:

$$\gamma(\theta) = \frac{\alpha\gamma n_2 cos\theta cot\theta}{2\pi r_1^2 cos^2\theta_c \sqrt{(sin^2\theta - sin^2\theta_c)}} \tag{4}$$

where θ_c is the critical angle of the unclad section $\theta_c = sin^{-1}\sqrt{n_1/n_2}$ and α is the absorption coefficient of the cladding material at the given wavelength λ given by[10]:

$$\alpha = Ae^{-\gamma v/v_0} \tag{5}$$

where v is the optical wave number $(1/\lambda)$ and A, γ and v_0 are constants given in data tables [11]. For a simple tube of constant radius, $\gamma(\theta)$ can be computed by integration of (4) over the power distribution of (2). This is very difficult and also inapplicable for a tapered section, where the incidence angles change at each collision with the interfacing surface especially when we use non-point source emitted rays.

C. Monte Carlo Approach

In the Monte Carlo simulation, rays are fired into the fiber according to the radial and angular distributions as per (1) and (2), respectively. Three Cartesian coordinates indicate the ray location and two angles define the direction of the ray movement. In order to define the new location, we define three variables:

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1) Location, defined by the vector $\vec{r}$
2) Direction of Movement

$$\vec{u} = (sin\theta cos\phi, sin\theta sin\phi, cos\theta)$$

where the angles θ, ϕ are defined relative to the Z axis.
3) Distance to the Geometric Boundary ds.

At the geometric boundary, we obtain changes in the direction of the beam and if the ray hits the fiber within the unclad section, the ensuing collisions are counted. The simulation process is based on the realization of the beam movement in a three-dimensional virtual fiber. We employ the Monte Carlo approach to FEWS by firing rays according to a given distribution into an optical fiber with an unclad section. In the simulation software tool, we modeled the absorbance at each point of reflection, and the net absorption - if θ is above the critical angle of the unclad section, the ray is discarded; otherwise, the number of collisions encountered within the unclad section are counted and multiplied by γ/α to provide the absorbance "weight." This figure is averaged (by histories) over a large number of rays fired into the fiber to yield the average relative absorbance.

III. THE PERFECTIVE MAINTENANCE RESULTS

The first software simulation tool was the FEWS application (Figure 4). The FEWS application was built in order to simulate effects on the absorbance of the evanescent field of an optical fiber with tapered thickness. The configuration consists of an IR source that plots rays into a tapered fiber that has had its cladding removed in its middle (tapered) part to allow contact with the sample.

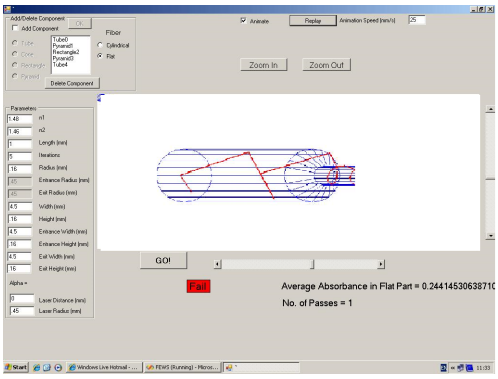

Figure. 4. The first software simulation tool

In order to improve the absorbance of the ray, one of the very first suggestions was to tapper the fiber by flattening the middle section so that the fiber would have a thinner and flattened midsection (Figure 2). Rachelin [1], who investigated experimentally the hypothesis that changes to a fiber optic, such as the narrowing of its midsection, will increase the absorbance value due to an increased number of reflections, found a correlation between the absorbance and the thickness of the flattened part.

The first simulation tool (FEWS) was built as a prototype in order to reproduce these results by calculating the effect of the tapered thickness of an optical fiber on the absorbance of the evanescent field of an infrared signal using a Monte Carlo approach. The prototype was found as a suitable [2] tool for analyzing FEWS when the results were in agreement with previous experimental and analytical calculations, that the absorbance increases as the narrowed thickness decreases (Figure 5).

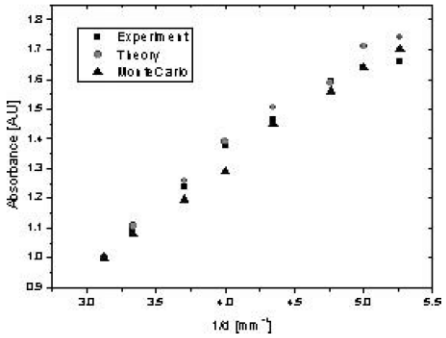

Figure. 5. Average Relative Absorbance for Fiber with Narrowed Midsection [2]

As a result, we were required to improve and to extend the capabilities of the tool for fiber with geometries that are more complex as well as to spectroscopy involving more complex physical phenomena.

Progress in the research required continuing development of the software simulation tool. Development demanded changes that focused mainly on the ability to examine the effect of bending the fiber on the absorbance level. This new requirement led to the construction of new software that can cope better with future changes to development requirements. Due to the relatively simple geometry that was being investigated (i.e., a cylindrical fiber with a trapped area), in the early version of the FEWS software, we were able to utilize the well-known geometric description method of CG fundamentals (e.g., bodies and regions).

The new requirements mandated allowing the user to change the spatial presentation of the tapered fiber in order to improve the efficiency of the fiber. These demands obligated the developer to substitute the geometrical description approach with more efficient approach and we choose to use the computer graphics approach. Utilizing the graphical approach, the user determines the geometrical dimensions of the fiber and can also deform the spatial presentation of the fiber. In order to meet these graphical demands, the FOPS3D [4] software tool was built. FOPS3D is a full three-dimensional tool utilizing a computer graphics approach that can simulate any geometrical manipulation of the fiber. The simulation tool was developed in Java language, utilizing the object oriented and event driven concepts of the language. The graphics were programmed using OpenGL. The FOPS3D simulation software product was approved only after passing all testing phases, including a black box testing phase process of validation and verifications against Rachelins [1] results and the FEWS software results [2].

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One of the conclusions that was reached during a FOPS3D study of a cylindrical fiber with a bended trapped area (Figure 6) was that the transition from a CG approach to a computerized geometric method resulted in a drastic, but still reasonable, delay in obtaining the results.

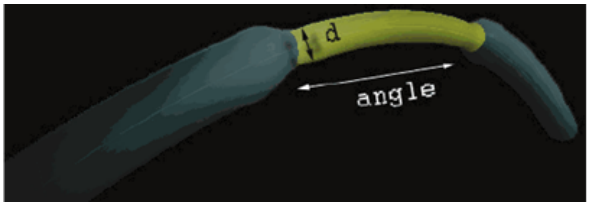

Figure. 6. FOPS3D a full three-dimensional tool [4]

As previously described, further research was required in order to improve the efficiency of the optical fiber. Progress in the research led to a focus on improving efficiency without the need for bending the fiber. One possibility was the addition of a diamond head to the fiber tip, based on the theory that a diamond head would increase the absorbance value due to the diamond characteristic of total internal reflection. That is, the diamond would reflect the ray back into the fiber to allow for greater fiber efficiency(Figure 7).

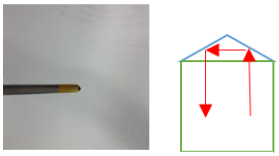

Figure. 7. (a) The real fiber used to build the simulated diamond head (b) Ray reflected from the diamond head back to the fiber

The requirement for the use of a diamond head led us to add a new functionality to the FOPS3D, functionality that allowed us to add a diamond head to the fiber. In other words, the new functionality was a perfective maintenance to the FOPS3D software(Figure 8).

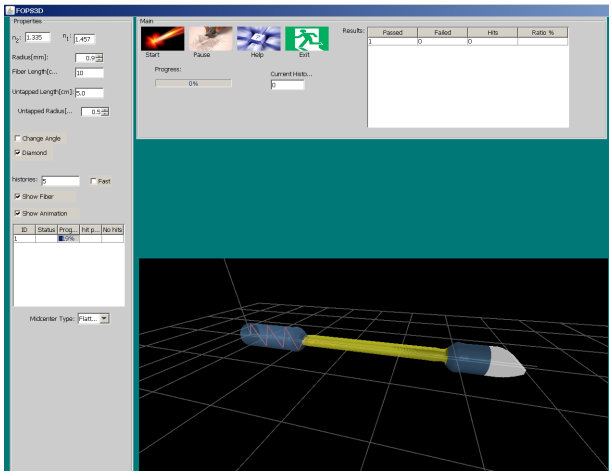

Figure. 8. The new version of FOPS3D with the diamond head

The new version of FOPS3D (containing the diamond head functionality), was utilized in the simulation of an un-tapered fiber in order to compare absorbance levels with and without a diamond head. We found that absorbance levels increased by a factor of 2.24 when the diamond head was utilized. In addition, in the case of a tapered fiber with a 0.3 radius, absorbance levels improved by a factor of 1.52, when the diamond head was utilized.

IV. CONCLUSION AND FUTURE WORK

The transition from combinatorial geometry to a computer graphics approach allowed us greater freedom and convenience in depicting the 3D geometric structure of the optical fiber. In developing the first version of FOPS3D, we found that it required a tremendous number of calculations which caused a very significant, but reasonable, delay in obtaining results. This fact did not prevent us from continuing the development of the software. Moreover, in order to reduce the CPU workload and increase performance, we decided to preform these calculations on a GPU.

However, we found that with the addition of the diamond head functionality in the new version of POFS3D, computing efficiency (measured as the average time to calculate one history) was 2.4 times slower, and above all, required much greater computational resources, such as the extension of RAM memory, the use of a dedicated GPU, and, ultimately, required utilizing computers with multiple processors working in parallel.

In our evaluation of the perfective maintenance process, we found that the required added functionality was successfully implemented. However, from a software engineering standpoint, our criteria were not met, especially because the perfective required considerably greater resources. This determination raised a question about the long-term feasibility of the entire process. In conclusion, extending the functionality of a scientific software product necessarily requires dedicated efforts to achieve the efficient use and management of computational resources (computing power, memory, GPU, processors, etc.), as well as efforts to mitigate the complexity of the algorithmic process. That is, particularly for long-term maintenance, the development process must take into account the corresponding need for improvements to the softwares capacity to contend with the increased complexity of the algorithmic process.

Scientific software product developers must confront a particular challenge at the initial stage of the perfective maintenance process in that, at the outset of the process, there is a circumscribed capacity to prognosticate the full scope, requirements, and efforts (including the necessary computational resources and algorithmic complexity) that will be mandated. Often, until the actual computation is preformed, it is not clear what the most appropriate configuration will be and what will be needed in terms of computing resources, as expressed in this study. Our work is at present continuing in order to improve the simulation process and to optimize the perfective process.

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One direction we have taken in our efforts is the modification of the simulation algorithms into distributed versions, such as would allow us to better utilize the resources of emerging cloud technologies.

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