

ABSTRACT

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A NEW APPROACH TO
COMPUTER MODELING AND ANALYSIS OF
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What Is This Thesis About?

About This Research

In this research, the author has *ab initio* developed a new conceptual and numerical approach for computational modeling of field theoretical problems. The new method has been given the name ‘FAQ’, which is an acronym for: fields as quanta.

What Is the Main Idea Here?

The basic idea here is to take any classical field pattern, and think of it as if a large collection of tiny quanta had gone into producing it. The quanta are imagined to be very simple entities, and their description is taken to include only the simplest attributes such as position, speed, phase, etc.

What Kind of Field Problems Can FAQ Address?

Thinking along these lines, initial success was obtained for the “Helmholtzian” class of field problems—i.e., the linear wave (hyperbolic), heat/diffusion (parabolic), and Poisson-Laplace (elliptic) equations, all taken together in a single class.

In all these equations, the space-related part is exactly the same—a Laplacian. So, the only difference between them pertains to the time variable. There is a systematic reduction in the order of the time differential term as we go from the wave to the Poisson-Laplace equation. In the present approach, this is significant, because the diffusion field is seen as obtained from the wave field by time-averaging the local variations due to phase. Similarly, the scalar potential field is seen as produced by a “particle” that has been diffusing for an infinitely long time. Thus, the three scalar/vector fields of the Helmholtzian class are seen to be very intimately related to each other.

On the question of whether this method can be extended to handle tensor fields or not, the opinion received from the stochastic elasticity community is not encouraging. However, based on several indirect arguments, the author believes that such an extension should be possible. Though not proven yet, a conjecture to this effect has been included in this thesis.

Why Think along the FAQ Line?

As a *conceptual* approach, the FAQ idea serves to integrate experimental facts, concepts and even theories, in a manner that is not possible otherwise.

As a numerical or *computational* approach, there are two basic reasons to pursue the FAQ idea. Firstly, it can be anticipated that through statistical sampling, comparatively fewer quanta should be sufficient to represent a given field pattern. Secondly, quanta can be anticipated to be simpler units to manipulate inside a computer. These two factors, when taken together, were expected to yield faster, more efficient, or otherwise

more desirable computations. As a matter of fact, the computer trials conducted in this research have well borne this anticipation. Further, FAQ algorithms are inherently parallelizable, and the availability of the hardware-based (i.e. the physically based) random number generators is anticipated to further reduce the cost of computation in FAQ algorithms.

How Does the Method Actually Work?

The method works through geometric sampling of a local process. The local process cascades through space and also involves an element of feedback. For time-dependent fields, the successive feedbacks are taken to be separated in time.

For Helmholtzian fields, the new approach starts with the wave field. For these fields, the idea is to apply the techniques of geometric probability to Huygens' principle. Accordingly, consider a source of waves in an infinitely extended space, radiating waves outwards. Applying Huygens' principle, each point on a wave-front radiates secondary spherical wavelets of radius λ . First, uniformly sample the surface of the initial wave-front so as to yield a point, say P_1 . Then, consider the secondary Huygens wavelet which will be radiated at P_1 . Once it is radiated, uniformly sample its surface as well to obtain a point, say P_2 . Join the two points using a displacement vector: $\vec{s} \equiv \overrightarrow{P_1 P_2}$. Note that the points on the surface of the secondary wavelet can, in turn, act as secondary sources. Accordingly, P_2 will go on to re-radiate yet another spherical wavelet whose surface is once again to be sampled, to yield P_3 . The process can be repeated to obtain a series of points: $P_1, P_2, P_3, P_4, P_5, \dots$

Now, imagine that sampling begins at the source, proceeds through all the successive Huygens wavelets, and finally ends at the sink. Due to randomness of sampling, if all the sampled points were to be joined in the sequence in which they occur, the connected zig-zag curve would be akin to a random walk traced by the motion of a point-particle. The complete wave field would be obtained by superposing all such random walks. The continuum solution is approached in the limit when (i) infinitely many particles originate at the source point; and (ii) the displacement vector for each pair of sampling is infinitesimally small.

In this manner, a collection of particles come to characterize the continuum field description of wave fields.

Of course, wave fields consist of undulations, and accordingly, the phase of the "particle" must change as it moves from one point to another. The change in phase is determined by the current value of the wave-vector and the local displacement vector. In this thesis, it is argued how the change of phase is a completely local issue even if it seems to carry instantaneous action-at-a-distance (IAD) about it. This argument is new. It has implications in clarifying the nature of quantum entanglement.

Some Comments

Obviously, the numerical technique corresponding to the abovementioned description is comparable to random walk (RW) and Monte Carlo (MC) methods. However, note that RW and MC are, theoretically, intermediate implications in the new approach—neither the starting point nor the exclusive focus. The thesis explains in detail precisely how.

The physical nature of the particle in this description will depend on the kind of field it represents. For example, the quanta of light (i.e. photons) have the electric field vector \vec{E} associated with them, but the conjectured quanta of stress field won't. Thus, in FAQ, the term “quanta” is to be taken in a broad sense.

The motion undergone by some forms of quanta may have an element of randomness associated with it. However, mathematically, the assumption of randomness is not always necessary—the motions of the “quanta” could very well be specified to be completely “deterministic.”

When FAQ is taken as a numerical approach, the quanta involved in it can be abstract quantities. When quanta do not have a *direct* physical interpretation but rather express abstract mathematical concepts, it is not necessary to continue considering them as indivisible entities. Similarly, it is not always necessary to regard them as indestructible entities—which happens to be the case only when the field in question is flux-conservative, i.e., when the field is linear and non-dissipative in nature.

Thesis Organization

This thesis is divided into eight parts and sixteen chapters. The part I is introductory in nature. Given below are sections dealing with the brief description of each part separately.

About Part II: An Overview of the Helmholtzian Fields

This part consists of Chapter 2.

Chapter 2 is devoted to an overview of the Helmholtzian fields. After introducing the physical motivation for the formation of such a class as Helmholtzian, some polemic against the traditional scheme of classifying PDEs (into the so-called hyperbolic, parabolic and elliptic categories) is offered. A review of linearity and well-posed-ness in respect of these equations is given. The diverse range of practical engineering applications of these equations is identified.

About Part III: The Research on Wave Fields

This part consists of Chapters 3 through 6.

Chapter 3: The Huygens-Fresnel Principle

The development of this principle through its 300+ years of history is traced, beginning with the original writings and illustrations of Huygens himself. Some details of Fresnel’s mathematical analysis of diffraction are given, so as to provide a background for understanding how the idea of obliquity factor was introduced in physics. The recent literature on proving this principle—or rather the various interpretations thereof—is reviewed. The inconsistencies in the various accounts are pointed out.

Chapter 4: The Obliquity Factor Is Not Essential to the Huygens-Fresnel Principle

While studying diffraction theory and simultaneously developing the concept of Huygens processes (discussed in Chapter 5), it seemed that certain simple symmetry considerations would go against the existence of the obliquity factor in diffraction theory.

The matter was therefore investigated further and it was found that obliquity factor is not a fundamental aspect of the *physical process* of diffraction[1]. Instead, it is a “measure” of the *integration scheme* followed in applying the Helmholtz-Kirchhoff theorem. The concept of obliquity factor refers to the particular geometrical relations that the sources and surfaces of integration have with each other, together with the imposed initial values and boundary conditions. But, obliquity factor is *not* a fundamental feature of waves or of diffraction.

Yet, that precisely has been the generally accepted view right since the time that Fresnel introduced the factor in his 1818 paper, i.e., for 187 years. In this sense, the new observation is a remarkably novel result. Further, taken from the practical angle, this result directly suggests a more efficient algorithm.

Chapter 5: The Three Huygens Processes

In this thesis, a completely rectified description of the Huygens principle has been given[2]. The new description is formulated in terms of an underlying physical *process*. In fact, three different variants of such a process are given here:

I: The Classical or the Continuum Huygens Process

II: The Continuum and Random Huygens Process

III: The Finitely Sampled (and Random) Huygens Process

Historically, there have been many subtle differences in the meaning of the term “Huygens’ principle.” As an example, secondary emissions have often been regarded as waves, not wavelets. A description couched in terms of a process emphasizes the fact that the theory must treat all points of space and all secondary emissions in a consistent manner. A thoroughly rectified and process-based description of the Huygens principle is a separate contribution that this thesis makes. The term “First Huygens process” refers to this new description.

The Second Huygens process then adds the idea of geometric sampling, and introduces certain differences that arise out of the randomness of the sampling. However, note that it still remains a *continuum* process, completely equivalent to the First process. The major difference between these two Huygens processes is primarily mathematical in nature. In other words, there won't be any difference in the end-consequence if either of the two processes were to be carried out in reality. The two are presented as separate processes only in order to help streamline the presentation of the theory.

In conceptual terms and by its physical implications, the Third Huygens process is in a different category as compared to the first two. Its development requires dealing with several additional considerations such as those of cardinality, uniformity of sampling, the possibility of introducing systematic errors (such as Moiré's fringes), the problem of reconciling the local aspects of photons with the global aspects of an all pervading aether, etc.

The Dirac delta pulse for wave fields: The old versus the new view[3]: According to the standard view of wave propagation, once a Dirac pulse is emitted at a source point, it translates outwards in space keeping its initial magnitude unchanged, which means that the instantaneous phase of the waveform it represents remains constant. This is possible because, in terms of space-time diagrams, the pulse entirely moves on the surface of the light-cone. Note that in this view, the pulse never travels backwards towards the source. Thus, the standard treatment takes cognizance of only the retarded part of d'Alembert's general solution—it *arbitrarily* drops the accelerated part out of theory.

In contrast, in the present view, an emitted pulse splits up at every instant into forward and backward moving sub-pulses. Put another way, for a given point of space, the instantaneous wave magnitude is a result of the superposition of all the sub-pulses which arrive there at that instant. Consequently, once a pulse is emitted, it is not possible to trace it in space using its distinctive magnitude. Further, in the new view, even the phase of the wave represented by a specific split-up part of a Dirac's pulse cannot remain constant—it continually suffers changes with every change in either space or time. Such a view of the propagation of Dirac's delta pulse is a new contribution made by the present research.

The thesis discusses the abovementioned differences in some detail. The new view can be applied over the entire range wherever the formalism of Dirac's delta "function" is useful—whether quantum or classical.

Chapter 6: The Resolution of the Wave-Particle Duality of Light

The Third Huygens process essentially involves point-phenomena. Once the systematic progression of the three Huygens processes was in place, it became possible to state precisely how classical and quantum mechanical ideas were related to each other. In

other words, the famous quantum wave-particle paradox was resolved![4] Chapter 6 of this thesis is concerned with this topic.

The new theory of photon propagation does not offend reason or dispense with causality. In the new theory, each photon traces a continuous path that passes through only one slit at a time. Thus, the photon has a particle character. Yet, as the number of photons increases, the interference pattern, characteristic of waves, *necessarily* emerges on the observation screen.

The resolution of the wave-particle paradox is so dramatic a result that it would be futile to even attempt providing any details here. Instead, reference is made to the relevant papers [2][4]. Chapter 6 itself provides a further fine tuning of those ideas.

The nature of randomness, and the philosophical viewpoint: Philosophically, in this research, the concept of randomness is taken to mean the absence of that specific kind of order which is not essential to system definition. Thus randomness does not mean the absolute lack of all orderliness.

As far as a general philosophical viewpoint is concerned, this thesis takes for granted Objectivism, e.g., the idea that the axiomatic concept of identity, including its corollary of causality, is at the root of any scientific theory, and that any attempt to establish or falsify philosophical truths through conclusions drawn in special sciences is a gross error involving an inversion of the entire knowledge-hierarchy. Consequently, quantum mechanics cannot reject reason, causality or reality.

The thesis also very briefly qualifies the position taken earlier in this research concerning the debate of determinism *vs.* indeterminism [2].

The necessity of aether in physics: In this research, aether has been shown to be necessary in physical theory on the basis of some *physical* considerations [2]. Those arguments are new. The present view of aether differs from all the previous views in the sense that the author takes luminiferous aether to be a physically existing but *non-material* substance.

Computational modeling: The double-slit interference pattern produced by photons: For simplicity, only a planar (or 2D) interference chamber was modeled. The results were compared with the celebrated experimental data put forth by Tonomura *et al.* The simulation was found to be in excellent agreement with the experimental data [4].

Further, the effect of switching on a detector near the diffracting slits was also studied computationally. The results were found to be in harmony with the finest available experimental results. This success is taken to provide a further support to the idea that a photon passes through only one slit at a time.

As one of the implications of the new theory, time-wise, there is a definite order in which a given photon covers the specific points lying on its path. Surprisingly, the

existence of such a temporal order is *distinctive* to the new theory. An entirely new kind of an experimentally testable prediction, therefore, could be made [4].

About Part IV: The Research on Diffusion Fields

This part consists of Chapters 7 through 9.

Chapter 7: The Classical and Stochastic Approaches to Diffusion Fields

This chapter is concerned with the two disparate approaches to the phenomenon of diffusion: (i) The classical analytical approach of Fourier, which is based on the technique of separation of variables, and (ii) The later-date stochastic approach, which is based on a random walking particle.

While both these theories are part of standard curricula, the review here is geared towards providing clues to the arguments rejecting instantaneous action at a distance (IAD). Accordingly, this chapter notes many points of physical basis and interpretation that are never found discussed in the literature.

Deriving the diffusion field from the wave field: As mentioned earlier, to get a diffusion field starting from a wave field, one only has to average out the local variations due to phases. In diffusion fields, the concept of period no longer applies. However, the notions of characteristic duration and characteristic distance still remain meaningful. However, the true significance of retaining these two concepts is that they serve to motivate and simplify the discussion related to finitude of support of Dirac's delta pulse.

Note the direction of the derivation: wave \rightarrow diffusion. The stochastic theory of diffusion has a 100 years of active history, and MC has a 50+ years of very active history. This was more than ample time for someone to have given a direct description of wave-fields in terms of either RWs or MC (i.e. a description that did not make a reference to a functional that was subsequently randomized). But, none seems to have even thought of giving a direct MC description of wave fields. The thesis discusses the reason why a derivation in the reverse direction, from diffusion to wave fields, would have been very difficult to think of[3].

Chapter 8: The Diffusion Equation Does Not Involve Instantaneous Action at a Distance

The Huygens process is an essentially local process. Therefore, one would expect also diffusion to be a local process. Further, from the meso and macro scale observations, diffusion is essentially a local phenomenon. For example, one can't expect scent molecules to *diffuse* to Cambridge, MA, as soon as a vinaigrette is opened in Pune, India. Yet, this is precisely what Fourier's theory predicts.

The thesis shows how the instantaneous action-at-a-distance (IAD) arises in the Fourier theory only because of the latter's mathematical method and structure [5]. In

particular, each spatial harmonic component of the Fourier series simultaneously suffers an exponential decay at all points of space. This *mathematical* fact (and its basis in separation of variables) involves IAD. However, there is no *physical* reason for supposing IAD—even if the standard treatment confuses between the two. The idea of IAD gains weight not because some “counter-intuitive” physical facts directly support it but because explanations have not been forthcoming as to how Fourier’s is a fundamentally ill-fitting theory when it comes to modeling phenomena like diffusion.

The thesis also looks into some meta-reasoning and proposes that IAD should be rejected out of physics in the same manner that perpetual motion machines once were—as a conclusion drawn after a process of inductive generalization.

Fourier’s was the first theory of diffusion. The implication of IAD has been present in physics theory for about two centuries by now. It was truly surprising not to find the abovementioned clarification (or implications thereof for quantum entanglement) discussed in prior literature. This result, therefore, once again, seems to be a new contribution made by the present research.

A discriminant to tell the existence of IAD in a theory: Another way to look at the issue of IAD is to say that it arises in Fourier’s theory because Dirac’s delta pulse has support everywhere in the domain. Once the issue of the finitude of support was thus understood, similar ideas could also be applied to Einstein’s stochastic theory of diffusion.

Einstein is generally taken to have been against the premise of IAD. Yet, the structure of his own theory of diffusion is such that IAD can very well creep into it unwittingly. The discriminant to decide whether a given stochastic theory carries IAD or not, is the extent of the support of the probability density function (PDF) of the displacements from the sink-point.

The identification of the possibility of introducing IAD in Einstein’s theory of diffusion, and the identification of the discriminant to tell if a theory of diffusion (analytic or stochastic) carries IAD or not, are the two additional new contributions that the present research makes [5].

Chapter 9: Computational Modeling of a Melting Snowman

To see how the local theory of diffusion might practically work out in computer simulation, the case of a melting snowman was taken up for study[3]. This seemingly simple problem still involves the following complexity: transient heat conduction, continuously changing size and shape of domain (i.e. a moving boundary and a moving source problem), and incipient heat absorption. Further, this case study was done in 3D—not just 2D.

The corresponding physical experiment also was conducted. The simulated and actual contours of the melting snowman were compared at different stages of melting.

It was found that the simulation qualitatively reproduced the following features: (i) the early melting near the sharp domain corners; and (ii) the general nature of the geometric contours assumed by the snowman. However, the simulation showed a comparatively late onset of melting. The thesis discusses the probable reasons for this discrepancy.

The actual computer implementation for this case did not employ the idea of the indivisible quanta. Instead, a discrete-lattice version of their motions, as in cellular automata (CA) modeling, was implemented.

About Part V: The Research on Scalar Potential Fields

This part consists of Chapter 10.

Chapter 10: Deriving the Potential Field from the Diffusion Field, and the Ideal Fluid Flow

The idea of deriving the potential field from the diffusion field is not at all new—the result is well known in prior work. What is distinctive here is the overall theoretical perspective and the physical abstraction underlying the derivation.

In particular, if a martingales-based view of the potential field is adopted, it becomes necessary to originate random-walking particles from each interior point of the domain. In contrast, if a Huygens process is taken as the basic physical abstraction, then the view it suggests is that particles are emitted only at the source-points and absorbed only at the sink-points. Thus, this thesis demonstrates how having an explicit physical abstraction makes it easier to both visualize field solutions and properly handle the various kinds of boundary conditions.

Computational modeling: The flow of the ideal fluid in finite and infinite domains: For finite domains, a simple 2D situation of the flow of the ideal fluid past a square obstacle inside a square cavity was studied. The velocity potential of the flow was numerically modeled using both FAQ and FEM.

A specially noteworthy feature of this study was that the entire FEM code (including the solver and the pre- and post-processors) was custom written in this research using C++. Even the non-uniform and high-quality mesh required for the FEM study was generated after adapting into C++, and debugging, a public domain software written in C.

For infinite domains, the problem chosen was: the flow of the ideal fluid towards a singular point-sink in an infinite planar domain. Here, the FAQ solution was compared with the available analytical (or “exact”) solution.

In both the cases, FAQ results were found [6] to be in very close agreement with the respective benchmarks. While the point-to-point variation was within $\pm 5\%$, visual inspection indicated the overall field distributions to be even closer. In view of the second fact, it seemed alright to use some suitable smoothening schemes. However, note

that if the quanta move at random and if the trial is not run for a sufficiently long time, then despite smoothening of the velocity-potential field, the FAQ approach may still show pronounced variations in the velocity field. The thesis discusses this and some other related points.

About Part VI: The Research on Tensor Fields

This part consists of Chapters 11 and 12.

Chapter 11: The Nature of Stress and Strain Tensor Fields: Why Are They So Difficult?

Chapter 11 provides a brief review of the system of elasticity and its displacement and traction formulations. It then asserts that the root cause that the stress field problems are so difficult to analyze by any means—analytical or numerical—is that their governing equations are, by definition, coupled across the spatial coordinate axes [7]. This particular feature shown by the stress/strain fields is completely unlike the usual scalar/vector fields. When it comes to stress fields, the governing equations for even the simplest theory of elasticity cannot at all be decoupled if expressed with reasonable generality, i.e., in 3D.

The thesis proposes that the *only* strategy fundamentally available to overcome this difficulty is to make the coupling implicit [7][8]. In the case of analytical techniques, it is easy to see how potential functions (e.g. stress functions) make the coupling implicit. But, unlike the prior literature, this thesis explicitly notes how the same strategy also underlies the *numerical* techniques of BEM, FEM and FDM.

The chapter discusses some of the finer details of the abovementioned points so that the difficulty of proving the conjecture, and the grounds for asserting its viability, may both be better appreciated.

Chapter 12: Tensor Fields and FAQ: A New Conjecture

This chapter first gives an overview of the very limited prior work that has sought to solve elasticity problems using stochastic approaches. Two main threads of development are briefly touched upon: (i) Random Walk on Spheres, and (ii) Random Walk on Boundary.

The applicability of the FAQ approach to model tensor fields such as stress-strain fields—in full generality and in the 3D context—still remains a matter of conjecture.

However, note that the conjecture itself is new. Other leading researchers seem to be of the opinion that such an approach would not be viable. Of course, this does not mean that they have proved its impossibility. Indeed, no known fact or principle goes against making the conjecture. Further, more than one indirect argument indicates that it might hold. This chapter briefly discusses these supporting arguments.

About Part VII: Computational Aspects

This part consists of Chapters 13 and 14.

Chapter 13: A Summary of the Software Written

In this thesis work, software not only for the FAQ method, but also for the FEM and cellular automata (CA) modeling was implemented starting from the scratch. Further, a mesh generator available in the public domain was adapted. This chapter provides a summary of the various programs written, and also shows a few illustrative screenshots.

It would have been impossible to provide the complete source code in this thesis because more than 10,000 lines of C++ code was written during the course of this PhD.

Chapter 14: Comparisons with Other Computational Methods

This chapter is to point out the relations that the present approach has with several other approaches:

(i) The transmission line matrix method (TLM, also known as the “discrete Huygens method” in acoustics research) is, in many ways, a closely related technique. For example, just like FAQ, TLM also addresses discretization of wave-fields, incorporates back-waves in its description, and is concerned with the entire range of Helmholtzian fields. Further, there is a valuable body of theoretical work put forth by the TLM researchers. (ii) The relaxation method developed by Southwell in 1940s is relevant. (iii) The cellular automata (CA) technique is also relevant in some ways. (iv) Further, inasmuch as CA algorithms are equivalent to iterative approaches like Liebmann’s method (i.e. the Gauss-Seidel iteration), a certain relation can also be seen to exist between FAQ and FDM. However, in spite of this relation, the Courant and von Neumann criteria (for wave and diffusion fields, respectively) are of only limited utility in analyzing the stability of the FAQ-based models [3]. The thesis briefly discusses all these subtle points.

Finally, some prominent differences of the core abstractions are also pointed out in this chapter. Just as an example, the TLM theory still remains couched in terms of electromagnetic fields; its beginning concepts remain concerned with lattice-based processes; and it apparently has not addressed either quantum mechanical or stress analysis-related problems.

Comparative Speeds of FEM and FAQ In this research, only preliminary and limited computer runs could be conducted towards comparing the run-time speeds of FAQ vs. FEM. For simplicity, all these trials were carried out only for the simplest Poisson fields, and only in 2D. Though there are certain qualifications to be applied, the preliminary results indicate that that by trading off a little bit of accuracy FAQ gains as much as 25 times in speed as compared with a naive $O(n^3)$ implementation of the

matrix inversion in FEM. A comparatively faster speed for the FAQ approach would seem to be against the anticipation created by the prior writing on this subject. Thus, this positive result, though encouraging, is somewhat unexpected. The FAQ approach is likely to retain the speed advantage even if the relative speedup factor might diminish with a better FEM solver technique.

About Part VIII: Conclusions

This part consists of Chapters 15 and 16.

Chapter 15: Main Contributions

Some aspects of the present work appear to be novel in 75–100, 187 and 199–202 years. This chapter provides a point-wise list of all the salient work that was performed in this research. The list is split up into two separate parts: (i) original work that is novel, and (ii) work that was done independently, but which is known not to be novel. It is hoped that the provision of these point-wise lists would help in understanding the main thrust of the present work, and also ease the task of assessing its merits.

Chapter 16: An Outline for Future Research

The thesis then concludes by outlining in Chapter 16 some possible directions that may be pursued in future research. The work that can be done in the shorter term (within approximately one to two semester's time or so) has been given separately from that which would require research over a much longer term.

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