应用数学新时代的曙光

The Dawning of a New Era in Applied Mathematics

鄂维南 / 文

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1. 开普勒范式和牛顿范式

自牛顿以来，科学研究基本上是按照开普勒和牛顿这两种不同的范式展开的。开普勒范式是一种数据驱动的研究方式，通过对数据的分析寻找科学规律并解决实际问题。其经典案例是行星运动的开普勒定律。生物信息学为开普勒范式在现代的成功提供了一个令人信服的例证。牛顿范式是一种基于第一性原理的研究方式，其目标是发现物理世界的基本原理。它的最佳案例来自牛顿、麦克斯韦、玻尔兹曼、爱因斯坦、海森堡和薛定谔等人的理论物理工作。时至今日，牛顿范式仍是许多顶级才智的主要用武之地。

随着统计方法和机器学习的发展，数据驱动的研究方法已经成为一种非常强大的工具。它能有效地帮助我们发现规律，但对于找到规律背后的原因却鲜有成效。

基于第一性原理的研究方法旨在从最基本的层面理解事物。对第一性原理的追求很大程度上驱动了物理学的发展。1929 年，随着量子力学的建立，这条道路出现了一个重大转折点：正如狄拉克[2]所宣称的那样，有了量子力学，除一些极端尺度下的情形以外（如核物理），我们已经掌握了大多数工

[2] Paul A. Dirac, Quantum mechanics of many-electron systems, Proc. Roy. Soc. London Ser. A 123 (1929), no. 792.

1. The Keplerian and Newtonian Paradigms

Ever since the time of Newton, there have been two different paradigms for doing scientific research: the Keplerian paradigm and the Newtonian paradigm. In the Keplerian paradigm, or the data-driven approach, one extracts scientific discoveries through the analysis of data. The classical example is Kepler's laws of planetary motion. Bioinformatics provides a compelling illustration of the success of the Keplerian paradigm in modern times. In the Newtonian paradigm, or the first-principle-based approach, the objective is to discover the fundamental principles that govern the world around us or the things we are interested in. The best example is theoretical physics through the work of Newton, Maxwell, Boltzmann, Einstein, Heisenberg, and Schrödinger. It is still a major playground for some of the best minds today.

The data-driven approach has become a very powerful tool with the advance of statistical methods and machine learning. It is very effective for finding the facts, but less effective for helping us to find the reasons behind the facts.

The first-principle-based approach aims at understanding at the most fundamental level. Physics, in particular, is driven by the pursuit of such first principles. A turning point was in 1929 with the establishment of quantum mechanics: as was declared by Dirac [2], with quantum mechanics, we already have in our hands the necessary first principles for much of engineering and the natural sciences except physics at exceptional scales.

程和自然科学所需要的第一性原理。

然而，也正如狄拉克所指出的那样，描述量子力学基本原理的数学问题异常复杂。困难之一在于它是一个多体问题：每加上一个电子，问题的维数便增加了三。事实上，第一性原理方法经常面临的困境是：尽管它很深刻，但它不太有用。因此，在实践中，我们常常不得不放弃严格优雅的理论，而采取经验的、非系统的近似方法。我们为此付出的代价不仅仅是丢失了严格和优雅，还有结果的可靠性和普适性。

讨论这两种范式的原因是因为应用数学正是沿着类似的路线发展起来的。由于物理学的基本原理通常是用微分方程来表述的，微分方程的分析和数值算法自然在应用数学中占据了中心地位，特别是在 20 世纪 50 到 80 年代期间。其目标有三重：解决实际问题，理解其背后的数学原理，为实际问题提供物理直觉。流体力学是一个非常典型的成功案例。不仅流体力学已成为偏微分方程研究的主要动力，计算也已经成为流体力学研究的一个基本工具。这个事实也证明了数值方法的成功。直到今天，对偏微分方程和数值方法的研究仍然是应用数学的一个中心课题。

However, as was also pointed out by Dirac, the mathematical problem that describes the laws of quantum mechanics is exceptionally complicated. One of the difficulties is that it is a many-body problem: with the addition of one electron, the dimensionality of the problem goes up by 3. This is the dilemma we often face in the first-principle-based approach: it is fundamental but not very practical. Consequently in practice we often have to abandon the rigorous and elegant theories and resort to ad hoc and nonsystematic approximations. The price we pay is not just the lack of rigor and elegance, but also the reliability and transferability of the results.

Applied math has developed along a similar line. Since the first principles of physics are formulated in terms of partial differential equations (PDEs), the analysis and numerical algorithms for PDEs has occupied a central role in applied math, particularly during the period from the 1950s to the 1980s. The objective is three-fold: solving practical problems, understanding the mathematics behind them, providing physical insight into these practical problems. A very compelling success story is fluid mechanics. Not only has fluid mechanics been a major driving force for the study of PDEs, the fact that fluid mechanics research has largely become a computational

我在加州大学洛杉矶分校读研究生时，我们的老师自豪地告诉我们，我们属于“柯朗风格的应用数学”阵营。这个词是为了与“英式风格的应用数学”相对应而创造出来的。两者都专注于流体力学。英式风格崇尚物理洞察力和渐近分析。领袖人物如泰勒、巴彻勒、林家翘、莱特希尔等，不仅是伟大的应用数学家，也是流体力学的领军人物。众所周知，他们一般不重视数值计算和严格的分析。柯朗风格则推崇数值计算和严格的数学理论（他们被另一阵营戏称为“证明定理的人”）。它的理念是只要基本的偏微分方程和数值算法是可靠的，我们就可以通过计算学到很多东西。毕竟，物理过程是非常复杂的；没有计算，我们不可能走得太远。他们的一些领袖，如冯•诺依曼、柯朗、弗里德里希和拉克斯，不仅是伟大的应用数学家，也是伟大的纯数学家。这两个学派之间的争执被认为是当时应用数学的主要矛盾。这也证实了那个时期流体力学在应用数学中所占的统治地位。

在数据方面，正统的研究团体是在统计学界。然而不知什么原因，直到不久前，统计学一直是独立于应用数学发展的。事实上，它也基本独立于数学。数学系或应用数学研究所很少有统计学方面的团队。直到最近几年才有人呼吁改变这个现象。

这并不意味着应用数学界对数据驱动的方法不感兴趣。相反，自 20 世纪 80 年代后期以来，随着对小波和压缩感知的研究，信号和图像处理在应用数学中占据了中心地位。事实上，过去三十年，这种应用数学版本的数据驱动方法一直是应用数学中最高产的领域之一。

也不是说流体力学是经典应用数学唯一成功的例子。事实上，有人会说固体力学同样成功：毕竟应用数学最重要的算法之一——有限元方法就是从固体力学中诞生的。另一个成功的例子是数值线性代数：人们只需看看 Matlab 的流行程度，就可以体会到它的广泛影响。这样的例子不胜枚举。

2. “柯朗学派”的危机

不幸的是，对于我们这一代“柯朗学派”的应

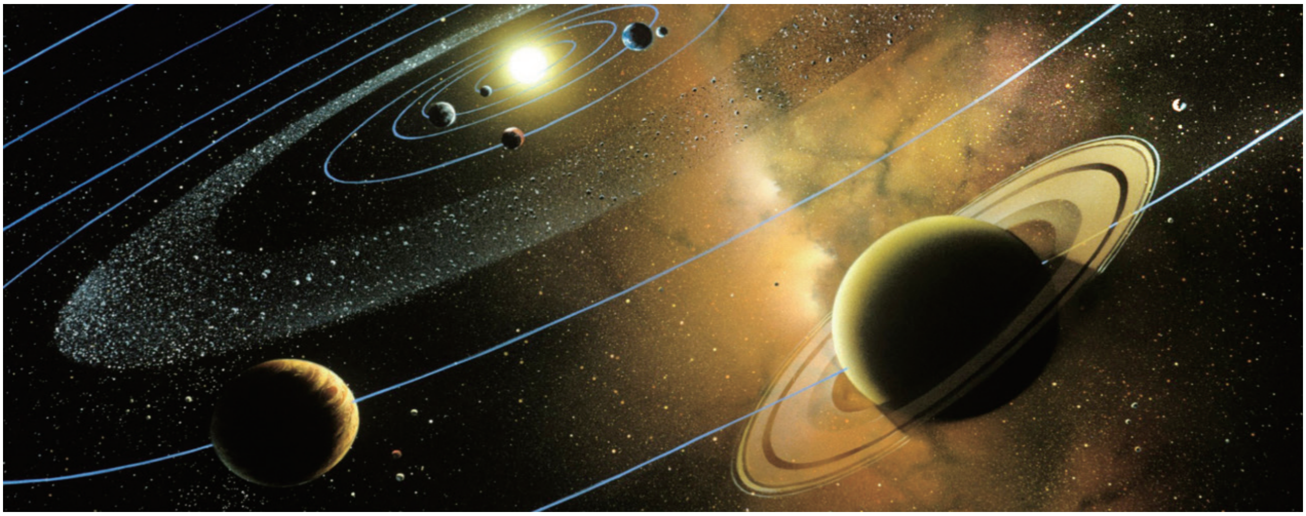
discipline is also testimony to the success of the numerical algorithms that have been developed. The study of these PDEs and the numerical algorithms have been a central theme in applied math for many years and it is still an active area today.

When I was a graduate student at UCLA, we were proudly told that we belonged to the camp of “Courant-style applied math.” This term was coined to make a distinction with the “British-style applied math.” Both focused on fluid mechanics. The British-style championed physical insight and asymptotics. The leaders, Taylor, Batchelor, C. C. Lin, Lighthill, et al., were not only great applied mathematicians but also leading theoretical fluid dynamists. It is also known that they generally did not hold numerics and rigorous analysis in very high regard. The Courant-style championed numerics and theorems (“theorem provers”). Its philosophy was that as long as the underlying PDEs and numerical algorithms are solid, much can be learned through computing. After all, the physical processes are very complicated; one cannot go very far without computing. Some of their leaders, such as von Neumann, Courant, Friedrichs, and Lax, are not only great applied mathematicians, but also great pure mathematicians. The fact that the feud between these two schools was considered the main animosity in applied math speaks for the dominance of fluid mechanics during those times.

The card-carrying data-driven research community has been statistics. For whatever reason, until quite recently, statistics has developed pretty much independently of applied math, and in fact, independently of mathematics. It was very rare that a math department or applied math program contained statistics. It is only in recent years that there has been a call for change.

This does not mean that the applied math community has not been interested in the data-driven approach. To the contrary, since the late 1980s, with research work on wavelets and compressed sensing, signal and image processing has taken a center stage in applied math. In fact, this applied math version of a data-driven approach has been among the most productive areas of applied math in the last thirty years.

Neither does it mean that fluid mechanics was the only



用数学家来说，流体力学的统治地位和成功带来的更多是挑战而非机遇。偏微分方程和流体力学的奠基性工作已被前辈们完成。我们面临的要么是解决遗留问题，如湍流，要么是开辟新的领域。事实证明，这两条道路都很艰难，更不要说重现应用数学在流体力学中的辉煌。

事实上，继流体力学之后，柯朗风格的应用数学已经扩展到许多其他科学与工程学科，如材料科学、化学、生物学、神经科学、地球科学和金融工程等，并取得了巨大成功。但总的来说，应用数学在这些领域的成功程度无法比拟我们在流体力学中所见到的。虽然我们的工作是受欢迎的，但这种贡献往往是增量性的，而不是变革性的。因此，科学家们为了解决他们所面临的核心问题，经常不得不采取既不可靠又很繁琐的近似方法。这种情况在量子力学、分子动力学、粗粒化分子动力学、化学反应、复杂流体模型、塑性力学模型、蛋白质结构与动力学、湍流模型、控制问题、动态规划等许多领域都可以看到。

对于上述的大多数（即便不是全部）问题而言，其共同点在于它们本质上是高维问题，而维数灾难是一个核心困难。

对其中的许多问题，高维是由问题的多尺度特性所导致的结果。二十多年前，多尺度、多物理建模的想法曾经给我们带来了一线希望：通过将小尺度下的无关紧要的自由度整合起来，人们应当能够直接使用更可靠的微观尺度模型，为我们感兴趣的

successful area for applied mathematicians interested in PDEs. In fact, some would argue that solid mechanics was equally successful: after all it was from solid mechanics that the finite element method, one of the most important success stories in applied mathematics, was originated. Another success story is numerical linear algebra: one just has to look at how popular Matlab is to appreciate its widespread impact. This list goes on.

2. Crisis for the "Courant-style Applied Math"

Unfortunately for my generation of "Courant-style" applied mathematicians, the dominance and success in fluid mechanics presented more of a challenge than an opportunity. The ground work for PDEs and fluid mechanics was already laid down by the generations before us. We were left to either address the remaining problems, such as turbulence, or conquer new territory. Both have proven to be difficult, not to mention reproducing the kind of success that applied math had before in fluid mechanics.

Indeed after fluid mechanics, the Courant-style applied math has spread to many other scientific and engineering disciplines, such as material science, chemistry, biology, neuroscience, geoscience, and finance, with a lot of success. But generally speaking, the degree of success in these areas has not matched what we saw in fluid mechanics. Our contributions are welcomed, but they tend to be incremental rather than transformative. As a result, to deal with the central issues that they face, scientists or