The Nature and Context of Exploratory Experimentation:

An Introduction to Three Case Studies of Exploratory Research

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Abstract: My aim in this article is to introduce readers to the topic of exploratory experimentation and briefly explain how the three articles that follow, by Richard Burian, Kevin Elliott, and Maureen O'Malley advance our understanding of the nature and significance of exploratory research. I suggest that the distinction between exploratory and theory-driven experimentation is multidimensional and that some of the dimensions are continuums. I point out that exploratory experiments are typically theory-informed even if they are not theory-driven. I also distinguish between research programs and experiments. Research programs that are largely exploratory, such as the ones discussed in these case studies, can involve both exploratory and theory-driven experimentation.

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This article introduces the topic of exploratory experimentation and briefly explains how the three articles that follow, by Richard Burian, Kevin Elliott, and Maureen O'Malley advance our understanding of the nature and significance of exploratory research[1].

Recent philosophical research on exploratory experimentation began with the observation that experimentation in science is not always guided by theory, that sometimes, experimentation is exploratory in nature. Friedrich Steinle (1997) set out to characterize exploratory experimentation by examining a difference between specific experiments in the early research of electromagnetism. Some experiments were designed to look for specific effects, which were expected because of theoretical ideas about electromagnetism. But other experiments were set up to discover rules about electromagnetic behavior about which the investigators had no theoretical ideas, and hence had no specific expectations. This difference, as Steinle showed, was reflected in experimental designs. The

[1] Kevin Elliott organized a session on exploratory experimentation at the 2007 conference of the International Society for the History, Philosophy, and Social Studies of Biology and invited Dick Burian and Maureen O'Malley to give papers. He asked me to introduce the session and comment on the papers afterwards. The session turned out to be very stimulating and Kevin, Dick, and Maureen decided to develop their papers and submit them to this journal. I would like to thank them for inviting me to write and submit an accompanying essay, and for writing provocative papers on a topic that is central to my research on genetics and allied sciences. My thinking has been advanced by this collaboration. In addition, we all benefited from stimulating discussion with the audience at the conference and from our sustained conversations about their papers. I would like to thank Kevin, Dick, and Maureen for commenting on an earlier draft of this essay, and my colleague Antigone Nounou for suggesting the term "theory-informed". I would also like to acknowledge Keith Benson's patient support of this project.

exploratory experiments were set up in ways that enabled investigators to intervene in a variety of ways. This made sense because investigators did not enter the inquiry with ideas about which kinds of interventions were likely to influence the phenomena and how they would influence the phenomena. In contrast, experiments directed by theory were set up in ways that restricted the ranges of intervention. This enabled experimenters to focus on the most promising interventions, that is, most promising from the perspective of their theoretical ideas about the phenomena being investigated.

Richard Burian (1997) made similar observations, but in the context of early research on the localization and function of nucleic acids. Burian, who was influenced by Hans Rheinberger's account of research on protein synthesis (1997), also used the term "exploratory experimentation" to describe a style of inquiry that is not guided by theory. Burian examined the extensive and fruitful research program of Jean Brachet, who investigated the distribution of nucleic acids through cell cycles and ontological development. Brachet's inquiry was not guided by theoretical speculations about the role nucleic acids might play in these processes or even hunches about how nucleic acids would be distributed. Unlike Francis Crick, Brachet's team did not employ theoretical speculation to guide their inquiry. They employed biochemical methods to systematically follow the distributions of these molecules through cell cycles and ontology in a variety of organisms. These experiments, Burian observed, were exploratory in nature.

There were differences between Steinle's and Burian's accounts. For example, Steinle proposed a narrower conception of "exploratory experimentation" than did Burian. But both philosophers argued that exploratory experimentation is an important activity in scientific investigation, an activity which has been obscured by traditional accounts of experimentation that stress the role of hypothesis testing, and by traditional accounts of scientific knowledge and practice that emphasize theoretical knowledge and theory-driven practice. Philosophy of science, as Ian Hacking (1983) complained, is theory-biased. Burian and Steinle both sought to understand the nature and role of a kind of experimentation, exploratory experimentation, that had been hidden by philosophers' preoccupation with theoretical reasoning.

In thinking about exploratory experimentation and the articles that follow, it is helpful to keep three points in mind. First, the line between exploratory and theory-driven experimentation, as Steinle mentions, should not be drawn between experiments aimed at testing hypotheses and experiments aimed at generating new hypotheses. Theoretical considerations can direct experimentation in a variety of ways. Second, exploratory experimentation is typically not free of theory. There is a subtle but importance difference between being theory-directed and being theory-informed. The distinction between exploratory and theory-driven experiments centers not on whether an experiment depends on theory, but on the way(s) in which it depends on theory. And third, the distinction between exploratory and theory-driven experimentation is not necessarily sharp. I will develop these points by briefly reviewing Thomas Kuhn's account of "normal science" (Kuhn 1970).

Kuhn's account of normal science, which Hacking (1983) criticized for being theory-biased, shows that theory-driven research encompasses much more than hypothesis testing. Although Kuhn articulated his account of normal science in terms of "paradigms", his account centered on the idea that the practice of normal science involved articulating and extending "paradigm theories". Kuhn's classification of the activities of normal science included two umbrella categories: theoretical activities and "fact-gathering" activities. His description of theoretical activities is not directly relevant to my present concerns, and I will not discuss it here. His broad characterization of the fact-gathering activities included both experimentation and observation. But his taxonomy of fact-gathering activities did not divide along these lines, or along a line between hypothesis testing and exploratory research.

Kuhn identified three classes of fact-gathering activities, each associated with an aim. The first class of activities identified by Kuhn are those aimed at uncovering facts about those things, such as periods of planets, specific gravities, spectral intensities, and boiling points that "the paradigm has shown to be particularly revealing of the nature of things." (Kuhn 1970, p. 25) These activities are theory-directed in at least a weak sense, and in varying degrees in a stronger sense as well. They are *theory-directed in the weak sense* that the theory directed experimenters to search for facts about some things and not about other things. Experiments falling under Kuhn's first class of fact-gathering activities can also be *theory-directed in the strong sense* that a theory generates expectations about what will be observed when the experiment is conducted. The second class of fact-gathering activities identified by Kuhn are aimed towards determining facts that can be compared to predictions from the paradigm theory. These are theory-directed, and in the strong sense that a theory generates expectations about what will be observed.

The aim of the third class of activities, which Kuhn claimed are the most important fact-gathering activities of normal science, is to "articulate the paradigm theory". (Kuhn, p. 27) Scientists do so by determining physical constants to greater degrees of accuracy (theory-directed in the strong sense), by revealing facts that can be used to select among alternative ways of extending the paradigm to closely related areas of inquiry (hypothesis testing), and by discovering new quantitative laws. The latter kind of activity might sound like "exploratory" rather than "theory-driven" experimentation. But here is how Kuhn described it:

> *Perhaps it is not apparent that a paradigm is prerequisite to the discovery of laws like these. We often hear that they are found by examining measurements undertaken for their own sake and without theoretical commitment. But history offers no support for so excessively Baconian a method. Boyle's experiments were not conceivable (and if conceived would have received another interpretation or none at all) until air was recognized as an elastic fluid to which all the elaborate concepts of hydrostatics could be applied. Coulomb's success depended upon his constructing special apparatus …. But that design, in turn, depended upon the previous recognition that every particle of electric fluid acts upon every other at a distance. (Kuhn, p. 28)*

Boyle's experimentation seems theory-directed in at least the weak sense that the theory about the underlying phenomena led scientists to conduct the experimentation, but it is unclear whether it was theory-directed in the strong sense (i.e. it is unclear whether from the quotation whether Boyle's theoretical ideas about hydrostatics generated expectations about what would be observed). The fact that Coulomb employed theory to construct an experimental apparatus, in itself, does not imply that experimentation utilizing the apparatus was theory-directed, even in the weak sense. If a scientist employs a theory about one kind of phenomenon to experiment on a separate kind of phenomenon, the experimentation on that separate kind of phenomenon is not necessarily directed by a theory about that separate kind of phenomenon. If it is not directed by such a theory, it would be more accurate to call the experiment *theory-informed* rather than *theory-directed*. But Kuhn, himself, did not explore this nuance, and did not entertain the possibility that exploratory research was a part of normal science. As he put it, "No part of the aim of normal science is to call forth new sorts of phenomena; indeed those what will not fit the box are often not seen at all." (Kuhn 1970, p. 24),

My aim here is not to argue that Kuhn was mistaken to dismiss the possibility that exploratory experimentation is an important part of normal science. This is amply accomplished in the articles that follow. I discuss Kuhn's account of normal science because it demonstrates the point that theory can drive research in a variety of ways. The style(s) of experimentation identified by Steinle and Burian, and investigated further by the articles that follow, falls largely outside the classes of experimentation and observation that Kuhn identified with the practice of normal science.[2]

The second point to keep in mind is that exploratory experimentation is not (typically) theory free. All kinds of background theories are used to set up experiments, generate data, and draw conclusions (as Kuhn's remark about Coulomb's apparatus attests). Exploratory experimentation is embedded within scientific inquiry that relies on a lot of theory. The point of difference, Burian (1997) and Steinle (1997) suggest, is that the experiments are not "directed" by the aim to test, develop, or otherwise articulate an existing theory or hypothesis. Roughly speaking, *the aim of exploratory experiments is to generate significant findings about phenomena without appealing to a theory about these phenomena for the purpose of focusing experimental attention on a limited range of possible findings*. The findings might be significant with respect to a variety of goals ranging from the practical goal to learn how to manipulate a phenomenon to the theoretical goal to develop a conceptual framework that will help focus future experimental attention.

[2] This raises a question of whether exploratory experimentation is what Kuhn meant by pre-paradigm science. The quick answer is no. Kuhn's account of pre-paradigm practice attributes a large role to theoretical speculation. The distinction between normal and pre-paradigm science in Kuhn's account centers on whether science is driven by a single paradigm associated with a uniform theoretical perspective or whether it is practiced in a disunified fashion associated with a number of conflicting theoretical perspectives. Experimentation in pre-paradigm science, according to Kuhn's account, is often theory-driven.

As Burian says in this issue, exploratory experimentation comes into play when theory does not provide expectations of what investigators will find. He does not deny that theory plays a role in exploratory experimentation. Instead, he claims that theoretically generated expectations do not direct research by guiding scientists to set up particular experiments. The vagueness of "direct" and "guide" in this context leads to the third point: the distinction between exploratory and theory-driven experimentation does not mark a sharp division. The fact that theory plays a multiplicity of roles in theory-driven research indicates that the difference between exploratory experimentation and theory-directed experimentation may involve multiple dimensions. And the fact that some of these roles admit degrees indicates that the difference between exploratory and theory-driven experimentation might represent continuums along these dimensions. Clearly, thinking about experimentation in terms of a simple dichotomy is too superficial.

In addition to these three points, it is also helpful to keep in mind the distinction between experiments and programs of research. Some research programs, such as the program of investigative research in genetics, involve stable meta-strategies of exploratory experimentation in which the experimental procedures themselves evolve over time (see Waters 2008). Appreciating the significance and continuity of experimentation, as the example of genetics shows, requires understanding the larger context of the research program in which they are carried out. And in the larger context, one and the same research program might include a combination of both exploratory and theory-driven experimentation. Some research programs are largely exploratory in nature, such as the ones discussed in the three articles that follow. And others are largely theory-directed, such as the ones that are emphasized in traditional philosophical discussions. But research programs that are largely exploratory might include some theory-directed experiments and programs that are largely theory-driven might include some exploratory experiments. Adding to the complexity is that fact that one and the same experimental procedure might be employed for the purposes of exploratory research in some situations and theory-driven research in others. The messy world of scientific practice may not yield to sharp distinctions aimed at partitioning research programs or experimental procedures into neat categories such as theory-driven versus exploratory.

In light of these sloppy complications, philosophers might be tempted to drop the topic of exploratory experimentation altogether. Perhaps this style of experimentation is relevant only in the very early contexts of scientific investigation. One might suppose that the progressive development of scientific practice depends on experimentation becoming increasingly directed by theory. If this were the case, then understanding the productivity of scientific practice would require understanding the ways in which experimentation becomes increasingly effective as it becomes increasingly theory-driven. One might argue that the exploratory experiments discussed by Steinle and Burian are outliers, not worthy of philosophical attention or analysis because the experimenters did not use the kind of reasoning that makes scientific experimentation so productive.

The reasoning that makes scientific experimentation so productive, on this view, is reasoning that employs theoretical considerations in ways that focus experimental attention on a limited range of possible findings. This seems to be Kuhn's explanation of the productivity of normal science.

Burian's contribution to this issue offers a new and compelling argument against the idea that exploratory experimentation is an outlier. Or to put it more positively, Burian offers good reason to think that the continued success of biological sciences will depend on the use of exploratory experimentation that will not be led by theory-generated expectations. His argument is based on ontology. He claims that biological systems, such as the system of a cell, are too complicated to be investigated by means of a theory-driven approach. Such systems contain a variety of mechanisms that work in such different ways that no single theoretical perspective can unify the details of their workings. Hence, knowledge of the details of some mechanisms in a system will not provide general insights that will help direct experimentation on other mechanisms in the system. Burian bases this claim on the way scientific investigation has proceeded in the study of microRNA, on recent discoveries about the mind-boggling complexities of molecular mechanisms in cellular biology, and on biologists' understanding of the highly contingent nature of the evolutionary process.

If Burian is correct, then exploratory research in biology is here to stay. The future success of experimental inquiry will depend on it. This motivates the project of investigating the styles of reasoning underlying exploratory investigations. And this is exactly what Elliott and O'Malley do in their contributions to this volume. Their case studies move our understanding of exploratory experimentation beyond simplistic dichotomies and call attention to nuances and complexities of exploratory experimentation in the broader context of exploratory research. Elliott's aim is to develop a taxonomy of exploratory experimentation by conducting a case study of nanotoxicology, a program of ongoing research rich in exploratory experimentation. The aim of nanotoxicology is to determine the biological and environmental effects of nanoparticles. Elliott analyzes a comprehensive plan of investigation for the field written by a leading investigator, Gunter Oberdörster and his collaborators (2005).

Elliott's analysis leads him to construct a taxonomy of exploratory experimentation which is strikingly different than Kuhn's taxonomy of the research activities of normal science. Nevertheless, there is overlap in the activities that Kuhn and Elliott identify. Kuhn, for example, includes the construction of experimental apparatus (e.g. Coulomb's device) as does Elliott. And Elliott includes the aim of resolving anomalies, as does Kuhn. This suggests that the difference between exploratory and theory-driven research practices is more subtle than a simple dichotomy. Elliott deals with the complexity of exploratory experimentation by constructing a taxonomy along three separate dimensions: (1) different goals, (2) different ways theory is employed, and (3) different experimental methods and strategies. One feature his taxonomy exemplifies is the lack of sharp distinctions among different styles of exploratory experimentation. He describes the differences in terms of continuums.

Careful readers will notice that Elliott's taxonomy includes classes of experimentation that seem to be theory-directed. For example, his dimension of different aims includes anomaly resolution, which appears theory-directed in at least the weak sense that theory directs experimenters to seek information about some things and not other things. His dimension of the different roles that theory can play in experimentation includes the role of being used as a starting point. This seems to cover theory-directed experimentation in the strong sense that theory generates expectations of what will be observed. Each of Elliott's categories is exemplified by an experimental strand in nanotoxicology. What the presence of these categories of apparently theory-directed experimentation indicates, I suggest, is that the research program of nanotoxicology, while largely exploratory, includes some theory-directed experimentation. One way to interpret Elliott's taxonomy, though not the way he originally intended, is as a taxonomy of experimentation in an exploratory *research program*. Under this reinterpretation, his taxonomy reveals that an exploratory *program* of research can include both exploratory and theory-driven experimentation. In addition, it shows that the difference between exploratory and theory-directed experimentation, as the difference between styles of exploratory experimentation, involves gradations of differences along multiple dimensions.

O'Malley, in her article that follows, explicitly examines the way exploratory and theory-driven experimentation interact within the context of an exploratory program of research. She examines metagenomics, a program of research that involves the sequencing and analysis of large amounts of DNA collected across a variety of specific environments containing a diversity of microorganisms. The aim of this "high through-put" research is to explore currently uncharacterized microbial entities and processes. Metagenomics has led to a number of important discoveries and O'Malley focuses on several strands of investigation that began with the accidental discovery of a proteorhodopsin gene in ocean microbes. Proteorhodopsin is associated with processes that produce energy from light (but not via the more complex processes of photosynthesis that involve chlorophyll). Prior to this discovery, scientists thought this kind of energy producing process was extremely rare and confined to microbes in highly unusual environments. The discovery, as O'Malley shows, led to a number of important discoveries ranging from concrete conclusions about the prevalence of light utilization in ocean waters to the abstract idea that functional properties ought to be studied as they relate to particular environments rather than to particular lineages of organisms. She also shows how this discovery led to new ideas about the dynamics of gene transfer and microbial evolution.

O'Malley's account shows that the research program of metagenomics involved exploratory experiments that were theoretically informed, but not theory-driven. But her account also shows that various strands of research led to theory-driven analysis of data (that led, for example, to conclusions about the selection of very small sequence changes) and the testing of theoretical ideas (that led, for instance, to the rejection of ideas about the evolution of rhodopsin molecules). She points out that the testing of theoretical ideas in the context of metagenomics sometimes fits the model of natural experimentation (which examines naturally existing patterns of variable combinations instead of patterns resulting from experimental manipulation). She calls this special kind of probing natural history experimentation. O'Malley concludes that the practice of metagenomics involves an interaction of a diversity of activities including exploratory experimentation, theory-driven experimentation, and natural history experimentation.

The picture of scientific practice that emerges from Burian's, Elliott's, and O'Malley's cases studies shifts attention to styles of experimentation that are obscured by the theory-biased perspective that currently dominates the philosophy of science. Burian offers a strong argument for the idea that exploratory experimentation is and will continue to be an essential part of experimental practice in biological sciences. It is not a fleeting feature of the early stages of scientific investigation. Elliott offers a taxonomy that helps make sense of the complexity of largely exploratory research programs without obscuring the important role of exploratory experimentation. His taxonomy offers an important starting point for organizing our understanding of scientific research practices that are not dominated by theory. O'Malley helps pave the way towards understanding how scientific research can involve a productive interchange of different styles of experimentation and observation. Together, these articles provide a strong corrective and should, I hope, lead all of us to adopt a less theory-biased, more inclusive, investigation of scientific practice.

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