

# On Sci-En-Math Computing and its Emerging Core Discipline of Algorithmic Science and Engineering (AS&E)

J.L. Nazareth\*

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## 1 Introduction

Algorithmic science is the theoretical and empirical study and the practical implementation and application of real-number algorithms, in particular for solving problems of continuous mathematics that arise within the fields of optimization and numerical analysis. Note that algorithms of discrete mathematics, which form a backbone for computer science, are not excluded, but they take second place to algorithms of continuous mathematics within this characterization.

We attach to ‘algorithmic’ the word ‘science’ in its fullest sense. Thus, as with *any* scientific field, the discipline has three main forms of expression:

- *Theoretical* algorithmic science establishes the convergence, complexity and numerical stability of algorithms and provides the foundations for underlying computational models.
- *Experimental* algorithmic science studies algorithms through the use of physical models and investigates the numerous manifestations of algorithms within nature.
- *Computational* algorithmic science uses the computer and the large body of associated software tools, for example, Mathematica, Matlab, etc., as a laboratory for the study of algorithms. Also included are practical implementation and the development of reliable, robust mathematical software, i.e., the ‘technology’ of the subject.

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\*Professor Emeritus, Washington State University and Affiliate Professor, University of Washington. Mailing address: CDSS, P.O. Box 10509, Bainbridge Island, WA 98110, USA. E-mail: nazareth@amath.washington.edu; Web: [www.math.wsu.edu/faculty/nazareth](http://www.math.wsu.edu/faculty/nazareth).

For additional background and discussion, see Nazareth [8].

In this essay, the broader context of algorithmic science within scientific, engineering, and mathematical computing is considered in detail. An emerging, core discipline of Algorithmic Science and Engineering (AS&E) is contrasted with its now well-established, complementary discipline of Computer Science and Engineering (CS&E).

## 2 A Visual Schema

In order to frame our discussion, we employ the visual schema shown in Figure 1. In this figure, each labeled loop, or band, with boundary perimeters defined by two adjacent squares, will be called an “arena.”

Mathematics, the core arena of Figure 1, is commonly partitioned into three broad areas—the real number system and algebra, geometry, and analysis—with many additional subdivisions and areas of intersection; see, for instance, the definitive, three-volume survey [2]. Within this integrated subject, the emphasis on “pure,” the heart of mathematics, could be symbolized by the inner perimeter of the mathematics arena, and the emphasis on “applied,” by the outer perimeter, bordering science and engineering.

Around mathematics is the arena of science,<sup>1</sup> often partitioned into the physical, chemical, and biological sciences. Further partitioning would identify the many specific sciences within each of these three broad subdivisions. “Mathematical science,” interfacing with mathematics, can be symbolized by the inner perimeter of the sciences arena, and “applied science” by the outer perimeter, at the interface with engineering. Observe, in particular, that “mathematical sciences” and “applied mathematics” are overlapping designations, the former reflecting the perspective of science and the latter the perspective of mathematics. For example, the region where applied mathematicians and physicists share common ground is called “mathematical physics”; or where applied mathematicians and biologists intersect is called “mathematical biology.”

Engineering corresponds to the outermost arena of Figure 1 and again it has many subdivisions: mechanical, chemical, electrical, and so on. Now the inner perimeter can serve to symbolize the interface with science and mathematics, specifically, “engineering science” and “mathematical engineering,”<sup>2</sup> and the outer perimeter can symbolize “applied” engineering in its usual sense: the development of “engineered objects” premised on science and mathematics, e.g., bridges, aeroplanes, and computers,

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<sup>1</sup>Here we are considering only the so-called “hard sciences,” in particular, the natural sciences.

<sup>2</sup>From the perspective of the mathematics arena, the relevant part of applied mathematics is called “engineering mathematics.” The diagonal lines within the science arena link the mathematics and engineering arenas and serve as a reminder that engineering borders on mathematics. They also add a visual dimension to the figure.

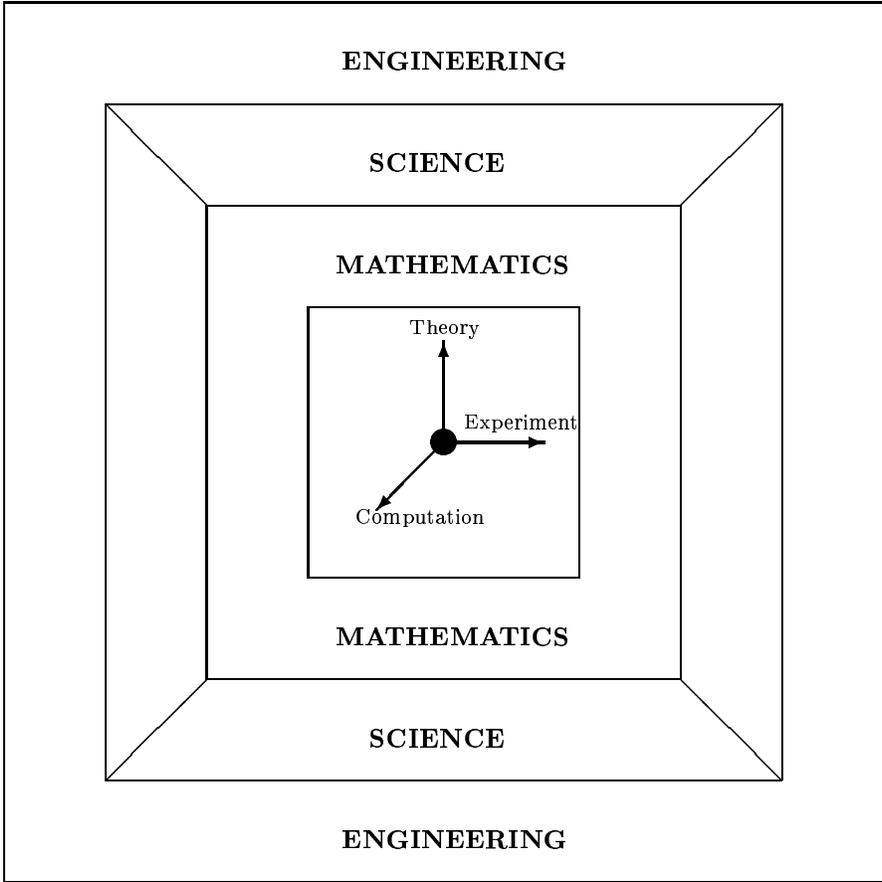


Figure 1: A Visual Icon

Some academic fields traverse arena boundaries in a natural manner. Computer science, for instance, has its origins in theoretical models of computation and complexity developed by mathematicians, which lie at its foundation. But the subject evolved subsequently, in tandem with the electronic computer, into a separate discipline<sup>3</sup> that unites science and engineering; the field is now commonly designated as computer science and engineering (CS&E); or electrical engineering and computer science (EE&CS).<sup>4</sup> Likewise, the discipline of statistics traverses the boundary between the mathematics and science arenas, uniting mathematical probability (measure) theory and the science of statistical data.

Finally, the three axes at the center of Figure 1 depict the three main *modus operandi*, or forms of investigation, that are employed within *any* branch of mathematics, science and engineering, namely, the theoretical,<sup>5</sup> experimental, and computational<sup>6</sup> modes; recall also Section 1. The central dot of the figure symbolizes any subfield within the arenas, for instance, evolutionary biology, which can be studied in theory, by experimentation in the laboratory, or via simulations on a computer. Or within mathematics, cf. the recent, landmark monograph of Borwein and Bailey [4] on the experimental/computational mode.

In summary, the inner perimeter of each arena—mathematics, science, or engineering—represents the “pure” side of its associated subject, and the outer perimeter represents the “applied.” Mathematics “applied” borders science (and engineering) “pure”; science “applied” borders engineering “pure.” And every subfield within the arenas, symbolized by the central dot, has three main *modus operandi* that correspond to the three axes: theory, experiment, and computation. Because the computer can be used as a “laboratory,” the distinction between the experimental and computational modes<sup>7</sup> can become blurred. Thus, the ambiguity within Figure 1 of three-dimensional axes being superimposed on a (shifting) two-dimensional portrayal of the arenas is, in fact, fortuitous.

Figure 1 will facilitate the discussion that now follows. We call this schema an “icon” because it is more closely akin to a “compound symbol” for the complex interrelationships between mathematics, science, and engineering than a strict pictorial representation of them.

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<sup>3</sup>The current interface between mathematics and computer science is discussed in Graham, Knuth and Patashnik [6].

<sup>4</sup>This union arises because the development of computer software and computer hardware are closely intertwined. Moreover, in the prescient definition of Newell, Perlis and Simon [10], modern computer science is best characterized simply as “the study of computers,” and the latter are themselves engineered objects in hardware and software.

<sup>5</sup>Note that “theoretical” does not necessarily imply the use of mathematics. For example, much of evolutionary biological theory is non-mathematical.

<sup>6</sup>Observe that even “computational computer science” is not redundant. For example, the properties of hashed symbol tables within computer science could be studied either theoretically or computationally (by simulation on a computer).

<sup>7</sup>The union of “experimental” and “computational” could be termed “empirical,” the counterpart of “theoretical.”

### 3 Algorithmic Science & Engineering (AS&E)

Let us turn to the positioning of algorithmic science within Figure 1, and first consider its foundational areas of numerical analysis and optimization. As the name “numerical analysis” suggests, the subject began within mathematics as the region of analysis where number representation and numerical processes play a central role, in particular, analysis of the effects of rounding error. This aspect is exemplified by the classic monographs of Wilkinson [14], [15]. The subject today enjoys a much broader interpretation—the study of numerical models and algorithms—and has diffused widely into most branches of the natural sciences and engineering. For further background, see the panel discussion in [11]. The field of optimization has enjoyed a similar success—its classic is the monograph of Dantzig [5]. These works, [5], [14], [15], which coincidentally appeared within the span of 1963–65, are the crown jewels of optimization and numerical analysis, two interrelated fields that have advanced rapidly, in tandem with computer hardware developments, during the past five decades. Key facets of the two fields are:

- The *art of modeling*, i.e., casting real applications into one of a wide array of basic mathematical (template) models. In the case of numerical analysis, these models generally take the form of linear or nonlinear equation-solving (including algebraic and differential), defined over finite-dimensional or infinite-dimensional (function) spaces. In the case of optimization, they generally involve the maximization or minimization of objective functions over feasible regions defined by equality and/or inequality constraints, again in finite or infinite dimensions.
- The *science of algorithmics*, i.e., the invention and implementation of efficient algorithms for solving models.
- The *mathematics of models and algorithms*, in particular, the analysis of solution sets and other properties of, and duality relationships between, various classes of models; and the analysis of algorithms from the standpoints of convergence, complexity, and numerical stability.

For a more detailed discussion within optimization, see [9].

While the modeling aspects of optimization and numerical analysis are often best conducted within, or in close partnership with, the scientific or engineering areas where the applications originate, the two fields continue to retain a strong *algorithmic core* and an *associated mathematics of (template) models and algorithms* for solving them. This subject is frequently subsumed nowadays under the rubric of *scientific computing*. In this term, “computing” broadly connotes “algorithms” and “software,” but its qualifying adjective “scientific” has an ambiguous interpretation and is used in two senses: “of, relating to, or exhibiting the methods or principles of science” and “as it applies to the sciences.” The

first interpretation, in conjunction with “computing” as “algorithmics,” yields the term “scientific algorithmics,” in other words, ‘algorithmic science.’ The second, oft-used interpretation of “scientific” within “scientific computing” is regrettable, because it only embraces the sciences arena of Figure 1. A more appropriate name would be, for example, “scientific, engineering, and mathematical computing,” which explicitly embraces all *three* arenas.<sup>8</sup>

The name “algorithmic science” has the advantage that it clearly identifies the *objects*<sup>9</sup> that lie at the heart of the discipline and are studied scientifically. As with any scientific discipline of Figure 1, the three modus operandi—theory, experiment<sup>10</sup> and computation—are readily evident, and the discipline interfaces with mathematics and engineering. From the viewpoint of science, the interface with mathematics would be mathematical algorithmic science; from the viewpoint of mathematics, it would be the relevant part of *algorithmic, or constructive*, applied mathematics. The intersection of algorithmic science and engineering involves the development, or engineering, of so-called mathematical software and is an *integral* part of the discipline. For this reason, we will use the name “algorithmic science and engineering,” abbreviated to AS&E, for the field in the discussion that follows. If the reader prefers, he/she can substitute the more recognizable name “scientific, engineering, and mathematical computing.”<sup>11</sup>

At the core of the discipline is the study of real-number algorithms of continuous mathematics, as characterized in Section 1, just as its counterpart study of algorithms of discrete mathematics—more specifically, “concrete” mathematics as defined in Graham, Knuth, and Patashnik [6]—is at the heart of computer science; see, in particular, the discussion in Knuth [7]. It is around this core area that AS&E can encompass a wide domain: *grand challenges of computing* (e.g., algorithmic investigations of protein folding or the intriguing near-optimality of the genetic code); *new computing paradigms* (e.g., the dramatic paradigm-shift proposed by Wolfram [16]); *cross-fertilizations* (e.g., the algebraic eigenproblem viewed from the standpoint of nonlinear optimization and equation-solving<sup>12</sup>); *foundations* (e.g., the real-number computational models of Blum, Cucker, Shub

<sup>8</sup>This alternative choice also has an appealing abbreviation: *sci-en-math computing*.

<sup>9</sup>Algorithms are finitely-terminating, teleological dynamical processes that are defined abstractly as mathematical objects or realized concretely in the form of computer software, or are found empirically within nature.

<sup>10</sup>For example, the experimental study of algorithmic processes involving annealing, spin glasses, or evolution based on genetic recombination and mutation.

<sup>11</sup>Algorithmic science can then be viewed as its *core area*. The public’s recognition of the word “algorithm” could well change in the future; see, in particular, Berlinski [1].

<sup>12</sup>For example, consider the symmetric eigenvalue problem. Given an  $n \times n$  symmetric matrix  $\mathbf{A}$ , let us view  $\mathbf{Ax} - \lambda\mathbf{x} = \mathbf{0}$  as a system of  $n$  polynomial equations in  $n+1$  unknowns for which all solutions  $(\mathbf{x}, \lambda)$  are sought. Add an  $(n+1)$ ’th equation,  $-\frac{1}{2}\mathbf{x}^T\mathbf{x} + 1 = 0$ , to obtain a square system with a symmetric Jacobian, and derive a potential function from the associated gradient mapping. Eigensolutions are the *stationary points* of the potential function. Are there any benefits to be accrued, conceptual or computational, from this optimization-based approach to the standard, or generalized, eigenproblem?

and Smale [3]); and so on. An emergent AS&E discipline within a university would help to integrate real-number algorithmic research, which is currently conducted within numerous departments, often in a disparate manner, with little intersection. Its recognition would thus have significant benefits for research.

In addition, significant educational advantages would be gained from the recognition of an AS&E discipline within the formal structure of a university, a counterpart of the now well-established discipline of computer science, or related CS&E and EE&CS. Requirements for graduate qualifying examinations could be set appropriately, to achieve the right balance between mathematical and computer science emphases. Coherent training could be provided for much-needed real-number computing professionals within academia and industry, producing graduating students that would be well-positioned in the job market. Mathematical software engineering would be a respectable activity within AS&E and would be officially recognized and rewarded, as is the writing of (non-mathematical) software within computer science.<sup>13</sup> Indeed, an AS&E discipline could comfortably embrace a full spectrum of orientations, ranging from theorem provers to mathematical software developers, all within the unifying rubric of “computing,” “algorithms,” and “software.”

Just as computer science, or its embracing CS&E and EE&CS disciplines, became established at universities during the past four decades, one can hope to see the discipline of AS&E, or an embracing scientific, engineering & mathematical computing, emerge in decades to come. In this regard, it is worth recalling Knuth’s original vision of computing and computer science as the “study of algorithms”; see his collected articles in [7]. This vision could be realized within a university by a full-fledged AS&E that works hand-in-hand with its counterpart CS&E, creating a situation whereby the study of algorithms for both continuous and discrete mathematics would receive more equal emphasis. Only time will tell, however, whether a desirable integration<sup>14</sup> of real-number algorithmic-oriented research and education will indeed become a reality, or whether fragmentation of its underlying fields of algorithmic numerical analysis and optimization will continue.

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<sup>13</sup>Writing a large piece of software is as challenging a task as proving a convergence theorem—harder perhaps, because the computer is an unrelenting taskmaster—yet mathematical software development receives little reward in a mathematics or mathematical sciences department.

<sup>14</sup>A blueprint for an informally-structured nexus for the emerging discipline—an algorithmic science and engineering research center—can be found at the web address: [www.math.wsu.edu/faculty/nazareth/aserc.pdf](http://www.math.wsu.edu/faculty/nazareth/aserc.pdf).

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