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ASSURING DATA QUALITY
AT U.S. GEOLOGICAL SURVEY LABORATORIES

Committee to Review the U.S. Geological Survey's Laboratories

Board on Earth Sciences and Resources

Division on Earth and Life Studies

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This Consensus Report was reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise. The purpose of this independent review is to provide candid and critical comments that will assist the National Academies of Sciences, Engineering, and Medicine in making each published report as sound as possible and to ensure that it meets the institutional standards for quality, objectivity, evidence, and responsiveness to the charge. The review comments and draft manuscript remain confidential to protect the integrity of the process.

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Although the reviewers listed above provided many constructive comments and suggestions, they were not asked to endorse the content of the report nor did they see the final draft before its release. The review of this report was overseen by **Paul Gilman**, Covanta Energy Corporation, and **Michael Ladisch**, Purdue University. They were responsible for making certain that an independent examination of this report was carried out in accordance with the standards of the National Academies and that all review comments were carefully considered. Responsibility for the final content rests entirely with the rapporteur and the National Academies.

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Contents

Summary

The U.S. Geological Survey (USGS) mission is to provide reliable and impartial scientific information to understand Earth, minimize loss of life and property from natural disasters, and manage water, biological, energy, and mineral resources. Data collection, analysis, interpretation, and dissemination are central to everything the USGS does. Among other activities, the USGS operates some 250 laboratories across the country to analyze physical and biological samples, including water, sediment, rock, plants, invertebrates, fish, and wildlife. The data generated in the laboratories help answer pressing scientific and societal questions or support regulation, resource management, or commercial applications. Consequently, it is important to maintain public trust in USGS data.

In 2016, an Inspector General report found scientific misconduct and data manipulation at a USGS laboratory in Colorado. Two laboratory analysts had adjusted values outside of protocols over two extended periods. To restore confidence in USGS data, the USGS began developing a quality management system (QMS) in 2016 and set an aggressive schedule for its implementation. A QMS is a structured system that establishes and documents the requirements for how work is to be managed, conducted, and monitored to assure data quality. A QMS is a paradigm shift for the USGS because all its laboratories will be required to implement a centrally defined quality standard in a similar and consistent way.

At the request of the USGS, the committee reviewed a representative sample of USGS laboratories, examined QMS and other approaches for assuring the quality of laboratory results, and recommended best practices and procedures for USGS laboratories. The specific tasks to the committee are given in Box S.1 and discussed below.

The tasks in Box S.1 specify two types of laboratories:

1. Research laboratories, which support innovation or scientific discovery and are typically led by a principal investigator (senior scientist). Some research laboratories also develop methods that are needed to answer a scientific question or that other laboratories can use for routine analyses.

2. Production laboratories, which carry out routine or repeated analyses for USGS or external customers, are sometimes supported by user fees, and are generally led by laboratory managers.

In practice, many USGS laboratories carry out a mix of these activities. Consequently, the committee sought to differentiate laboratories that primarily serve scientists, and thus likely support research activities, from laboratories that serve external customers (regulators, resource managers, and private companies), and thus likely support production activities.

Box S.1
Committee Tasks

An ad hoc committee will review a representative sample of USGS laboratory facilities, covering energy and minerals, natural hazards, surface and groundwater, ecosystems, and environmental health. The review will focus primarily on production laboratories that serve both USGS users and external customers, and secondarily on laboratories that support research and method development. Specific tasks for the committee are given below.

1. Provide an overview of USGS laboratory facilities across the nation, including their science and applications objectives, budget, staff and user profiles, and history of sample throughput for the past 5 to 10 years.
2. Describe the laboratory protocols, analytical procedures and standards, and data management processes for USGS laboratories, relevant laboratories hosted by other federal agencies (e.g., National Institute of Standards and Technology, U.S. Army laboratories, and National Institutes of Health), and geological surveys in other countries (e.g., Canada, United Kingdom, Australia, and Norway).
3. Assess the extent to which resources (operational and personnel) are sufficient to meet the scientific and applications objectives of USGS laboratories (production, research, and method development).
4. Develop criteria for assessing protocols and procedures used by the organizations in Task 2, and use them to identify relevant best practices and procedures for USGS production laboratories.
5. Provide recommendations on best practices and procedures for achieving scientific and applications objectives and ensuring the integrity and reliability of results from USGS production laboratories.
6. Comment on best practices and procedures for USGS research and method development laboratories.

The analysis will be based on USGS-provided profiles of its laboratory facilities and protocols, preliminary results from the USGS assessment of quality management procedures at its laboratories, and other information gathered by the committee at site visits, teleconference meetings, and elsewhere.

USGS LABORATORIES

Tasks 1 and 3 concern USGS laboratory characteristics. Before 2016, the USGS did not have a complete inventory of its laboratories and their capabilities. Consequently, the agency issued two data calls to its employees: one on basic laboratory information and one on data quality procedures. In responding to the questionnaires, laboratory managers and principal investigators defined their own laboratory boundaries, with some grouping similar activities into a single laboratory, and others splitting similar activities into more than one laboratory. This exercise yielded 257 analytical laboratories. The committee examined the USGS 2016 laboratory inventory in the context of its tasks.

Task 1

Task 1 was to provide an overview of USGS laboratories, including scientific objectives, budget, staff, user profiles, and sample throughput rate. The committee found substantial diversity in all of these factors. Collectively, the laboratory science and applications objectives cover all USGS mission areas: core science systems, ecosystems, energy and minerals, environmental health, land resources, natural hazards, and water resources. Some laboratories focus on a mission area, a region (e.g., Grand Canyon), or a measurement technique (e.g., stable isotopes or molecular genetics). Sample throughput, which depends on the type of sample being analyzed and the analytical procedures being performed, ranged from 60 samples per year to 33,000 samples per year for the laboratories visited by the committee.

Most laboratories have multiple sources of funding, such as the USGS, grants from other federal agencies, or user fees. Analyses may also be traded for other services. Similarly, most laboratories serve multiple types of users, including scientists (USGS, other federal agencies, and academic), regulators and resource managers (federal, state, and local), and private companies. A few serve only USGS scientists.

All of the laboratories supply analytical data to USGS researchers, external users, or both. The laboratories focused primarily on supporting research are generally small (two or three full-time equivalents [FTEs] on average), have low annual budgets (typically $0.2 million or less), and serve USGS scientists as well as scientists in other federal agencies and academic institutions. In contrast, laboratories that serve regulators, resource managers, and commercial users in addition to scientists generally have more staff (seven FTEs on average) and larger annual budgets (typically two to four times higher) than laboratories primarily supporting research. The largest USGS laboratory—the National Water Quality Laboratory—primarily provides sample analyses and specialized services to customers, and it has 134 FTEs and an annual budget of $6 million or more. Finally, all of the USGS laboratories have some quality assurance and quality control procedures in place, but those procedures are generally more comprehensive and better documented in laboratories supporting production activities than in laboratories primarily supporting research.

Task 3

Task 3 was to assess the extent to which operational and personnel resources are sufficient to meet the scientific and applications objectives of USGS laboratories. The 2016 USGS laboratory inventory was not sufficiently detailed to carry out this assessment. Consequently, the USGS asked the committee to draw high-level conclusions on the adequacy of resources based on the views of laboratory staff and committee's observations at its laboratory visits. The committee found that staff in the 17 laboratories visited were skilled in what they do and took pride in their science, their reputation, and the societal impact of their work. Most of the laboratories had state-of-the art instruments as well as older equipment purchased over their long history. The laboratories appeared be to meeting their science and applications objectives. However, staffing shortfalls and turnover were a common resource problem. Adding responsibilities for implementing a complex QMS, especially without adding sufficient resources, may hinder their future ability to meet their science goals.

APPROACHES FOR IMPROVING LABORATORY DATA QUALITY

Tasks 2 and 4 concern data quality assurance procedures and best practices at laboratories in a variety of institutions. An extensive literature from biomedical science and other scientific fields evaluates research practices that affect data quality, assesses laboratory procedures, and recommends best practices for laboratories. These publications show that errors and poor habits occur frequently enough to affect data reliability, and that these problems could be mitigated by systematically managing laboratory processes to assure the quality and integrity of data and records. Quality assurance programs are designed to establish the criteria for assessing and improving laboratory performance, and to ensure that best practices are routinely identified and adopted across laboratory activities.

Task 2

Task 2 was to describe the laboratory protocols, analytical procedures and standards, and data management processes for laboratories at the USGS, other federal agencies, and geological surveys in other countries. Evaluating analytical and data management procedures in hundreds of laboratories was not feasible in the confines of this study. Consequently, the USGS asked the committee to focus on laboratory QMS procedures in order to provide a benchmark for its QMS effort. The committee invited eight organizations that are using a QMS for at least some of their laboratories to share their approach and experiences at open meetings. The organizations chosen were the USGS, Navy, Centers for Disease Control and Prevention, Environmental Protection Agency, the French and Norwegian geological surveys, Texas A&M University, and Duke University Medical Center. Each of these organizations had different motivations for developing a QMS, different QMS challenges (e.g., number and diversity of laboratories and laboratory activities), and different QMS implementation strategies (e.g., top down or bottom up, and fast or slow).

Despite these differences, some common themes emerged. The presenters told the committee that implementing a QMS provides benefits, such as improving documentation, reliability, or reproducibility of laboratory data; finding and correcting data quality problems; and enhancing the organization's reputation for quality data. However, these benefits come with substantial monetary and personnel costs. The high costs and paperwork burden associated with implementing a QMS, as well as the need to learn a new way of doing things can create resistance among laboratory scientists and staff. Institutional commitment and strong leadership are required to gain buy-in and to change the organization's culture. Consistent messaging is important for explaining why a QMS is needed, and good two-way communication between managers and laboratory staff is essential for developing a QMS that meets the needs of the laboratories. Finally, implementing the QMS slowly allows the system to evolve in response to lessons learned and thus ensure that the system fulfills its intended purpose.

Task 4

Task 4 was to develop criteria for assessing protocols and procedures used by the organizations in Task 2, and use them to identify relevant best practices and procedures for USGS production laboratories. Criteria for assessing laboratory procedures are typically developed by managers, regulatory agencies, or professional organizations that offer laboratory inspection and accreditation programs. However, numerous assessments of laboratory procedures and recommended best practices have been published, and the committee drew from these to address Task 4.

A variety of approaches can be taken to assure data quality in laboratories. Approaches range from highly autonomous scientific oversight programs designed to meet individualized requirements to centrally controlled quality management systems designed to meet the requirements of an organization. Examples of approaches relevant to the USGS include the following:

1. *Scientist-defined procedures and protocols that are implemented at the individual laboratory level.* With this approach, scientists have the autonomy and flexibility to be creative and innovative in developing their laboratory methods. However, the practices may be ad hoc, may be highly variable across laboratories, or may not cover quality planning, quality control, and quality improvements for all processes that contribute to data quality. This approach is common in academic laboratories and was used by most USGS laboratories prior to 2016.
2. *Institution-defined best practices that are implemented at the individual laboratory level.* Best practices are procedures that have been shown by research and experience to produce optimal results and that are established or proposed as a standard for widespread adoption. With this approach, institutional management establishes its general

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expectations for how data quality should be maintained and demonstrated, and the laboratory lead scientist develops a program to meet those expectations. Having standardized expectations for data quality should improve the consistency, reliability, and efficiency of processes across the laboratory system. However, implementation requires more time, effort, training, and oversight than the previous approach. A variety of generalized guidelines and best practices for implementing this approach are available.

3. *Institution-defined QMS requirements that are implemented throughout the institution.* This centralized approach is used to achieve consistency, efficiency, and a shared quality culture across the laboratory network. However, it increases cost because quality assurance professionals are needed to coordinate and monitor activities (document control, change control, personnel, equipment, methods, materials, error management, and internal or external audits) across the organization, and staff require training and support to take on additional quality assurance activities. The USGS is implementing this approach.
4. *Externally-defined QMS requirements that are implemented at the institution or individual laboratory level to demonstrate compliance with an external quality standard.* With this approach, an institution adopts an external standard to carry out a particular line of work or to meet the specific requirements of clients, collaborators, or regulatory agencies. It demonstrates a high level of research accountability, but expensive, periodic external reviews (audits) are required for laboratories to maintain accreditation. The USGS National Water Quality Laboratory is using this approach.

Approaches 2 through 4 are examples of organization-wide quality assurance programs, which describe the activities put in place to meet the requirements and expectations of a data quality standard. Implementation of a quality assurance program is a recommended best practice because it is systematic, process oriented, and addresses all aspects of the work being done. Approach 1 does not take this system-wide approach to data quality.

RECOMMENDATIONS

The committee's last two tasks concern best practices and procedures for achieving scientific and applications objectives and assuring the integrity and reliability of results for USGS laboratories. Task 5 was to recommend best practices for production laboratories (those carrying out routine analyses for USGS or external users), and Task 6 was to comment on best practices for research laboratories (those supporting innovation or scientific discovery).

Tasks 5 and 6: Best Practices

Institution-defined expectations of data quality are important for generating data of known and consistent quality across large organizations such as the USGS, which has to manage some 250 diverse laboratories around the country. The USGS is already implementing one

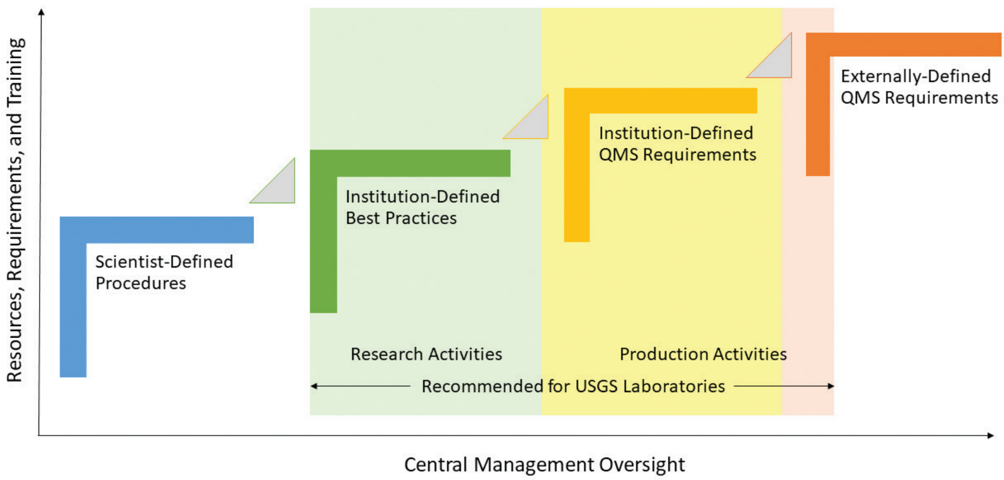

FIGURE S.1 Four approaches (steps 1–4) for assuring the quality of results from laboratories that support research, method development, or data production. The triangles represent training opportunities. Prior to 2016, most USGS laboratory practices were consistent with scientist-defined procedures (blue, step 1). The USGS is now implementing an institution-defined QMS (yellow, step 3). The committee recommends that USGS laboratories follow institution-defined best practices (green, step 2) and QMS, as appropriate (primarily step 3, with a few in step 4, orange).

type of institution-defined approach (QMS; step 3 in Figure S.1) for its laboratories. This is a good fit for laboratories that carry out well-characterized and routine analyses for internal or external users (production activities). A few of these laboratories may also need to meet additional externally-defined QMS requirements (step 4 in Figure S.1) for some procedures, based on client requirements.

Approximately half of USGS laboratories are used primarily by researchers. In these laboratories, methods are frequently adjusted as research hypotheses unfold, or as the process of optimization and validation proceeds. Creative experimentation is necessary before processes can be standardized. For these laboratories, institution-defined best practices (step 2 in Figure S.1) are appropriate to accommodate continually developing and improving analytical procedures while still meeting the best practice guidelines chosen by the USGS. Moving from scientist-defined procedures to institution-defined best practices would mean the research-oriented laboratories would fully participate in a centralized USGS laboratory culture committed to accountability and data quality and integrity. Adding periodic independent data quality checks (e.g., peer review, internal audits, and sample exchange with external laboratories) would confirm that institution-defined best practices have become routine in research and method development laboratories at the USGS.

Few USGS laboratories support only research activities or only production activities. Consequently, the USGS, in consultation with its laboratories and their users, will have to decide which laboratories need a QMS and which need institution-defined best practices.

Recommendation 1. The USGS should implement institution-defined best practices (step 2) or institution-defined QMS (step 3), as appropriate, for its laboratories.

Resources

A key responsibility of management is to support implementation and maintenance of the quality assurance program. However, current USGS resource commitments, quality assurance staffing, and training are insufficient to implement the central QMS for all USGS laboratories. The USGS expects its laboratories will devote an estimated 20 percent of their resources for about 2 years to implement the QMS and about 10 percent annually thereafter to maintain the system. This substantial effort should be recognized, supported, facilitated, and rewarded by USGS management.

Institution-defined best practices are less expensive to implement than a comprehensive QMS. Consequently, implementing institution-defined best practices for the laboratories focused primarily on research would free up central USGS resources to support QMS implementation and maintenance for the subset of laboratories engaged in production activities.

Recommendation 2. The USGS should optimize and prioritize centralized resources for the subset of laboratories doing production activities that would most benefit from a QMS.

Timeline

The USGS is developing and implementing its QMS too quickly. QMS development began in 2016 and the system was implemented in 11 energy laboratories in mid-2017. Quality assurance programs such as QMS and institution-defined best practices are relatively new concepts in most academic and government research environments. Such systems are complex and take time to develop, implement, and evolve. The USGS will need to take the time to

- Communicate more extensively with staff, including explaining the quality goals of the organization and gaining staff input and feedback on system design and implementation;
- Provide staff training, including meetings with quality assurance experts;
- Establish mechanisms to recognize, support, and reward the substantial time and resources invested by laboratory scientists and quality assurance experts to meet USGS data quality goals;
- Develop QMS champions who would help lead the necessary culture change; and
- Learn from implementation experiences and continually improve the system.

Recommendation 3. The USGS should slow implementation of its QMS and allow ample time to develop institution-defined best practices, take advantage of lessons learned, provide training, and obtain input and buy-in from USGS laboratory staff.

Conclusion

The committee commends the USGS for pursuing recognized best practices to produce data of known and documented quality. A well-resourced and gradual implementation of a flexible approach that incorporates institution-defined best practices for research activities and QMS for production activities would meet the quality goals of the USGS and the diverse needs of its laboratories, foster staff buy-in, and cultivate an enduring quality culture across the agency.

1

Introduction

The U.S. Geological Survey (USGS) mission is to provide reliable and impartial scientific information "to describe and understand the Earth; minimize loss of life and property from natural disasters; manage water, biological, energy, and mineral resources; and enhance and protect our quality of life."[1] Data collection, analysis, interpretation, and dissemination are central to everything the USGS does.

The USGS operates some 250 laboratories to analyze physical or biological samples, including water, sediment, rock, plants, invertebrates, fish, and wildlife. The data generated in the laboratories help answer pressing scientific and societal questions associated with energy and mineral resources, natural hazards, surface and groundwater quality and quantity, biology and ecology, environmental health, and other topics. A growing number of these topics touch on controversial issues, such as those concerning environmental pollutants or climate change, and USGS scientific results are coming under increasing scrutiny. For these issues especially, the USGS reputation and the self-correction of science through peer-reviewed publications may no longer suffice to maintain public trust in USGS research results.

The importance of providing reliable information came to the fore in 2016, when an Inspector General report found scientific misconduct and data manipulation at a USGS laboratory in Lakewood, Colorado (IG, 2016). Two laboratory analysts had adjusted values outside of protocols over two extended periods. Reports of such incidents are rare, but they highlight the importance of data quality assurance and quality control procedures. To restore confidence in USGS data, the USGS has begun implementing a quality management system (QMS)—a structured and documented system that establishes the requirements for how work is to be managed, conducted, and monitored to assure data quality. A QMS is a paradigm shift for the USGS because instead of each laboratory developing its own quality assurance procedures, all USGS laboratories will be required to implement a centrally defined quality standard in a similar and consistent way, as applicable to the work performed (USGS, 2018). The laboratory elements typically managed in a QMS are illustrated in Figure 1.1.

[1] See https://www.usgs.gov/about/about-us/who-we-are.

FIGURE 1.1 Laboratory elements typically coordinated and managed using a QMS developed to ensure compliance with a quality standard.

In addition to developing a QMS, the USGS has commissioned external reviews of its QMS implementation, including this report.

COMMITTEE TASKS AND APPROACH

At the request of William Werkheiser, then USGS Deputy Director, the National Academies of Sciences, Engineering, and Medicine established a committee to review a selection

Box 1.1
Committee Tasks

An ad hoc committee will review a representative sample of USGS laboratory facilities, covering energy and minerals, natural hazards, surface and groundwater, ecosystems, and environmental health. The review will focus primarily on production laboratories that serve both USGS users and external customers, and secondarily on laboratories that support research and method development. Specific tasks for the committee are given below.

1. Provide an overview of USGS laboratory facilities across the nation, including their science and applications objectives, budget, staff and user profiles, and history of sample throughput for the past 5 to 10 years.
2. Describe the laboratory protocols, analytical procedures and standards, and data management processes for USGS laboratories, relevant laboratories hosted by other federal agencies (e.g., National Institute of Standards and Technology, U.S. Army laboratories, and National Institutes of Health), and geological surveys in other countries (e.g., Canada, United Kingdom, Australia, and Norway).
3. Assess the extent to which resources (operational and personnel) are sufficient to meet the scientific and applications objectives of USGS laboratories (production, research, and method development).
4. Develop criteria for assessing protocols and procedures used by the organizations in Task 2, and use them to identify relevant best practices and procedures for USGS production laboratories.
5. Provide recommendations on best practices and procedures for achieving scientific and applications objectives and ensuring the integrity and reliability of results from USGS production laboratories.
6. Comment on best practices and procedures for USGS research and method development laboratories.

The analysis will be based on USGS-provided profiles of its laboratory facilities and protocols, preliminary results from the USGS assessment of quality management procedures at its laboratories, and other information gathered by the committee at site visits, teleconference meetings, and elsewhere.

of USGS analytical laboratories and identify best practices and procedures for assuring the integrity and reliability of laboratory results. The specific tasks to the committee are given in Box 1.1.

When the tasks in Box 1.1 were developed, USGS managers had only begun collecting information about its laboratories and their quality assurance practices. As their knowledge grew, it became clear that some of the information needed to address the tasks would not be available for the study. Consequently, some tasks could not be addressed exactly as written. At the first committee meeting, the USGS deputy director suggested ways to address the intention, rather than the exact wording, of these tasks. With those guidelines, the committee addressed the tasks as described below.

Task 1 was to provide an overview of all USGS analytical laboratories, including their science and applications objectives, budget, staff and user profiles, and history of sample throughput. The USGS collected and analyzed this and other information (e.g., data quality procedures) in 2016 (see Phillips et al., 2018). Consequently, the committee used the 2016 USGS laboratory inventory as a baseline and supplemented it with information gathered at site visits to USGS laboratories. Site visits and associated committee meetings were held in four cities: Reston, Virginia; Denver, Colorado; Menlo Park, California; and Kearneysville, West Virginia (see Table 1.1). Only 17 laboratories (6 percent), 16 active and 1 inactive at the time, could be visited in the confines of the study, and they were chosen to sample a diversity of sizes and activities. Visits to a small number of diverse laboratories cannot yield a comprehensive picture of the USGS laboratory landscape. However, a number of common themes emerged that informed the committee's response to Task 1.

TABLE 1.1 USGS Laboratories Visited by the Committee

Date	Location	Laboratories Visited
June 2018	Reston, Virginia	• Energy Environmental Labs • Environmental Organic Geochemistry Lab (inactive) • Microbiology Lab • Reston Stable Isotope Lab • Wetland Ecosystems Ecology and Biogeochemistry Laboratory
August 2018	Denver, Colorado	• Analytical Chemistry Project • Gas Chromatography/Mass Spectrometry • National Water Quality Laboratory • Plasma Laboratory • Radiogenic Isotope Laboratory • Spectroscopy Laboratory
November 2018	Menlo Park, California	• Benthic Lab • Rock Physics Laboratory • Tephrochronology Project Laboratory • Unsaturated Zone Flow Processes Lab
February 2019	Kearneysville, West Virginia	• Fish Health Laboratory—Fish Culture and Pathology • Functional Genomic, Biomarker, and Environmental Contaminant Bioanalysis

Task 2 was to describe analytical procedures, standards, and data management procedures for laboratories at the USGS, other federal agencies, and other geological surveys. Describing analytical and data management procedures in hundreds of laboratories was not feasible in the confines of this study. Consequently, the USGS asked the committee to focus on laboratory QMS procedures in order to provide a benchmark for its QMS effort. The committee addressed the task by asking a selection of U.S. federal agencies and academic institutions and geological surveys in other countries to discuss a set of questions on QMS and alternative approaches for assuring data quality at committee meetings.

Task 3 was to assess the extent to which laboratory resources are sufficient to meet their objectives. The USGS-collected data were not sufficiently detailed to carry out this assessment. Laboratory budget information was available in ranges, staff (principal investigators, laboratory managers, analysts, and students) were grouped into total full-time equivalents, and research and applications objectives were general. Consequently, the committee used the opinions of laboratory staff and its own observations at the laboratory visits to draw high-level conclusions on the adequacy of resources.

Tasks 4, 5, and 6 concern the identification of best practices for assuring data quality in USGS laboratories. Best practices and data quality terms used in this report are defined in Box 1.2. The USGS distinguishes two types of laboratories:

1. Research laboratories support innovation or scientific discovery and are typically led by a principal investigator (senior scientist). Some research laboratories also develop methods that are needed to answer a scientific question or that other laboratories can use for routine analyses.
2. Production laboratories carry out routine or repeated analyses for USGS or external customers, are sometimes supported by user fees, and are generally led by laboratory managers.

The USGS data do not indicate which laboratories do routine analyses or are led by laboratory managers, but they do specify which have external users, such as regulators and resource managers, which is an indication of production activities.

Task 4 was to develop criteria for assessing laboratory protocols and procedures used by the organizations mentioned in Task 2 and to use them to identify best practices for USGS production laboratories. Numerous assessments of laboratory procedures and recommended best practices have been published, and the committee drew from these to address Task 4.

Task 5 was to recommend best practices and procedures for achieving objectives and assuring the integrity and reliability of results for USGS production laboratories, and Task 6 was to comment on best practices and procedures for research and method development laboratories. The committee used what it learned from the laboratory site visits, meeting presentations, and the published literature to address Tasks 5 and 6.

Box 1.2
Data Quality Terms Used in This Report

Best practice—A procedure that has been shown by research and experience to produce optimal results and that is established or proposed as a standard suitable for widespread adoption

Data integrity—The degree to which the data are complete, consistent, accurate, trustworthy, and reliable throughout the data life cycle

Data quality—The characteristics of data that bear on its fitness for purpose, including accuracy, completeness, reliability, traceability, and relevance

Data quality descriptors:

- Reliable—The data are sufficiently complete, consistent, and error free to be convincing for its purpose and context
- Reproducible—Measurements made at different times and/or by different people using the same measuring device yield similar results within specified boundaries
- Verifiable—The data can be tested and proven accurate and free from errors

Data quality standard—The requirements, specifications, guidelines, or characteristics that can be used to establish best practices and ensure that materials, processes, and data are fit for their purpose

Quality assurance—A proactive managerial tool used to monitor and improve processes so that defects, problems, or errors do not arise when the product is being developed

Quality control—A component of quality assurance that is focused on identifying (and correcting) defects in the actual product or procedure before a product is released

Quality Management System—A formal system that documents the structure, processes, roles, responsibilities, and procedures required to achieve effective quality management

SOURCES: https://asq.org/quality-resources/quality-glossary and dictionaries.

U.S. GEOLOGICAL SURVEY

The USGS has a federally funded budget of roughly $1 billion and has some 8,000 employees. The USGS is organized in a matrix structure that involves seven mission areas chosen to reflect USGS science and applications objectives and seven regional offices chosen to reflect geographic variations in geological, biological, and hydrological characteristics (e.g., northeast, southwest, and Alaska). The mission areas are core science systems, ecosystems, energy and minerals, environmental health, land resources, natural hazards, and water resources. The USGS is headed by a director, under whom are a deputy director and seven associate directors corresponding to the mission areas (Figure 1.2). The directors of the seven regional offices report to the USGS deputy director. Each regional office has several science centers, which manage the science activities of the region and also oversee most of the laboratories.

Line management, personnel management, and science center management are organized through the regional offices. However, the QMS is being implemented by mission area. The reporting structure is complex. Although QMS implementation plans are being developed by the mission areas, QMS reporting lines flow through the Deputy Director. The Bureau QMS Coordinator and staff—who oversee implementation of the QMS—report to the Deputy Director through the director of the Office of Science Quality and Integrity (Figure 1.3). The other QMS staff, including QMS champions, report to their Deputy/Associate Science Center Director, and not to the Bureau QMS Coordinator.[2]

ORGANIZATION OF THIS REPORT

This report examines approaches to managing laboratory data quality and recommends best practices and procedures for assuring the integrity of USGS laboratory results. The report is organized to emphasize the information that USGS most needs to develop its quality assurance program. Chapter 2 summarizes the literature on systematic approaches for assuring data quality, including assessments of laboratory procedures and best practices (Task 4), and describes example approaches that are relevant for USGS laboratories. Chapter 3 provides an overview of the approximately 250 USGS laboratories being examined, including the adequacy of resources to meet their science and applications objectives, and their approach to assuring data quality (Tasks 1, 2, and 3). Chapter 4 highlights experiences with quality management systems at the USGS, other federal agencies, other geological surveys, and research institutions (Task 2). Chapter 5 provides the committee's recommendations for the USGS, including the development and implementation of its QMS, and best practices and procedures for USGS laboratories (Tasks 5 and 6). The report concludes with a list of references and biographical sketches of committee members (Appendix).

[2] The language of this sentence was modified after release of the publication version to reflect current USGS staffing plans.

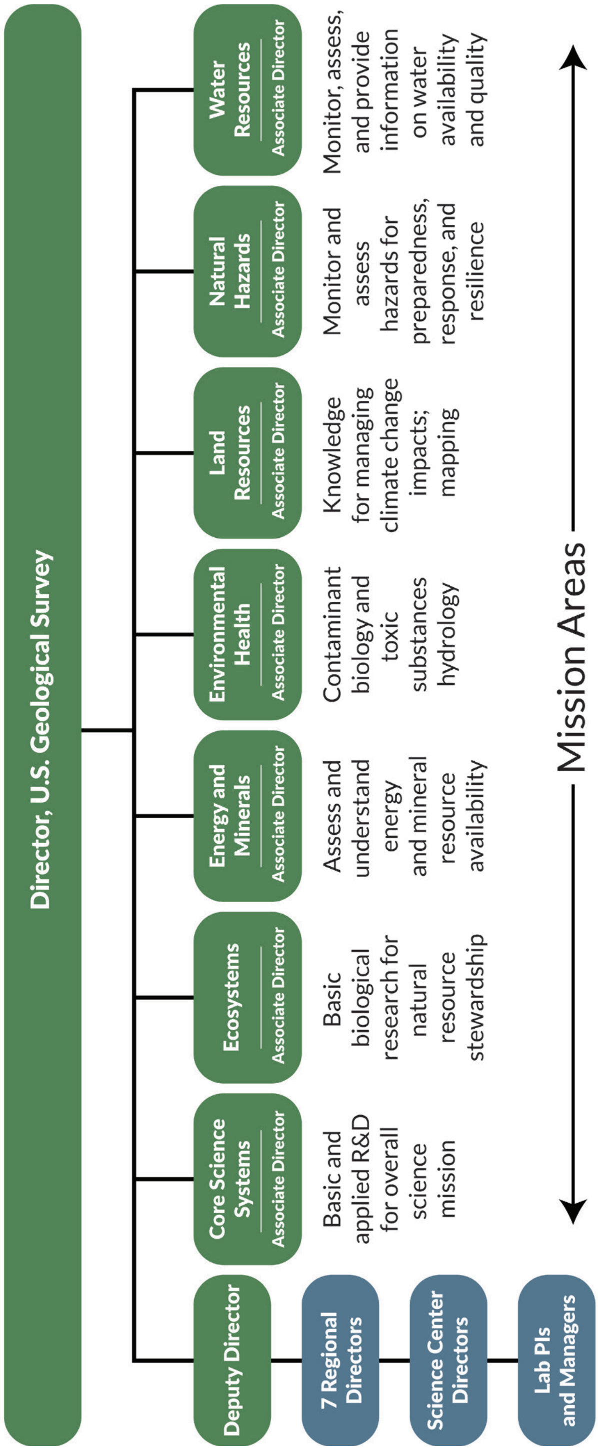

FIGURE 1.2 Simplified representation of key organizational elements and reporting relationships of USGS upper-level management.
SOURCE: Modified from USGS.

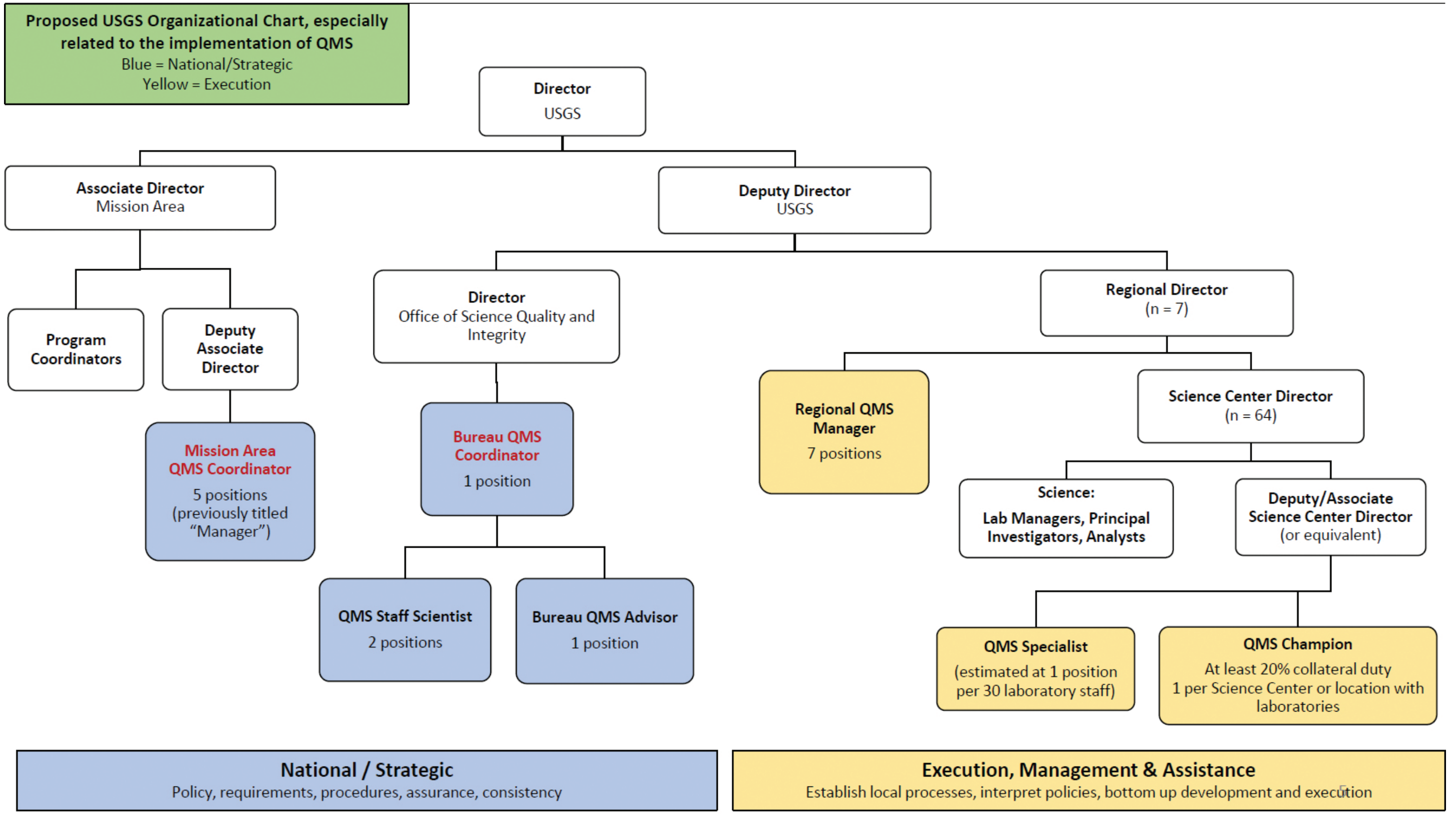

FIGURE 1.3 Proposed QMS staffing and reporting structure for the USGS.[3]
SOURCE: USGS.

[3]This figure was replaced with a current organizational chart after release of the publication version.

2

Improving Data Quality and Integrity

Every organization has quality management activities, whether they have been formally planned or not. An organizational quality standard provides guidance on how to develop a formal system to manage these activities (ISO 9000:2015 (E).2.4.2).

The committee's fourth task was to develop criteria for assessing laboratory protocols and procedures used by the organizations mentioned in Task 2 and to use them to identify best practices and procedures for U.S. Geological Survey (USGS) laboratories. Laboratory procedures are typically assessed using criteria developed by managers, regulatory agencies, or professional organizations. The criteria may incorporate formal quality standards, consensus-based best practices, input from subject matter experts, or feedback from laboratory personnel, collaborators, users, and scientific peer review.

Numerous assessments of laboratory procedures and recommended best practices have been published, and the committee drew from these to address Task 4. This chapter introduces the use of systematic approaches for assuring quality, explains reasons for implementing quality assurance programs, describes example approaches used to do so in research settings, and discusses the training and support needed to integrate and maintain such systems.

INTRODUCTION TO QUALITY ASSURANCE PROGRAMS

A process or product that conforms to requirements or to a quality standard is recognized as a quality process or product (Crosby, 1979). This conformance to requirements demonstrates the ability to meet expectations and is the foundation for establishing value (Guaspari, 2002). The requirements used to define and measure quality can either be established by management (a lead scientist, group, or institution) or adopted from an externally developed, consensus-based quality standard. In either case, management has complete control over, and flexibility around, what the requirements are and how to change them in response to evolving experience or needs. Once the requirements are defined, a quality assurance program is

ASSURING DATA QUALITY AT U.S. GEOLOGICAL SURVEY LABORATORIES

developed to direct and coordinate the organizational, managerial, and technical activities needed to ensure that the requirements are met.

The steps to build a quality assurance program generally include the following:

1. Identify the quality objectives related to a product;
2. Assess the risks that may threaten the quality of a product;
3. Establish the requirements to reduce the likelihood that risks will be realized;
4. Check processes and outcomes to ensure that requirements are met;
5. Evaluate, reduce, and learn from errors or problems that occur; and
6. Routinely reevaluate risks, processes, and requirements to capture opportunities for improvement.

This systematic approach to managing quality arose from the field of manufacturing in post-World War II Japan. Quality management based solely on individual product inspection (quality control) was replaced by systems that manage quality (including quality planning, quality control, and quality improvements) across all manufacturing processes (Deming, 1982; Juran, 1986; Ortner, 2000; Smith, 2009). These principles underlie modern quality assurance programs used to maintain and demonstrate the quality of a product or process.

REASONS FOR IMPLEMENTING QUALITY ASSURANCE PROGRAMS

Implementation of a laboratory quality assurance program is a recommended best practice because a standard for work is established to assure that the best quality data are generated. Determining whether the work conforms to the standard is part of quality assurance. Standardizing routine activities has the benefit of aligning laboratory scientists around a consensus-based approach for assuring data quality, while avoiding problems stemming from uncontrolled or unintended variation (GBSI, 2013).

A quality assurance program can be implemented by an organization of any size and applied to any kind of work that produces a product (Cochran, 2008; Westgard and Westgard, 2014). In laboratories, the products are primarily analytical data generated and published in reports or journal articles. These data products are typically the outcome of multiple processes executed by different people under different conditions using similar or different methods. For these reasons, standardized and transparent processes that enable accurate reconstruction of all analytical activities and their associated data and metadata are critical for demonstrating data quality and for testing reproducibility of results within and across laboratory environments.

Laboratory quality assurance programs are systematic, process oriented, and intended to address all aspects of the work being done, including management, personnel, equipment, methods, materials, laboratory records and documentation, data management, error management, and facility and environment. The expectation is that data and metadata (the primary work products) will be managed to assure data quality and integrity throughout the data life cycle, from generation and recording, to processing and analysis, to use, to archive or destruction, as appropriate (MHRA, 2018). Data and information management processes are put in place to ensure that data and metadata are described (who, what, where, when, how, why), documented (e.g., attributable, accurate, complete, and consistent), and preserved for publication, sharing, and re-use. Collectively, these processes contribute to a data governance system and laboratory culture that supports the generation of a complete, consistent, accurate, and secure research record (Wiggins et al., 2013; WHO, 2016; MHRA, 2018).

Quality assurance programs facilitate effective research and data management in laboratory environments because they address organizational, managerial, and technical activities; support data completeness and accuracy; promote process standardization when possible; and assure work transparency and traceability. The key benefits from implementing quality assurance programs include the following:

- Standards for work are established and communicated;
- Activities are planned, managed, documented, and monitored;
- The assessment and mitigation of risks associated with error and uncontrolled or unintended variation are built in;
- An accurate, complete, transparent, and secure data record is maintained and available;
- Re-work is reduced due to reduction in errors and unaccounted variation; and
- Confidence in laboratory processes and competency is increased (Ehrmeyer, 2015).

Standardization and systematic oversight of laboratory practices are considered "good institutional practice" (Begley et al., 2015) because they are designed to reduce variability, manage risks specific to the work being conducted, increase work transparency, and increase the reliability of results within and across laboratory settings (Adams et al., 1998; Trotter et al., 2012; GBSI, 2013; Freedman and Inglese, 2014).

In some manufacturing, clinical, or other regulated laboratory environments, the quality of processes and products must be strictly controlled according to a specified consensus-based or regulatory standard. However, even research laboratories that do not need to comply with regulatory or accreditation requirements are increasingly integrating quality assurance programs and best practices into their operations (Adams et al., 1998; Holcombe et al., 1999; Vermaercke, 2000; Vermaercke et al., 2000; Abad et al., 2005; Robins et al., 2006; Poli et al., 2015; Baker, 2016a; Dirnagle et al., 2018). One driver of this shift are questions raised about the quality and reproducibility of research in disciplines including chemistry, biology, medicine, psychology, economics, physics, engineering, and earth and environmental sciences (Chalmers and Glasziou, 2009; Gratzer, 2013; Ioannidis et al., 2014; Macleod et al., 2014; Begley et al., 2015; Baker, 2016a,b; Bergman and Danheiser, 2016; Bustin and Nolan, 2016; Freedman et al., 2015, 2017; Moher et al., 2016b; Davies et al., 2017; NASEM, 2018b; Ellis et al., 2019).

In response, a number of papers have called for the development and expanded use of consensus-based standards and standardized vocabularies and approaches that support scientific quality (Steneck, 2006; Zimmerman, 2010; Poste, 2012; GBSI, 2013; Plant et al., 2014; Rüegg et al., 2014; Begley et al., 2015; Giesen, 2015; Nosek et al., 2015; Sené et al., 2017). Many laboratories already use available reference standards (purified and traceable biological, physical, or chemical materials) to calibrate equipment or to validate, verify, or authenticate methods. Similarly, written consensus standards that describe optimal practice for specific methods or tests are available. For example, standardized systems for data collection, analytical methods, quality control, and archive have been developed for some procedures by the Long Term Ecological Research program (e.g., Fahey and Knapp, 2004; Robertson et al., 2009). It will take time for such standards to be developed, approved, and adopted within multiple scientific disciplines. However, the adoption of a quality assurance program can facilitate the development and use of standardized approaches for routine activities in a laboratory or laboratory system. For example, some scientists are using quality assurance activities to reduce the potential for errors and uncontrolled or unintended variation in a wide range of factors (e.g., personnel, methods, equipment, or record keeping) that could affect the quality of data (Robins et al., 2006; Zapata-Garcia et al., 2007; Riedl and Dunn, 2013; Bongiovanni et al., 2015; Baker, 2016a; Dirnagl et al., 2016; Hooper et al., 2018; Molinéro-Demilly et al., 2018).

EVIDENCE THAT QUALITY ASSURANCE PROGRAMS SUPPORT DATA QUALITY

Evidence that quality assurance programs are appropriate and effective strategies for maintaining and demonstrating data quality comes from meta-research and reports by organizations and scientists who have integrated quality assurance best practices or programs into their laboratories. Key results from meta-research are summarized below. Examples of scientists' experiences integrating quality assurance programs into their laboratories appear in "Options for Designing Laboratory Data Quality Programs" below.

Meta-Research on Scientific Practices Associated with Data Quality

Meta-research (research on research) examines the strengths and weaknesses of scientific practices and looks for opportunities for improvement. Scientists have studied how science is conducted (methods), reported (communication), verified (reproducibility), evaluated, and rewarded, and they have recommended improvements that can be applied across scientific disciplines (Casadevall and Fang, 2012; Bond, 2013; Casadevall et al., 2014; Ioannidis et al., 2014, 2015; Casadevall et al., 2016). For example, the scientific community is being encouraged to adopt "open science" policies that make research data and methods freely available so they can be reused and reproduced (e.g., Nosek et al., 2015; Casadevall et al., 2016; Munafò, 2016; NASEM, 2018a; Kretser et al., 2019). As expectations for open science grow, the importance of being able to assure and demonstrate the quality and integrity of data and metadata becomes even more critical.

Much meta-research on the quality and integrity of data focuses on the biomedical field, which is highly dependent on laboratory-generated analytical data. However, biomedical laboratory methodologies share commonalities with all research disciplines (e.g., method development, equipment and materials management, quality control, and documentation), and so conclusions of meta-research studies are likely applicable to other types of laboratories.

Meta-research shows that routine and careless errors and poor habits occur frequently enough to affect data reliability. For example, Toker et al. (2016) examined 70 human gene expression studies and found discrepancies between the sex indicated by gene expression and the sex identified in the metadata in nearly half of data sets. They also found that "an alarming degree" of sample mislabeling was not being discovered by laboratories, even though detection is straightforward. Zieman et al. (2016) analyzed 35,175 supplementary Excel files from 18 journals. They determined that Excel default settings converted gene names to dates or numbers in about one-fifth of papers with supplementary files containing lists of genes. This problematic Excel feature has been recognized for more than 10 years and yet the errors continue. Ellis et al. (2019) conducted a study to determine whether previously reported and unexpectedly high steroid concentrations in river water could be confirmed. The authors concluded that calculation error (especially related to spreadsheet use) was the most probable cause of the high values reported in the initial study. However, the errors could not always be traced to the source because processing spreadsheets or written laboratory notebook records were not available. Finally, Martinson et al. (2005) examined survey data from a large and representative sample of early- and mid-career U.S. scientists funded by the National Institutes of Health. A substantial fraction of scientists reported engaging in "inadequate record keeping related to research projects" (28 percent) or "dropping observations or data points from analyses based on a gut feeling that they were inaccurate" (15 percent). Typical quality assurance activities, risk assessment, and standardizing and monitoring routine processes would likely have identified and reduced the frequency of these problematic research practices.

APPROACHES FOR DESIGNING LABORATORY DATA QUALITY PROGRAMS

The design and implementation of any process to assure research data quality requires substantial input from scientists to ensure that the process is science centered (incorporates general and field-specific scientific best practices), realistic for the research environment, and fit for purpose (Leonelli, 2017). Likewise, the design and implementation of a system-level approach to assure data quality across an organization needs to be designed to ensure that scientists have the infrastructure and resources needed to demonstrate that they have identified, established, adopted, and maintained appropriate best practices for the work they do.

A variety of approaches can be taken to assure and maintain data quality in laboratory environments. Options range from highly autonomous scientific oversight programs designed to meet individualized requirements to centrally controlled quality management systems (QMSs) designed to meet the requirements of an organization. The committee created four models to illustrate the range of approaches that could be adopted to provide confidence in the quality of data generated in analytical laboratories. The four approaches are

1. Scientist-defined procedures and protocols that are implemented at the individual laboratory level,
2. Institution-defined best practices that are implemented at the individual laboratory level,
3. Institution-defined QMS requirements that are implemented throughout the institution, and
4. Externally-defined QMS requirements that are implemented at the institution or individual laboratory level to demonstrate compliance with an external quality standard.

These four approaches are illustrated in Figure 2.1 and discussed below.

Approach 1: Scientist-Defined Procedures

Principal investigators and staff scientists establish their data quality procedures through personal oversight of laboratory-specific processes that are commensurate with scientific practices, in which methods are developed, shared, and adapted among research groups and honed through peer review. Laboratory processes may be managed using a combination

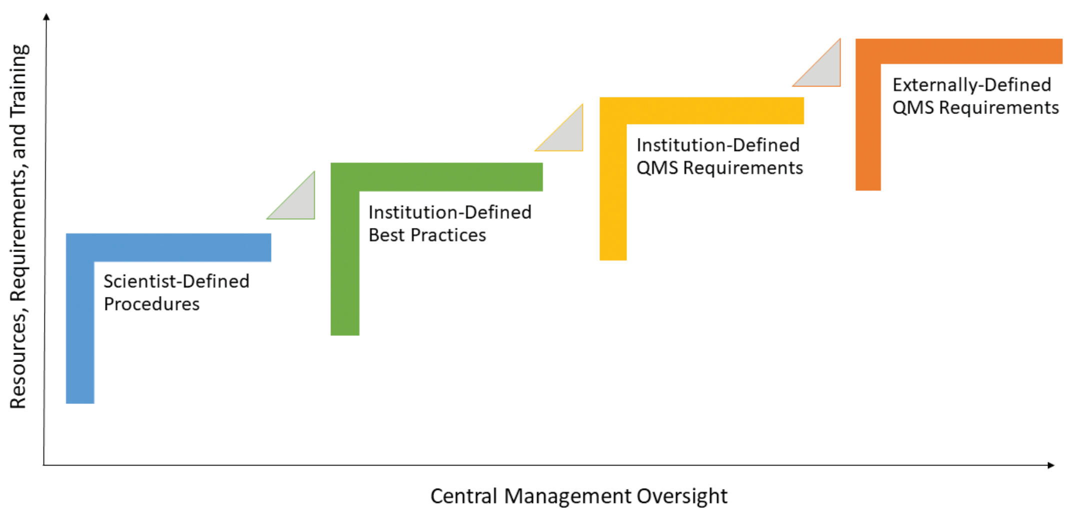

FIGURE 2.1 Four approaches (steps 1–4) for assuring the quality of results from laboratories that support research, method development, or data production. The triangles represent training opportunities.

Box 2.1
Examples of Scientist-Defined Procedures

The following examples were developed by committee members, based on personal observations or experiences.

Example 1: Lead scientist oversight

Scientist A manages staff through initial training activities, periodic laboratory meetings where work progress and problems are reviewed, and participation in round robins with other laboratories to cross-check analyses.

Example 2: Laboratory web page

In addition to training and laboratory meetings, Scientist B created a laboratory web page for project, records, and data management. The web page has folders for data management and review, methods, procedures and protocols, training records and resources, laboratory meeting minutes, and equipment maintenance and calibration records.

Example 3: Electronic notebooks

In addition to training and laboratory meetings, Scientist C provides staff with electronic laboratory notebooks to facilitate collaboration, data review and sharing, and collection and maintenance of data and metadata. The electronic notebooks also serve as a records repository for methods, notes, problems, issues, interpretations, conclusions, and plans.

of tools, including written and unwritten policies and procedures, personnel training and mentoring, proficiency testing, the use of electronic laboratory notebooks, automated quality control, and the use of software programs to maintain sample and data records. Examples of this approach are given in Box 2.1.

Advantages and disadvantages of scientist-defined procedures. The primary advantages of this approach to an organization are that

- Scientists have autonomy and flexibility to be creative and innovative in their laboratory methods;
- Scientists develop the procedures needed to address the specific complexity and risk in their environment; and
- Integration of best practices, procedures, and protocols is efficient and inexpensive because scientists follow community practice and there are no additional organizational requirements.

The primary disadvantages of this approach to an organization are that

- Individual practices applied to maintain data quality are highly variable and depend on the commitment, knowledge, training, and resources of the lead researcher and his/her team;
- Quality planning, quality control, and quality improvements may not be integrated across all processes that contribute to data quality and integrity;
- Self-assessment and peer review may not catch data problems quickly;
- Scientists may develop their procedures independently, which creates inefficiencies and may reduce the likelihood for sharing of best practices, tools, and resources within the organization; and
- The lack of consistent or recorded protocols among scientists may hinder the ability to reproduce results across multiple laboratories.

Approach 2: Institution-Defined Best Practices

Best practices are "procedures that have been shown by research and experience to produce optimal results and that are established or proposed as a standard suitable for widespread adoption."[1] In this approach, institutional management establishes and communicates its general expectations for how the quality of data should be maintained and demonstrated across the organization (e.g., Begley et al., 2015). It is then the responsibility of the lead scientist and his or her team to develop a program to meet those expectations. The institutional expectations are directed toward generalized laboratory best practices rather than compliance with a centrally controlled quality standard. For example, the guidelines for nonroutine work (i.e., research) could be flexible and be presented as a toolbox from which relevant best practices could be drawn (Krapp, 2001), whereas guidelines for routine work could include more detailed specifications and policies to assure consistency of the laboratory product.

This approach increases the uniformity of data quality throughout the institution because expectations for quality work and laboratory and data management are communicated and consistent, and awareness of quality assurance is maintained across the scientific organization. In addition, the organizational commitment impels the institution to provide training, tools, and resources to ensure that scientists can successfully meet the expectations.

Many institutions use this approach to encourage the adoption of safety best practices. Safety is frequently managed by requiring individuals to demonstrate that they meet the regulatory or institutional requirements that apply to their specific work. However, scientists are also expected to demonstrate that they have adopted the general best practices that apply to any kind of laboratory work. Typically, institutions offer training and resources to encourage the recognition and adoption of the recommended best practices.

Examples of this approach are given in Box 2.2.

[1] See https://www.merriam-webster.com/dictionary/best%20practice.

Advantages and disadvantages of institution-defined best practices. The primary advantages of this approach to an organization are the following:

- Standardized expectations for data quality and tools, training, and guidelines for scientists should improve the consistency, reliability, and efficiency of processes across the laboratory system.
- The organization demonstrates a commitment to data quality as a core value.
- The approach meets the diverse needs of the laboratory network because scientists have autonomy, creativity, and flexibility in how they meet organizational expectations.
- The alignment of centralized expectations creates opportunities to share training, tools, and resources.

The primary disadvantages of this approach to an organization are the following:

- Institutional management, in accordance with their objectives and in consultation with its scientists, must make the effort to identify the best practices necessary to assure effective data management and quality.
- Scientist-designed programs and their effectiveness will vary across the institution and will be affected by the commitment, training, or resources of the individual researcher.
- If programs do not include an independent or external audit activity, then self-assessment and peer review may not catch data problems quickly. In addition, opportunities to improve working habits may not be realized.
- Costs, support, implementation time, and oversight are higher than for scientist-defined procedures because scientists have to adapt their processes to the recommended guidelines. They will likely need extra time and support to change their routine approach.

Approach 3: Institution-Defined QMS Requirements

An institution-defined QMS is a centrally controlled system designed to assure that the quality objectives of the institution are met. In the laboratory setting, a QMS describes the manner in which a laboratory manages operations to assure the quality of the test results. The system is intended to ensure that all processes that contribute to the laboratory production of data (e.g., raw materials, training, instruments, procedures, sample collection and handling, quality control, and proficiency testing) are managed, conducted, documented, and monitored so that results meet specified quality criteria (Westgard and Westgard, 2014).

This approach differs from the two approaches discussed above because responsibility for managing and demonstrating research quality is shared among (1) the scientists that supervise research activities, (2) the independent quality assurance specialists that support and monitor the quality assurance processes, and (3) the organizational management that establishes the quality standard and provides the resources and oversight necessary to sustain the QMS.

Box 2.2
Examples of Institution-Defined Best Practices

Institution-defined best practices are only beginning to be implemented in research environments. The first example below describes an institution that set quality expectations and developed best practices for its research laboratories. In the second example, the institution is a science collective that identified some best practices for assuring data quality through tools for managing data across multi-investigator science projects. Although the science collective operated like an institution, it did not have the power of enforcement.

Example 1
Balancing quality assurance and scientific innovation at the Ferring Research Institute
(from Riedl and Dunn, 2013)

The goals of the Ferring Research Institute, the research arm of Ferring Pharmaceuticals, were to "implement quality assurance mechanisms that assure the quality and integrity of critical (impactful) data while avoiding the potential threat to scientific ingenuity from excessive regulations" and to "eliminate preventable errors, oversights, or misinterpretations in data analysis and final reporting." The hope was that scientists would adopt quality practices across all research activities as they became more experienced applying data quality best practices.

Ferring Research defined best practices through an audit standard and communicated them program wide. Only some processes were audited, but centralized expectations for data quality were made clear. Quality assurance activities were mandatory for one phase (lead optimization) of the research effort. Ferring Research:

- Defined the specific processes that generate critical data and would most benefit from quality assurance procedures (e.g., data used in key reports and for patents, investigator brochures, or strategic decision making).
- Defined a quality standard based on four requirements: traceability, accuracy, clarity or completeness, and timeliness.
- Provided tools (electronic notebooks to improve record-keeping, data capture, and transparency) and training in quality assurance awareness to everyone to help them meet quality expectations program-wide.
- Developed a quality audit process to confirm compliance with the standard.
- Ensured improvements by establishing a researcher-quality assurance partnership to find and fix problems.

Reidl and Dunn (2013) reported that Ferring Research's system added value while minimizing disturbance to research activities. It also changed scientists' attitudes toward quality assurance, in part by providing training and rewarding compliance with the system. An internal data audit has been voluntarily requested by scientists who are not required to participate. Finally, it reduced the number and severity of problems found in audits.

Example 2

Completing the data life cycle: Using information management in macrosystems ecology research (from Rüegg et al., 2014)

Rüegg et al. (2014) illustrates how a scientific collective can use community-developed and well-documented standards and information management protocols and procedures to assure the quality and integrity of data across collaborations and past the lifetime of an individual project. They examined macrosystems ecology projects on wetlands connectivity and grasslands sensitivity to climate change, which synthesize data (e.g., air and soil temperature, carbon dioxide flux, and land cover) from multiple sources and disciplines, using complex analytical and diverse data management approaches.

Rüegg et al. (2014):

- Chose to focus on two parts of the data life cycle: (1) describe and document and (2) preserve and publish.
- Defined best practices for transparent documentation, use of a standardized vocabulary across different research settings, and for quality control and storage of sensor data across projects.
- Used a MATLAB toolbox to perform data manipulation tasks and to apply quality assurance and quality control rules.
- Addressed data integration problems by using federated data repositories, standard metadata and data exchange formats, and existing database formats, as well as by developing workflow tools and ontologies.
- Encouraged collaboration between ecologists and data information professionals during all steps of data consolidation.
- Participated in developing the IsoMAP toolkit, which facilitates access to environmental isotope data and enables the standardization and version-controlled documentation of analyses.

Rüegg et al. (2014) found that standardized approaches to data and information management can be applied as best practices within and across projects and programs. They demonstrated the advantages of collaborating with information management experts and incorporating information management early in the research process. The authors emphasize the need for additional training, incentives, and support for data and information management.

ASSURING DATA QUALITY AT U.S. GEOLOGICAL SURVEY LABORATORIES

This centralized approach to managing quality is used to achieve consistency, efficiency, and a shared quality culture across the research network. A centralized QMS approach will increase the cost and complexity of research activities because quality assurance professionals are needed to coordinate and monitor multiple managerial and technical activities (e.g., document control, change control, internal auditing, equipment, environment, and error management) across the organization. In addition, staff will require training and support as they take on new or additional quality assurance activities as required within a QMS. The USGS is following this approach. Other examples are given in Box 2.3.

Box 2.3
Examples of Institution-Defined QMS Requirements

Example 1
Development of a research QMS for the French National Institute for Agronomic Research (from Molinéro-Demilly et al., 2018)

The French National Institute for Agronomic Research's goal was to implement a common QMS across a large, multidisciplinary, and regionally diverse research structure to improve risk management and increase the reliability of results. The Institute:

- Created a policy that summarized the organization's objectives related to research and data quality.
- Created easy-to-read guidelines on quality management and responsibilities, research conduct, resource management, documentation control, and measurements, analysis, and improvement that could be used to meet the data quality objectives.
- Provided implementation tools (including self-assessment metrics) and implemented the QMS over several years, beginning with support laboratories and extending to basic research laboratories.
- Created a "quality network" of research scientists, scientists with quality assurance expertise, and scientists with specific equipment and metrology expertise to support implementation and collaboration.
- Established internal audits for all teams, including a review of the quality system itself, to assess trends, monitor the effectiveness of solutions, and determine quality objectives for the coming year.
- Underwent an external audit every 5 years.

Molinéro-Demilly et al. (2018) reported that the QMS had a positive impact on the functioning and activities of the laboratory. Scientists were able to measure the effectiveness of their procedures for managing risks, and to establish action plans to make necessary changes. The French National

Advantages and disadvantages of institution-defined QMS requirements. Advantages of this approach to an organization include the following:

- A QMS is a recognized and accepted method for assuring confidence in laboratory results.
- The use of a centralized QMS should improve quality, reliability, work transparency, and consistency across the institution.
- An internally defined quality standard can be customized to address the specific needs of an organization.

Institute for Agronomic Research was able to prioritize laboratory activities and to identify future needs (e.g., resources, training, a Laboratory Information System, and incentive structures).

Example 2

Development of a QMS for Merck Serono Research (from Pohl et al., 2008)

The goal of Merck Serono Research was to develop a QMS that covered all exploratory research areas and locations to optimize planning and implementation of research projects, work flow, and service production. Merck Serono:

- Defined a quality standard to apply to all research units.
- Established guidelines and basic research rules for planning and documentation, reporting results, training personnel, managing data and errors, using well-controlled systems and methods, and improving the system.
- Allowed each research department to create a policy to meet the requirements of the quality standard. The department head was responsible for data quality.
- Reviewed the department policies for compliance with the quality standard and created an action plan to address any issues.
- QMS coordinators provided training, and local "Quality Delegates" coordinated the QMS implementation and improvement activities at the research sites.

Pohl et al. (2008) reported that the QMS improved protocols for validating computerized equipment, sped the production of reliable results, and minimized the need for repeat testing, thereby allowing more efficient use of resources. In addition, being able to demonstrate data quality made it easier for the organization to settle patent disputes. Staff viewed training in quality principles as a benefit that would enhance their future employability.

Additional examples of quality assurance activities that have been successfully implemented in basic research settings can be found in Adams et al. (1998), Vermaercke et al. (2000), Volsen et al. (2004), Volsen and Masson (2009), Bongiovanni et al. (2015), and Dirnagl et al. (2016).

- Quality assurance experts are available to help scientists implement required QMS procedures and identify and solve data quality problems before they become a larger concern.
- An effective QMS promotes opportunities for self-assessment and improvement of work habits through independent auditing and process review.

Some disadvantages of this approach to an organization include the following:

- QMS requirements established for an entire system may be more applicable to some laboratory activities than to others. For example, laboratory activities directed toward exploratory research or method development will not require the same level of management oversight as routine analytical testing for clients will require. This mismatch may lead to inefficiencies, increased costs, and the loss of flexibility and creativity in exploratory research environments.
- Scientists may be reluctant to adopt a system that they perceive as adding work or restricting their autonomy, flexibility, and creativity (e.g., Vermaercke, 2000; Riedl and Dunn, 2013).
- A fully centralized QMS that spans a diverse and distributed network of laboratories is complex and requires substantial ongoing commitment of management, dedicated quality assurance personnel, and financial resources to implement and sustain.
- Quality assurance specialists with the necessary information management expertise may be hard to find (Rüegg et al., 2014), especially in the numbers needed to support QMS implementation, audit activities, and training initiatives.

Approach 4: Externally-Defined QMS Requirements

With this approach, an institution adopts one or more externally-defined quality standards and develops its QMS to ensure that the requirements of those standards will be met. A laboratory or laboratory system may choose to comply with an external standard because it seeks accreditation by an external agency to carry out a particular line of work, enhance credibility, or meet the specific requirements of clients, collaborators, or regulatory agencies. The laboratory has some flexibility in how it addresses the requirements of the standard in light of its resources, skills, and mission. However, adopting an external quality standard is the most stringent approach for implementing a QMS because the laboratory undergoes accreditation or credentialing assessments.

Multiple standards that apply to laboratory testing have been developed. Examples include the International Organization for Standardization (ISO) standards and the National Environmental Laboratory Accreditation Conference (NELAC) Institute (TNI) standard. Compliance with the ISO 17025 standard (as demonstrated by accreditation status) enables laboratories to "demonstrate they operate competently, and are able to generate valid results"[2] using the accredited method. Compliance with ISO 9001 enables laboratories to demonstrate that they have implemented an effective QMS to ensure that customer and regulatory requirements are met.[3] The TNI standard encompasses ISO 17025 requirements, but focuses specifically on environmental data. It is used by the National Environmental Laboratory Accreditation Program to "foster the generation of data of known and documented quality" through the accreditation of environmental laboratories according to consensus standards "representing the best professional practices in the industry."[4]

It is possible for laboratories to comply with multiple standards within the same environment. For example, some TNI-accredited laboratories may also have to comply with the additional quality standards established by their own organization. In addition, it is possible for some methods within laboratories to be accredited, while others are not. For example, some quality standards like ISO 17025 are used to accredit individual tests within laboratories, and some standards like ISO 9001 are used to accredit the entire laboratory management system. Experience with either standard will typically build the culture of quality and drive best practices throughout the laboratory (e.g., Abad et al., 2005; Zapata-Garcia et al., 2007; Cutler and Scott-Dupree, 2016).

Examples of the use of externally-defined QMS requirements are described in Box 2.4.

Advantages and disadvantages of externally-defined QMS requirements. The primary advantages of this approach to the institution are the following:

- Compliance with an external quality standard allows a laboratory to conduct analyses that meet regulatory or other consensus-based requirements (e.g., from a professional society) to support high-risk applications and to demonstrate a high level of research accountability through accreditation by independent and external assessors.
- Most formal consensus-based standards are written with the understanding that there are many ways to comply with a given requirement. Therefore, the laboratory can customize how it will meet the requirements.
- Accreditation provides external recognition that the measurement was made under conditions that optimize the likelihood that the measurement is verifiable.
- A laboratory may have both accredited and nonaccredited test methods. If so, the QMS put in place to support the accredited tests is likely to enhance the management of the nonaccredited tests as well.

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[2] See International Organization for Standardization ISO/IEC 17025:2017(E); General requirements for the competence of testing and calibration laboratories (current edition 2017-11).

[3] See International Organization for Standardization ISO/IEC 9001: 2015-09-15; Quality management systems- Requirements.

[4] See National Environmental Laboratory Accreditation Conference Institute (TNI), Management and technical requirements for laboratories performing environmental analysis (2016). http://nelac-institute.org/content/NELAP/index.php.

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Box 2.4
Examples of Externally-Defined QMS Requirements

Example 1
Implementation of a QMS at the Environmental Radiology Laboratory, University of Barcelona (from Zapata-Garcia et al., 2007)

The Environmental Radiology Laboratory's goal was to obtain ISO 17025 accreditation for some of the analytical chemistry assays developed to monitor radiation around nuclear power plants. The laboratory:

- Implemented the standard in phases, starting with the management requirements and ending with the technical requirements.
- Decided which methods would undergo accreditation.
- Developed QMS infrastructure, including a document repository system, a quality manual, and 73 procedures related to research management, for the geographically distributed research units.
- Developed an internal audit program to conduct annual audits.

Zapata-Garcia et al. (2007) reported that additional resources were required to sustain accreditation-level quality assurance activities. The QMS provided several benefits, including better control of equipment and routine training in quality assurance. Standard procedures made the work easier, prevented improvisation, and reduced the number of sample treatment documents needed for routine processes.

The primary disadvantages to the institution are the following:

- Demonstrating compliance with an external quality standard requires substantial resources to address the complex array of management, performance, and monitoring requirements.
- An organization may need to maintain more than one quality standard if the scope of the external QMS accreditation does not cover the entire quality system. The result can be (a) a confusing array of requirements, which could lead to inconsistent adoption of requirements, or (b) universal application of potentially unnecessary requirements, which raise costs.

Example 2

Implementation of a QMS at the Materials Characterization analytical laboratory of the Fondazione Bruno Kessler, Trento, Italy (from Iacob, 2016)

The goals of the mineral characterization laboratory were to standardize procedures, develop technical competencies, and gain international acceptance of the reliability and credibility of analytical test results through accreditation to the ISO/IEC quality standard. The laboratory:

- Based its quality standard on ISO/IEC 17025/2005.
- Selected the methods that would be accredited, based on which methods are most frequently requested, could be standardized, or have market interest.
- Created a quality manual to describe the quality system framework and a documentation scheme to define general procedures, operative procedures, internal methods, and forms.
- Designed a bottom-up QMS by starting from existing research procedures as described by the personnel who perform them. Supportive documentation was then built around the staff descriptions to formalize and standardize the activities.

Iacob (2016) reported that the QMS improved measurement, record keeping, equipment management, and quality control processes, and also greatly reduced mistakes. Customer satisfaction reports were positive. The accreditation process created new tasks for quality management, extra work for staff, and increased testing. The system took 2 years to implement, and a full-time researcher was required to keep up with monitoring and evaluating the system. Although the benefits of method-specific accreditation were worth the costs, the laboratory is reducing the number of individual methods being accredited and looking for more cost-effective standards to guide its laboratory-wide research activities.

Quality management systems that meet externally-defined requirements have been implemented effectively in many basic research settings. Examples include research on radioactive waste (Vermaercke, 2000; Vermaercke et al., 2000), food safety (Henri et al., 2009), and cardiovascular disease (Poli et al., 2015) as well as QMS implementation in biomedical (Abad et al., 2005; Lacalamita et al., 2008; Solis-Rouzant, 2015; Jena and Chavan, 2017) and toxicology (Cutler and Scott-Dupree, 2016) laboratories.

Choosing the Right Approach

Individuals or organizations will choose an approach to maintain laboratory data quality based on their commitment to quality objectives, the inherent risks associated with laboratory activities and outcomes (data, results, reports), their implementation timeline, and the availability of resources needed to plan, implement, and sustain their program. Approaches 1–4 discussed above reflect the increasing complexity, cost, requirements, and oversight needed to assure confidence in the data. Approaches 2–4 are quality assurance programs and recommended best practices, with centralized expectations that a sufficient management system will be in place for all laboratories, and that the effectiveness of the program can be demonstrated throughout all laboratory processes. Scientist-defined procedures and institution-defined best

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practices offer the most flexibility and can be implemented at the lowest cost. The centrally controlled QMS approaches provide the most stringent strategies for maintaining and demonstrating data quality, but require the greatest institutional adjustments, the most resources (time, expertise, and funding), and the highest level of support and collaboration.

In some cases, hybrid approaches may meet the needs of an institution. For example, an organization may add independent internal or external auditing to institution-defined best practices to assure that data of known and documented quality are produced and that opportunities for improvement are created. Such monitoring could take the form of independent peer audit, quality assurance review at periodic intervals, round robins (sharing samples at multiple laboratories), or benchmarking (systematically comparing an organization's practices and procedures with those in other organizations). A quality approach that encompasses both basic research and method development (nonroutine) and production (routine) activities needs to be specifically and carefully designed to be fit for its purpose in each environment. Organizations may also use more than one quality approach. For example, a laboratory may use an institution-defined QMS for most of its methods and externally-defined standards for selected methods. These options may help institutions and scientists balance their needs for flexibility, creativity, productivity, and sustainable quality.

Inherent in the development of any approach is the understanding that not all aspects of research activity can be predicted or predetermined. Science progresses through frequently changing conditions. As a result, the approach used to support and manage data quality needs to be efficient, adaptable, and flexible while also enhancing the scientist's ability to generate accurate, transparent, complete, and reproducible data (Herman and Usher, 1994; Mathur-De-Vre, 1997; Holcombe et al., 1999; Petit and Muret, 2000; Krapp, 2001; Robins et al., 2006; Abdel-Fatah, 2010; Dirnagl et al., 2018).

MAINTAINING DATA QUALITY PROGRAMS

Implementing quality assurance programs as an organizational strategy to maintain and demonstrate data quality requires a strong and sustained commitment from leadership, management, and laboratory scientists. Every published account describing the integration of quality assurance programs in basic research laboratories stresses the critical need for effective training, communication, collaboration, and support to ensure success and participant buy-in as these changes to laboratory culture and practice are introduced. Scientists and quality assurance professionals need to be able to work together to establish quality assurance programs that will add value to the individual laboratory and to the organization as a whole. They can also combine their subject matter expertise to develop a training program that works. Training is required not only for the data quality approach an organization initially chooses, but also to support different approaches that may be implemented later. These training opportunities are indicated as the triangles between steps in Figure 2.1. For example, adoption of institution-defined best practices would be strengthened by providing training programs that illustrate how the guidelines can be implemented within individual laboratories, and by creating self-assessment, independent peer-assessment, or quality assurance assessment opportunities and resources. Examples are trainer and trainee handbooks (WHO, 2010a,b) intended to support adoption of the World Health Organization's quality practices in basic biomedical research (WHO, 2006).

Maintaining quality assurance programs also requires an infrastructure that supports the types of activities needed to comply with the program. For example, quality assurance activities can be supported through the use of tools that make it easier and faster to meet quality requirements. Examples include the use of electronic notebooks, centralized data collaboration and sharing sites, quality management software (record repository and working environment for quality assurance activities), and equipment or laboratory information systems that make the automatic collection of data and generation of records more consistent and reliable. Multiple publications provide examples of programs, procedures, checklists, tools, or guidelines that can be applied in research, development, and production-oriented laboratories to improve data quality (e.g., Herman and Usher, 1994; Adams et al., 1998; Holcombe et al., 1999; Volsen et al., 2004, 2009; Robins et al., 2006; Berwouts et al., 2010; Zimmerman, 2010; Davis et al., 2012; Trotter et al., 2012; Westgard and Westgard, 2014; Giesen, 2015; Dirnagl et al., 2016; Davies et al., 2017; Sené, 2017; Lanati, 2018; Plant et al., 2018)[5] or its management (e.g., WHO, 2006; Wiggens et al., 2013; Goodman et al., 2014; Nussbeck et al., 2014; Rüegg et al., 2014; Sandle, 2014; Perkel, 2015; Dirnagl and Przesdzing, 2016; Wilkinson et al., 2016; MHRA, 2018).[6] An example of a checklist is given in Table 2.1.

Quality assurance programs succeed when the activities become a routine and rewarded part of the laboratory culture. Therefore, an incentive structure needs to recognize scientist efforts to improve and document data quality (e.g., Casadevall and Fang, 2012; Rüegg 2014; Begley et al., 2015; Moher et al., 2016a). New strategies may be needed to encourage a culture that embraces quality assurance activities.

SUMMARY AND ANSWER TO TASK 4

The committee's fourth task was to develop criteria for assessing laboratory protocols and procedures and to identify relevant best practices and procedures for USGS laboratories. An extensive literature in biomedical research and other fields evaluates scientific practices that affect data quality, assesses laboratory procedures, and recommends best practices for laboratories. These publications show that errors and poor habits occur frequently enough to affect data reliability, and that this problem could be mitigated by systematically managing

[5] See also the Michelson Prize and Grants Research Quality Assurance toolkit website, https://www.michelsonprizeandgrants.org/resources/quality-assurance-toolkit/.

[6] See https://www.dataone.org/best-practices.

TABLE 2.1 Laboratory Quality Assurance Documentation Checklist

Project Management: Establish research plan and assess risk to data quality and integrity	**Yes**	**No**
1. Project plan (roles and responsibilities, objectives, timeline)		
2. Research management plan/process/procedures (communication, facilities, environment, security, confidentiality, etc.)		
3. Data governance plan/process/procedures		
4. Risk assessment and research review plan/process/procedure		
5. Research publication plan/process/procedure		
Personnel Records: Ensure that records can be traced to competent and appropriate personnel	**Yes**	**No**
1. Job descriptions, resumes, or CVs		
2. Signature and initials identification log		
3. Training and ongoing competency policies, standard operating procedures (SOPs) for processes related to data management, methods, equipment, quality assurance, and quality control		
Equipment Records: Ensure that data and records are traceable to critical equipment	**Yes**	**No**
1. Equipment inventory log (unique identification)		
2. Equipment use, maintenance, verification, and calibration records		
3. SOPs for use, care, and management of equipment		
4. Computer systems used to capture, process, generate, and report data are secure, working as expected, and fit for their intended purpose		
Method/Procedure Records: Ensure that data can be traced to methods or procedures that are approved, described, working as expected, and fit for their intended purpose	**Yes**	**No**
1. SOPs for routine research methods		
2. Laboratory notebook (paper or electronic) procedure for non-routine research records		
3. Method validation records		
4. Quality control records		
5. Research monitoring records (other quality checkpoints throughout the research life cycle)		
Standard Operating Procedures: Ensure that procedures are performed consistently, changed as needed, and maintained as historical records	**Yes**	**No**
1. Routine work instructions for laboratory and data management, established technical procedures, and equipment use are documented and controlled		
2. Document control procedures are in place (creation, revision, and archive) to ensure that only the current and approved method is in use		
3. SOPs are linked to associated data recording forms		

TABLE 2.1 Continued

Other Research Records (paper/electronic): Ensure that research data and critical work (who, what, where, when, how, and why) can be reconstructed	**Yes**	**No**
1. Reagent inventory, authentication and preparation records (receipt, verification, storage, expiration, and disposition), supply records		
2. Facilities data (temperature, water/air quality) if quality critical		
3. Unique identification for specimens and sources (data and metadata)		
4. Sample handling and storage instructions (SOPs) and records		
5. Transparent, reliable, and traceable records (accurate, legible, contemporaneous, original, attributable, consistent, available, and secure)		
6. Error management procedures (detecting, recording, managing errors, outliers, and nonconforming work or data)		

NOTE: Modified from Davies et al., 2017.

laboratory processes to assure the quality and integrity of data and records. Quality assurance programs are designed to ensure that the requirements for assessing and improving laboratory performance are met, and that best practices for laboratory activities are routinely identified and adopted. The goal is to establish a quality assurance program that is valued by scientists because of the opportunities it presents to safeguard and demonstrate the quality of their data, rather than one that is resented because it may limit their freedom and creativity.

Approaches to laboratory management vary according to the scope and objectives of the laboratory and organization overseeing it. Best practices relevant to the USGS include

- Institution-defined best practices that are implemented at the individual laboratory level,
- Institution-defined QMS requirements that are implemented throughout the institution, and
- Externally-defined QMS requirements that are implemented to demonstrate compliance with an external quality standard.

Each of these approaches to laboratory data quality has strengths and weaknesses. What they have in common is the expectation that all laboratories will have a sufficient management system in place, and that the effectiveness of that system can be demonstrated throughout all laboratory processes. The success of any of these approaches depends on the full support of management, staff commitment, acceptance of a quality culture, and a system that is simple, flexible, modular, non-redundant, self-sustaining, and value-adding (Vermaercke, 2000).

3

USGS Laboratories

The committee's first tasks were to provide an overview of all U.S. Geological Survey (USGS) analytical laboratories (Task 1), their analytical and data management procedures (Task 2), and the extent to which resources are available to meet their science and applications objectives (Task 3). Before 2016, the USGS did not have a complete inventory of its laboratories and their capabilities. Consequently, the agency issued two data calls to its employees: one on basic laboratory information (e.g., budget, staff, users, scientific objectives, and analysis capabilities) and one on the quantity of data produced and quality assurance and quality control procedures. In responding to the questionnaires, laboratory managers and principal investigators defined their own laboratory boundaries, with some grouping similar activities into a single laboratory, and some splitting similar activities into more than one laboratory. This exercise yielded 257 analytical laboratories. Some of these laboratories were inactive at the time, so the total number is an approximation.

The USGS provided a redacted version of the laboratory responses to the two data calls (USGS, 2016, unpublished laboratory inventory) to the committee to address Task 1. However, the questionnaires do not lend themselves to quantitative analysis. For example, some questions allow multiple answers (e.g., mission areas served), and some answers encompass multiple variables (e.g., regulators and resource managers are grouped together, and fee for service can include external payments and USGS staff reimbursements). Some answers are given in broad ranges (e.g., budget ranges and data recorded rates), and others are given in relative terms (e.g., high, medium, low, or none user categories). Finally, some questions, particularly those related to quality assurance practices, were sometimes answered inconsistently or not at all. For example, some laboratories reported having a quality management system (QMS), but were missing essential elements (e.g., documentation and independent monitoring for quality assurance; see Chapter 2). Such misunderstandings are not surprising, given that QMS is a relatively new concept in research organizations. With the subsequent QMS rollout, many laboratories now know more about QMS and some have even implemented the system. Despite these limitations, the USGS 2016 laboratory inventory provided invaluable information to broadly characterize the USGS laboratories.

This chapter provides an overview of the USGS laboratories, based on the USGS 2016 laboratory inventory provided to the committee, and summarizes insights on 17 laboratories, based on committee observations at site visits and additional data provided by the USGS.

OVERVIEW OF USGS LABORATORIES

The USGS 2016 laboratory inventory shows that the USGS laboratories are distributed throughout the United States (Figure 3.1), with the largest clusters near USGS headquarters (Reston) and other major USGS offices (Denver and Menlo Park). Some laboratories are focused on a mission area (e.g., Environmental Behavior of Mineral Deposits), although most laboratories support multiple mission areas. Other laboratories are focused on a region (e.g., Grand Canyon Monitoring and Research Center Sediment Lab) or a measurement technique (e.g., Stable Isotope Laboratory).

Most laboratories have multiple sources of funding—such as the USGS, other federal agencies, or user fees—and they may also trade analyses for other services. Similarly, most

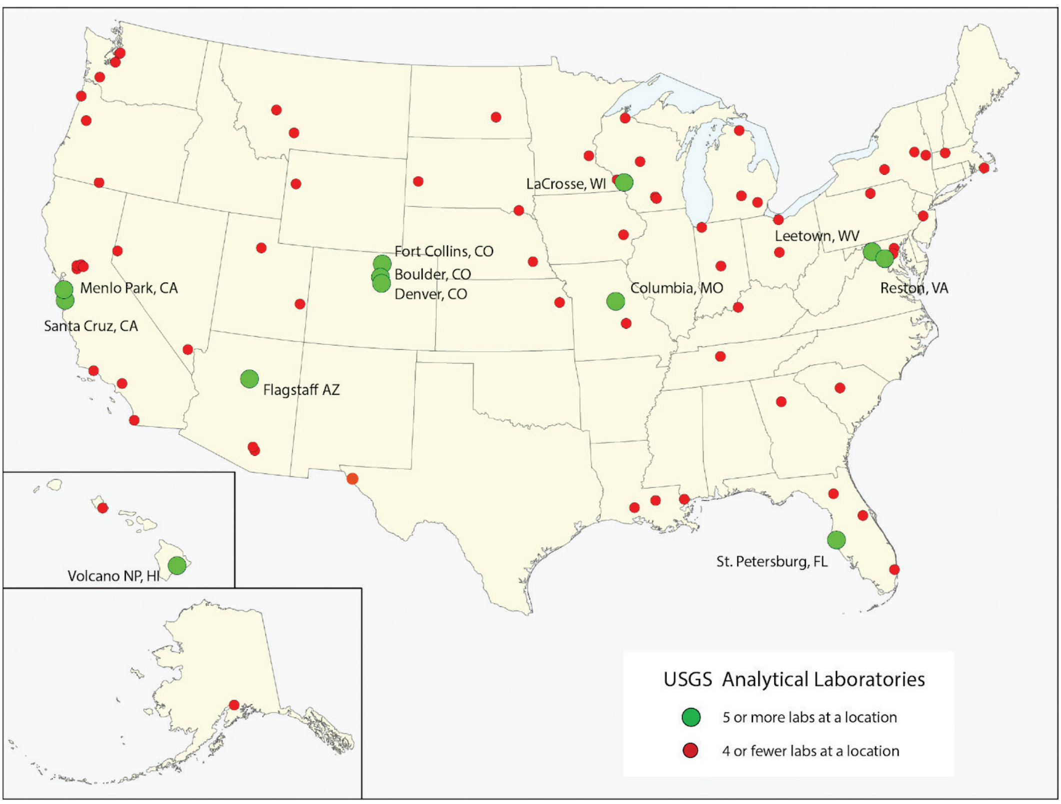

FIGURE 3.1 Locations of USGS laboratories in 2016.
SOURCE: USGS.

laboratories serve multiple types of users, including scientists (USGS, other federal agencies, and academic), regulators and resource managers (federal, state, and local), and private companies. A few serve only USGS scientists.

All of the laboratories support research and nearly half also supply analytical data to external users. The laboratories focused primarily on supporting research are generally small (two or three full-time equivalents [FTEs] on average), have low annual budgets (typically $0.2 million or less), and primarily serve USGS scientists and secondarily scientists in other federal agencies and academic institutions. In addition to carrying out analyses, some of these laboratories develop methods to study processes (e.g., fate and transport of organic contaminants), detect quantities of interest (e.g., microbes in water or fish disease), or improve the speed and accuracy of measurements (e.g., hydraulic conductivity).

In contrast, laboratories that serve federal and state regulators and resource managers and commercial users in addition to scientists generally have more staff (seven FTEs on average) and larger annual budgets (typically two to four times higher) than laboratories primarily supporting research. The largest USGS laboratory—the National Water Quality Laboratory—has 134 FTEs and an annual budget of $6 million or more (Table 3.1). Three-quarters of its work focuses on providing sample analyses and specialized services to its customers. Private companies use data from a handful of USGS laboratories, particularly those focused on remote sensing and earthquake science and engineering. Regulators and resource managers tend to use data from laboratories focused on other subject areas.

Before 2016, the data quality practices of USGS laboratories were largely determined by the laboratory principal investigators, as is generally the case in academic laboratories. Such practices are designed to meet the quality assurance and quality control needs of a laboratory, given its scientific objectives and user needs. All of the laboratories focused primarily on supporting research had at least some written quality assurance and quality control procedures (e.g., standard operating procedures and analysis of duplicate samples, standards, and blanks), and some had developed relatively comprehensive and documented approaches to data quality assurance. Sixteen of the laboratories primarily supporting research reported having a QMS, but committee visits to two of them showed otherwise, suggesting that the QMS concept was not well understood. One of these had many QMS elements in place, but the other was far from implementing a QMS (e.g., only one standard operating procedure had been developed).

Regulators and commercial users often have defined quality standards, and so laboratories that do production work often have more rigorous and documented data quality assurance and quality control procedures than laboratories focused primarily on research. Before 2016, some USGS laboratories with production activities even had a fully implemented QMS. These laboratories had a better understanding of QMS. The committee visited three laboratories with production work that stated they had a QMS in place and found that two had a QMS and one was just beginning to implement one.

TABLE 3.1 USGS Laboratories Visited by the Committee (from USGS)[a]

Laboratory Name	Budget	FTEs	Users[b]	Average Annual Sample Throughput 2013–2017[c]	QMS Status[d]	Science Applications
June 2018, Reston						
Energy Environmental Labs	\$0.6M to \$2M	4	Scientists, regulators, commercial	3,000	Implemented	Chemical, microbiological, and toxicological studies to support studies on energy resources, environment, ecosystems, and human health
Environmental Organic Geochemistry Lab (inactive)	NA	2	Scientists, regulators	146	Not applicable	Transport and fate of organic pollutants in the environment, and development of tracers and new methods
Microbiology Lab	\$0.3M to \$0.5M	2	Scientists, regulators, commercial	3,500	Not started	Microbiological, biogeochemical, and hydrological analyses to understand interactions between microbes and their environment
Reston Stable Isotope Lab	\$0.6M to \$2M	8.5	Primarily scientists	12,600	Not started	Development of new stable isotope techniques and reference materials, and measurement of light element isotopic compositions
Wetland Ecosystems Ecology and Biogeochemistry Laboratory	\$0.3M to \$0.5M	7	Scientists	2,500	Not started	Biogeochemical analyses to understand material transport in watersheds, coastal and estuarine processes, and wetland management
August 2018, Denver						
Analytical Chemistry Project	\$0.6M to \$2M	10	Scientists, regulators, commercial	12,000	In progress	Analyses of bulk solid chemistry, mineralogy, or physical properties, and chemical analysis of inorganic or biological media
Gas Chromatography/Mass Spectrometry	\$0.2M or less	1	Scientists	4,500	Implemented	Gas chromatograms to better understand the origin, maturity, and secondary alteration of petroleum system components

National Water Quality Laboratory	$6M or more	134	Scientists, regulators	33,908	Implemented	Environmental analytical chemistry in water, sediment, and tissue to support national assessments and trend analysis
Plasma Laboratory	$0.6M to $2M	5	Primarily scientists	125	In progress	Analyses of radiogenic and heavy stable isotopes in geological, biological, and hydrological materials
Radiogenic Isotope Laboratory	$0.6M to $2M	10	Primarily scientists	1,500	Not started	Radiogenic isotopic analyses to support geochronology and tracer studies in rock, mineral, soil, water, and biological materials
Spectroscopy Laboratory	$0.6M to $2M	3	Scientists	200–600	In progress	Spectral measurement of samples, ultraviolet to far infrared, to support spectroscopic and remote sensing research
November 2018, Menlo Park						
Benthic Lab	$0.3M to $0.5M	3	Scientists, regulators, commercial	650	Not started	Analysis of benthic samples to help characterize the benthic community of San Francisco Bay
Rock Physics Laboratory	$0.3M to $0.5M	5	Scientists, regulators, commercial	~60	Not started	Determination of physical, mechanical, and chemical properties of rocks and fault zone materials at elevated temperature and pressure
Tephrochronology Project Laboratory	$0.3M to $0.5M	3	Scientists	83	Not started	Geochemical analysis of volcanic glass shards to determine provenance, date geologic events, and support geologic reconstructions
Unsaturated Zone Flow Processes Lab	$0.2M or less	3	Scientists	NA	Not started	Geochemical analysis to study aquifer recharge, contaminant transport, slope stability, preferential flow, and ecohydrology

continued

TABLE 3.1 Continued

Laboratory Name	Budget	FTEs	Users[b]	Average Annual Sample Throughput 2013–2017[c]	QMS Status[d]	Science Applications
February 2019, Kearneysville						
Fish Health Laboratory—Fish Culture and Pathology	$0.2M or less	8	Scientists, regulators	400	Not started	Aquatic animal disease diagnosis, monitoring, and research investigations
Functional Genomic, Biomarker, and Environmental Contaminant Bioanalysis	$0.6M to $2M	6	Scientists, regulators	400	Not started	Development and application of molecular, protein, and cellular analytical approaches to evaluate fish health

[a] Data from USGS 2016 laboratory inventory, except the annual sample throughput, which was collected by USGS in 2018 and 2019 for the committee site visits.
[b] Regulators is short hand for federal, state, or local government regulators or resource managers.
[c] The nature of sample analysis varies widely among laboratories, and thus sample throughput does not necessarily reflect laboratory productivity.
[d] Laboratory reported status of USGS-defined QMS implementation on the date of the site visit.

INSIGHTS FROM VISITS TO USGS LABORATORIES

The committee visited 17 USGS laboratories, including one inactive laboratory. The laboratories were chosen to cover different budgets and staff levels, mission areas, stages in implementing the QMS, and types of laboratory activities (Table 3.1).

Although the site visits offered an opportunity to spot-check the USGS 2016 laboratory inventory, they were intended to learn about the day-to-day operations of the laboratories, their opportunities for advancing knowledge, and the challenges they face. The conversations covered sample flow, quality assurance and quality control practices, adequacy of resources, and accomplishments and concerns. Some common themes that emerged from those conversations are summarized below, and information collected by the USGS in 2018 and 2019 for the site visits is presented in Table 3.2.

The committee met with a principal investigator and/or laboratory manager at each laboratory and also talked with analysts working in the laboratory. The laboratory staff were welcoming and candid with the committee. In all the laboratories visited, the staff were excited to share their work, were skilled in what they do, and took pride in their science, their reputation, and the societal impact of their work. Many of the laboratories had been operating for more than 40 years (Table 3.2), sometimes in different guises, pointing to their ongoing usefulness. Most of the laboratories had state-of-the-art instruments as well as older equipment purchased over their long history. The committee was impressed with the laboratory capabilities and staff.

The staff expressed some concerns about the day-to-day operations of their laboratories. Many staff believed their laboratory is under-resourced, with a shrinking workforce and a limited ability to hire permanent staff. Laboratory information management systems—which are used to efficiently manage samples, data, and workflows—are expensive, and so most laboratories visited are using Excel spreadsheets to manage data. Retirements and the shift toward short-term contractors increase turnover and adversely affects institutional memory and training. In the water mission area, reporting lines are shifting, further complicating staffing issues. A few laboratories suffer from problems associated with aging infrastructure, such as leaking pipes that threaten equipment and samples.

Laboratory staff understood the importance of their results being accurate and reproducible, and they had generally put in place some standard operating procedures and quality assurance and quality control measures. In all of the laboratories visited, the vast majority of standard operating procedures described technical methods (Table 3.2). The National Water Quality Laboratory also had a substantial number of standard operating procedures for laboratory management. Quality assurance and quality control measures varied widely in comprehensiveness across laboratories, and some staff recognized the need to strengthen their procedures.

Some staff in laboratories that had implemented the QMS found that it improved their data quality practices. This observation dovetails with laboratory comments made during

TABLE 3.2 Data Collected in 2018 and 2019 for Committee Laboratory Visits (from USGS)

			Standard Operating Procedures	
Laboratory Name	Age (years)	QMS Status[a]	Number[a]	Type(s)[b]
Energy Environmental Labs	28	Implemented	10	9 technical methods and 1 laboratory management
Environmental Organic Geochemistry Lab (inactive)	29	Not applicable	38	34 technical methods, 1 equipment management, and 3 laboratory management
Microbiology Lab	34	Not started	44	40 technical methods, 1 equipment management, and 3 laboratory management
Reston Stable Isotope Lab	40	Not started	28	21 technical methods, 6 equipment management, and 1 laboratory management
Wetland Ecosystems Ecology and Biogeochemistry Laboratory	16	Not started	33	33 technical methods
Analytical Chemistry Project	22	In progress	15	14 technical methods and 1 laboratory management covering multiple processes
Gas Chromatography/ Mass Spectrometry	44	Implemented	16	14 technical methods and 2 laboratory management
National Water Quality Laboratory	41	Implemented	100	65 technical methods, 8 equipment management, and 27 laboratory management
Plasma Laboratory	6	In progress	1	1 technical method
Radiogenic Isotope Laboratory	60 years; current form since 2016	Not started	4	4 technical methods
Spectroscopy Laboratory	45	In progress	4	3 technical methods and 1 laboratory management
Benthic Lab	43	Not started	2	1 technical method covering multiple processes and 1 laboratory management covering multiple processes
Rock Physics Laboratory	49	Not started	0	
Tephrochronology Project Laboratory	45	Not started	6	1 technical method and 5 laboratory management

TABLE 3.2 Continued

			Standard Operating Procedures	
Laboratory Name	Age (years)	QMS Status[a]	Number[a]	Type(s)[b]
Unsaturated Zone Flow Processes Lab	50	Not started	1	5 technical methods
Fish Health Laboratory—Fish Culture and Pathology	40	Not started	2	2 laboratory management
Functional Genomics, Biomarker and Environmental Contaminant Bioanalysis	40	Not started	24	24 technical methods

[a] As of the site visit date.
[b] Committee interpretation from the titles of the standard operating procedures.

an external audit of QMS implementation in the Energy Resources Program (Meeks et al., 2018). Many of those laboratories found that the QMS process and documentation corroborated data quality.

In contrast, the committee found that laboratories that had not yet begun implementing the USGS QMS had a poor understanding of what was involved. Most laboratory staff expressed a willingness to adopt additional quality assurance procedures in their laboratories if it would improve the defensibility and transparency of their work. However, there was considerable hesitation about whether the USGS QMS would achieve this objective, and fear that it would create unnecessary burdens on their laboratory, detracting from valuable time and limited resources for research activities. In addition, the staff were concerned that the USGS would adopt a "one-size-fits-all" approach to a QMS that would not meet the needs of their laboratory, despite the stated purpose of accommodating the diverse research needs and user profiles of individual laboratories. Such concerns arose because (a) few laboratory staff were involved in QMS development and implementation, and (b) their laboratory has few similarities with the National Water Quality Laboratory (the primary model for the USGS QMS).

A common theme among the 17 laboratory visits was staff dissatisfaction and frustration regarding the USGS QMS implementation process thus far. The primary sources of dissatisfaction included the following:

1. *Short implementation timeline*. USGS staff in the Energy and Minerals Mission Area were expected to learn new procedures and implement the QMS in their laboratory in only about 1 year. Staff believed that meeting such a short timeline was unrealistic and would pull them away from their already demanding schedules.
2. *Inadequate resources and training to effectively adopt new requirements*. No monetary resources are being provided to the laboratories for QMS implementation, stretching

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already tight budgets and staff time. In addition, laboratory staff implementing the QMS noted that it took weeks or even months to have their standard operating procedures reviewed, and that the reviewers often did not have subject matter expertise, requiring iteration between laboratory staff and reviewers. Many staff scientists wanted QMS training opportunities, frequent access to a quality assurance expert, and discussions with laboratories developing similar standard operating procedures during the implementation phase. Although the USGS plans to hire more QMS personnel (see Figure 1.3), they will not be in place quickly enough to meet the QMS rollout timeline.[1]

3. *Ineffective communication from the USGS leadership*. Staff in laboratories that had implemented QMS or were next in line were well informed of the USGS implementation process. However, staff in other laboratories further down the rollout queue were largely unaware of the details, suggesting they are not paying attention to USGS communication efforts or that those communications efforts were unsuccessful. The more informed staff were often frustrated by what they perceived as shifting plans, deadlines, and expectations for adopting QMS requirements. For example, a few staff mentioned receiving different instructions at different USGS information sessions over the course of a week. Staff attributed some of these communication problems to inadequate QMS staffing, the rapid rollout, and the sense that the USGS was making up the process as they went along, analogous to "building the plane while it is rolling down the runway."

These three concerns were also highlighted in the external audit of Energy Research Program laboratories, which made recommendations for resolving them (Meeks et al., 2018; see Chapter 4).

SUMMARY AND ANSWERS TO TASKS 1, 2, AND 3

The committee's first tasks were to provide an overview of all USGS analytical laboratories (Task 1), their data quality assurance and quality control procedures (Task 2), and the extent to which resources are available to meet their science and applications objectives (Task 3). These tasks are related and are discussed together below.

The approximately 250 USGS analytical laboratories are diverse in their science and applications objectives, budget, staff and user profiles, and sample throughput. Collectively, their science and applications objectives cover all USGS mission and core science areas. All of the laboratories support USGS researchers, and about half also support the needs of federal, state, and local regulators and resource managers. The laboratories primarily supporting

[1] The language of this sentence was modified after release of the publication version to reflect current USGS staffing plans.

research have fewer staff, lower budgets, and fewer and less documented quality assurance and quality control practices than the laboratories that also serve regulators and research managers. Sample throughput depends on the type of sample being analyzed and the analytical procedures being performed, and ranged from 60 samples per year to 33,000 samples per year for the laboratories visited by the committee.

Before the USGS QMS rollout began, most of its laboratories operated like academic research laboratories, with principal investigators obtaining funding and establishing quality assurance and quality control practices. Although laboratory staff recognize that more formal and comprehensive practices may have benefits, many are concerned that the USGS QMS will not meet their specific needs and that QMS implementation is moving too fast with inadequate staff, resources, and communication to roll it out properly.

The laboratories the committee visited are mostly long lived (decades) and had state-of-the-art instruments as well as older equipment purchased over their long history. The laboratories appeared to be meeting their science and applications objectives. However, staffing shortfalls and turnover were a common resource problem. Adding responsibilities for implementing a complex QMS, especially without adding sufficient resources, may hinder their future ability to meet their science goals.

4

Experiences with Quality Management Systems

The committee's second task was to describe the analytical procedures and data management practices in laboratories at the U.S. Geological Survey (USGS), other federal agencies, and geological surveys in other countries. Because the USGS is implementing a quality management system (QMS), it asked the committee to focus on laboratory QMS procedures. The data quality assurance practices of USGS laboratories are summarized in Chapter 3. This chapter focuses on the experiences of selected organizations in implementing and maintaining a QMS.

The committee invited eight organizations to share their approach and experiences with a QMS. The committee heard from four U.S. federal agencies with a substantial number of analytical laboratories using a QMS: the USGS, the Navy's Environmental Laboratory Accreditation Program (ELAP) and Naval Sea Systems Command (NAVSEA) Shipyard Laboratory Program, the Centers for Disease Control and Prevention (CDC), and the Environmental Protection Agency (EPA). A QMS is less common in geological surveys and is rare in academic institutions. Two of five geological surveys from other nations that the committee consulted (France and Norway) use a QMS. Finally, the committee heard from the Geochemical and Environmental Research Group (GERG) Laboratory at Texas A&M University and a group of laboratories under quality assurance oversight of Duke University Medical Center that use a QMS. This group includes laboratories at Duke and other academic institutions. For simplicity, they are referred to in this chapter as the Duke University Medical Center laboratories.

This sample of organizations is small and cannot be considered representative of all organizations. However, the committee sought diversity in terms of scientific focus, number of laboratories under the QMS umbrella (see Table 4.1), and position of the presenters. Presentations by federal agencies were given by QMS-related managers, and presentations by geological surveys and academic institutions were given by scientists or laboratory managers. The diverse perspectives and experiences of these organizations are highly relevant to the USGS, which is incorporating lessons learned into its own QMS.

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TABLE 4.1 Scientific Focus and Number of Laboratories in the Presenting Organizations

Organization	Number of Laboratories with QMS	Number of Staff	Scientific Focus
USGS	~250 planned	~1,300	Geology, hydrology, and ecosystems
CDC	~200 proposed	~1,700	Infectious disease
Navy	85 ELAP	NA	Environmental restoration and ship materials
	5 NAVSEA	~130	
EPA	NA (100 percent)	NA	Public health and the environment
Duke University Medical Center	16	NA	Human clinical trials
Texas A&M GERG Laboratory	1	15	Contaminants, petroleum markers, and metals
French Geological Survey	1	77	Geophysics and the environment
Norwegian Geological Survey	1	18	Geology

NOTE: ELAP = Environmental Laboratory Accreditation Program; NA = not available; NAVSEA = Shipyard Laboratory Program.

PERSPECTIVES ON QMS FROM SELECTED FEDERAL AGENCIES, GEOLOGICAL SURVEYS, AND RESEARCH INSTITUTIONS

Each organization was asked to address the following points in their presentation:

- Why did you establish a QMS?
- Describe your current QMS.
- Is a QMS applied in all of your internal laboratories?
- How is the QMS resourced, managed, and assessed?
- Challenges in initially integrating QMS (what did you learn?)
- Challenges in maintaining the QMS (what are you learning?)
- Has the QMS evolved significantly and why?
- Has the QMS added value (e.g., examples where it either thwarted significant problems, saved money, created efficiencies, or produced defensible results that held up to scrutiny)?
- Opportunities or needs for interagency collaboration on developing consensus-based approaches for QMS in nonregulated laboratories.

The diverse perspectives of these organizations and common themes that emerged from the presentations are summarized below.

1. *Organizations have different motivations for having a QMS, and they find different benefits in it.*

All four federal agencies presenting had developed a QMS to improve the quality, reliability, and reproducibility of laboratory data. In addition, the USGS, EPA, and CDC sought to preserve or enhance their reputation for providing high-quality data. USGS data support policy making and CDC data support public health, and so high-quality data are needed to avoid unaccounted-for risk and error and to maintain public trust. EPA data support regulation, and so the data must be scientifically and legally defensible. The French and Norwegian geological surveys also cited enhancing customer confidence in laboratory results as a key motivation for implementing a QMS. The Navy mentioned the benefit of a QMS for continually improving processes.

Some laboratories adopted a QMS to pursue contract work and research projects in fields that require compliance with specific data standards. The Texas A&M GERG laboratory complies with EPA standards for work on contaminants (e.g., pharmaceuticals, pesticides, and dioxin), petroleum biomarkers, and metals. The Duke University Medical Center laboratories comply with National Institutes of Health requirements to support clinical trials.

A key QMS benefit identified by many of the presenters was the value of good documentation. A documented, step-by-step quality assurance process allows consistent performance, data verification, and proof that accepted protocols were followed. The need for consistent performance was emphasized by the Norwegian Geological Survey, where multiple team members carry out analyses and need uniform standards for quality assurance and quality control. The value of documentation for retaining institutional memory through staff turnover was noted by staff in several laboratories visited by the committee (see Chapter 3).

Several presenters noted that a QMS does not prevent all data quality problems, but it can leave clues that help laboratory staff identify and respond to problems relatively quickly. Some of the problems mentioned concerned sample or instrument contamination, and the loss of original data through machine overwriting or human editing. The built-in external audit feature of a QMS is intended to catch problems. For example, an external audit of USGS Energy Mission Area laboratories identified a data quality problem related to anion concentrations measured using ion chromatography (Meeks et al., 2018).

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2. *Some organizations are not implementing QMS for all their laboratories.*

Four of the presenting organizations have implemented or plan to implement QMS for all of their laboratories. EPA has one QMS that covers EPA organizations as well as other organizations that receive EPA funds, but allows flexibility in how these external organizations implement the system. The CDC is slowly implementing QMS through pilot programs that recruit successively more laboratories. Each CDC laboratory in the pilot program chooses from three QMS options: standard, customized, or both. The USGS has begun implementing a single QMS for all of its laboratories. The Norwegian Geological Survey has a QMS for its one laboratory.

The other organizations are implementing a QMS for only part of their enterprise. The Navy laboratories that operate under the Environmental Laboratory Accreditation Program and NAVSEA Shipyard Laboratory program require a QMS, but other Navy laboratory programs do not. The French Geological Survey laboratories are accredited for some environmental chemistry and mineral characterization activities, but not for isotope geochemistry or multiscale experimentation activities. The Texas A&M GERG laboratory embraced a flexible approach to support its diversity of programs. It maintains a QMS for most contract work, but not for research and development projects. Half of the 32 laboratories under the quality assurance oversight of Duke University Medical Center use the QMS.

3. *A QMS requires substantial resources. The cost of implementation and maintenance may be covered by the organization or by its laboratories.*

The USGS has found that its laboratory staff spent about 20 percent of their time to implement the QMS. This figure is in line with the experiences of other presenters—who estimated that their laboratories spent 10 to 20 percent of their time implementing a QMS and 5 to 10 percent thereafter maintaining it—and with published time estimates (e.g., Vermaercke, 2000). A substantial part of the investment involves record-keeping requirements. Laboratory Information Management Systems or electronic QMS provide a higher level of traceability than traditional spreadsheets for data management, but they may require procurement and maintenance funding or dedicated staff. External audits required in some QMSs can also be costly.

The organizations have different approaches for paying the costs of the QMS. The French and Norwegian geological surveys fund their QMS centrally. The USGS and the CDC pay for training and support all quality assurance staff. No additional funding is provided to their laboratories for QMS implementation and maintenance. The laboratories under QMS programs at the Navy, EPA, Texas A&M GERG, and Duke University Medical Center pay all QMS costs, including training and quality assurance specialists. The Duke University Medical Center laboratories are also covering information technology support for their electronic QMS.

4. *Implementation and maintenance of an effective QMS requires institutional commitment, leadership, and buy-in from the staff.*

A point made by several presenters was the role of leadership and culture in implementing a QMS. Initial resistance from laboratory staff was not unusual, and a substantial amount of institutional change was often required. The Texas A&M GERG Laboratory presenter noted that implementing a QMS was a huge undertaking, and getting staff to buy into the QMS was a major challenge. The Navy encountered resistance from laboratory staff, particularly those in smaller laboratories, when a QMS was introduced. The Norwegian Geological Survey stressed the importance of ongoing leadership support and laboratory staff awareness for maintaining their QMS.

EPA leadership set out to persuade scientists that a QMS supports science, rather than interferes with it. Some of the desired cultural shift toward a QMS occurred as management and scientists made decisions together. At the Duke University Medical Center, the participating laboratories were involved from the beginning to change attitudes and create buy-in. The CDC also involved agency managers and scientists in developing laboratory quality management policies. The well-respected principal investigators in the pilot laboratories served as "QMS champions," who were able to demonstrate the feasibility and benefits of a QMS and thus help facilitate cultural shift. The Navy accelerated culture change by first showing its laboratories a functioning QMS that yielded benefits, then requiring the laboratories to adopt it.

5. *Effective two-way communication between laboratories and management is important for developing and evolving a QMS.*

Presenters pointed out that communication between laboratories and management is important for explaining why a QMS is needed, creating buy-in, developing a QMS that meets the needs of the laboratories, and evolving the QMS to accommodate new equipment or meet new user needs. The USGS found communication a challenge, given the complexity of the organization and the rapid development and implementation of its QMS. USGS leadership is working to provide training and communication plans that focus on why a QMS is necessary. The CDC noted the importance of consistent messaging about the QMS from both leadership and QMS staff. EPA found it helpful to keep quality assurance jargon to a minimum. The French Geological Survey noted the importance of reminders of why the QMS was put in place, especially in light of staff turnover.

6. *Starting small and taking advantage of lessons learned helps the system evolve over time.*

   The Navy's NAVSEA Shipyard Laboratory Program experienced significant growing pains, including a struggle to develop documents and maintain records, as it implemented a top-down QMS for its laboratories. The USGS faced a steep learning curve by developing and implementing a QMS on an accelerated schedule. In contrast, the CDC found that implementing a QMS slowly and in stages increased the likelihood of success because it allowed the agency to test and modify its approach, measure the necessary level of effort and investment, and demonstrate the feasibility and benefits of the QMS. It also provided an opportunity to develop guidance documents, templates, and expertise to support implementation across the agency. The number of laboratories under the Duke University Medical Center QMS expanded from 3 to 16 as it was determined that the research would benefit from standard operating procedures and QMS.

SUMMARY AND ANSWER TO TASK 2

Task 2 was to summarize data management practices, specifically QMS, for laboratories at the USGS, other federal agencies, and geological surveys in other countries. The committee chose eight organizations that had different motivations for developing a QMS for some or all of its laboratories, different QMS challenges (e.g., number and diversity of laboratories and laboratory activities), and different QMS implementation strategies (e.g., top down or bottom up, and fast or slow). Despite these differences, some common themes emerged. First, implementing a QMS provides benefits, such as improving documentation, reliability, reproducibility of laboratory data; finding and correcting data quality problems; and enhancing the organization's reputation for quality data. However, these benefits come with substantial monetary and personnel costs. The high costs and paperwork burden associated with implementing a QMS, as well as the need to learn a new way of doing things, can create resistance among laboratory staff. Institutional commitment and strong leadership are required to gain staff buy-in and to change the organization's culture. Consistent messaging is important in explaining why a QMS is needed, and good two-way communication between managers, quality assurance staff, and laboratory staff is essential for developing a QMS that meets the needs of the laboratories. Finally, implementing the QMS slowly allows the system to evolve in response to lessons learned and thus fulfills its intended purpose.

5

Recommendations and Conclusions

The previous chapters described the U.S. Geological Survey's (USGS's) motivations for developing a quality management system (QMS) for its laboratories (Chapter 1), examples of approaches used to assure the quality of laboratory data (Chapter 2), current USGS laboratory quality assurance practices (Chapter 3), and the experiences of federal agencies, research institutions, and geological surveys in implementing a QMS (Chapters 3 and 4). The committee drew on this information to develop recommendations and conclusions on quality assurance programs for the USGS.

This chapter recommends best practices for USGS production and research laboratories (Tasks 5 and 6), the allocation of resources for implementing quality assurance programs, and the timeline for their implementation.

BEST PRACTICES

The committee's last two tasks concern best practices and procedures for achieving scientific and applications objectives and assuring the integrity and reliability of results for USGS laboratories. Task 5 was to recommend best practices for production laboratories (those carrying out routine analyses for USGS or external users), and Task 6 was to comment on best practices for research laboratories (those supporting innovation, method development, or scientific discovery). Below, the committee uses the step diagram introduced in Chapter 2 and simplified in Figure 5.1 to illustrate best practices for both types of laboratories.

Before QMS development began in 2016, most USGS laboratory principal investigators defined their own quality assurance procedures and best practices (step 1 in Figure 5.1), similar to the practices of academic laboratories (see Chapter 3). The other laboratories had quality assurance procedures more consistent with a QMS (step 3), although some QMS elements might be missing, and a few met externally-defined QMS requirements (step 4). The current USGS plan is to require that all of its laboratories follow institution-defined QMS requirements (Step 3). This change would mean a substantial increase in management oversight, resources, and requirements for most USGS laboratories.

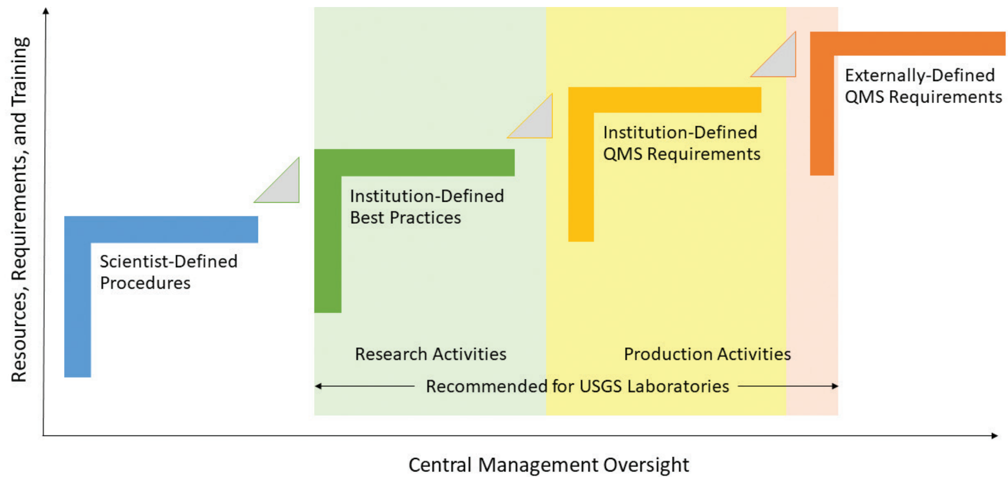

FIGURE 5.1 Four approaches (steps 1–4) for assuring the quality of results from laboratories that support research, method development, or data production. The triangles represent training opportunities. Most current USGS laboratory practices are consistent with scientist-defined procedures (blue, step 1). The USGS is now implementing an institution-defined QMS (yellow, step 3). The committee recommends that USGS laboratories follow institution-defined research best practices (green, step 2) or QMS, as appropriate (primarily step 3, with a few laboratories in step 4, orange).

Institution-defined expectations of data quality are important for generating data of known consistent quality across large organizations such as the USGS, which has to manage some 250 diverse laboratories across the country. The committee found two approaches that would meet this goal for most USGS laboratory activities: institution-defined best practices (step 2) and institution-defined QMS (step 3).

For laboratories focused on supporting research and method development, which need the flexibility to innovate and experiment, institution-defined best practices (step 2) are appropriate. This approach would allow the USGS to set general expectations for how its research-oriented laboratories are managed, while providing flexibility to principal investigators to develop a program that meets those expectations. Examples of how this might work are given in Box 5.1. Moving from step 1 to step 2 would retain the ability of these laboratories to experiment and innovate, while fully participating in a centralized USGS laboratory culture committed to accountability and data quality and integrity. Adding periodic independent data quality checks (e.g., peer review and internal audits) would confirm that institution-defined best practices have become routine in research and method development laboratories at the USGS. This innovative approach would also provide a leadership opportunity for the USGS, since relatively few large government organizations or academic institutions have attempted such broad-scale implementation of a quality assurance program in basic research settings.

BOX 5.1
Tips on Getting Started with Institution-Defined Best Practices

To develop general expectations for its laboratories, the USGS would begin by identifying the best practices they wish to adopt, drawing from the scientific literature, organizations developing consensus-based laboratory practices, or formal laboratory or data management standards or guidelines. The USGS would then provide guidelines, an infrastructure for managing research records (e.g., electronic notebooks, information technology support, or a laboratory information management system), and training, consultation, and formative monitoring to support the adoption of the guidelines in each laboratory. Models for defining institution-based guidelines, expectations, or policies include *Quality in Research, Guidelines for Working in Non-regulated Research* (RQA, 2014) and *Handbook: Quality Practices in Basic Biomedical Research* (WHO, 2006). Examples of different approaches appear in Box 2.2 (Chapter 2).

An example of a USGS expectation might be for each laboratory to develop a written laboratory management plan that describes approaches for managing people (e.g., safety and training), communication (e.g., laboratory meetings and result review), equipment (maintenance, calibration, and use), methods (e.g., approval, quality control, and validation), and research records (e.g., metadata and archives). Another example expectation might be for each USGS laboratory to implement a data management plan to ensure that data quality and integrity are preserved across all research activities. Both of these examples require a defined plan and processes to ensure that the plan is followed.

Individual laboratories could meet these generalized USGS expectations in different ways. For example, some laboratories may choose to have a single Standard Operating Procedure (SOP) that addresses all the elements of laboratory management and multiple SOPs that describe technical activities. Other laboratories may break down their processes into critical elements (e.g., equipment, personnel, or methods) and develop element-specific management and technical SOPs. Some laboratories may establish web-based and version-controlled folders containing work policies, procedures, and work records, and others may use electronic notebooks with embedded procedures. Regardless of the approach adopted by an individual laboratory, the key is to make sure that procedures are documented, effective, and monitored to ensure that data quality and integrity are maintained across all activities.

In contrast, laboratories that carry out well-characterized and routine analyses for internal or external users (production activities) would benefit from an institution-defined QMS (step 3), which the USGS is already implementing. Because of organizational objectives or user demands, these laboratories typically need to meet the most stringent strategies for maintaining and demonstrating data quality. A few of these laboratories (e.g., the National Water Quality Laboratory) may also need to meet externally-defined QMS requirements (step 4) for some procedures.

All USGS laboratories support research and perhaps half also carry out production activities. Available data do not distinguish which laboratories do production work or in

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what proportion. The USGS, in consultation with its laboratories and their users, will need to decide which laboratories need a centrally controlled QMS and which need institution-defined best practices.

Recommendation 1. The USGS should implement institution-defined best practices (step 2) or institution-defined QMS (step 3), as appropriate, for its laboratories.

RESOURCES

A key responsibility of management is to support implementation and maintenance of the quality assurance program. However, current USGS resource commitments, quality assurance staffing, and training are insufficient to implement a centrally controlled QMS for all USGS laboratories, especially on a fast timeframe. The USGS plans to cover the shortfall by splitting costs with its laboratories: the USGS will provide central training and quality assurance experts, and the laboratories will devote an estimated 20 percent of their resources for about 2 years to implement the QMS and about 10 percent annually thereafter to maintain the system. The USGS had considered having as many as one quality assurance expert for every 30 laboratory staff.[1] However, it has been able to hire only a half dozen quality assurance experts, not nearly enough to support QMS implementation for all of its laboratories. These personnel shortages and financial costs were a common concern of staff in the USGS laboratories the committee visited (see Chapter 3).

An additional reason for adopting the two quality assurance programs recommended above is that doing so would reduce the immediate resources required because it is less expensive to implement institution-defined research best practices than it is to implement a centrally administered QMS. Implementing institution-defined best practices for the laboratories focused primarily on research would free up central USGS resources to support QMS implementation and maintenance for the subset of laboratories engaged in production activities.

Recommendation 2. The USGS should optimize and prioritize centralized resources for the subset of laboratories doing production activities that would most benefit from a QMS.

TIMELINE

The USGS is embarking on one of the largest QMS efforts attempted by a national research organization. The organizations with smaller QMS programs that the committee

[1] The language of this sentence was modified after release of the publication version to reflect current USGS staffing plans.

consulted took substantial time (years) to implement a QMS and create a quality culture. It will likely take longer for the USGS to achieve these goals, given the scale and complexity of the USGS QMS effort. However, the USGS is developing and implementing its QMS more quickly. QMS development began in 2016, and the system was implemented in 11 energy laboratories in mid-2017. The USGS's goal is to complete QMS implementation in all USGS laboratories in 2024. Both QMS and institution-defined best practices are relatively new concepts in academic and government research environments and require the development of new systems to support production of data of known and documented quality. In addition, training programs are needed to increase knowledge and support the development of quality assurance skills. Such systems take time to develop, implement, and evolve.

Adopting QMS and institution-defined best practices requires a gradual shift in laboratory and agency culture and is more likely to succeed with buy-in from USGS staff at all levels of the organization. The USGS will need to take the time to gain substantive input and feedback from laboratory principal investigators, laboratory managers, quality assurance experts, and other organizations using these approaches to develop the systems, as well as to use lessons learned to make course corrections. Slowing implementation of the QMS would also make resources go further.

Recommendation 3. The USGS should slow implementation of its QMS to allow ample time to develop institution-defined best practices, take advantage of lessons learned, provide training, and obtain input and buy-in from USGS laboratory staff.

CONCLUDING REMARKS

The USGS is to be commended for pursuing recognized best practices to produce data of known and documented quality. The agency has chosen to implement a centrally controlled QMS to achieve consistency and a shared quality culture across its approximately 250 analytical laboratories. The QMS was developed from existing QMSs in laboratories doing routine production work (e.g., National Water Quality Laboratory). However, approximately half of USGS laboratories support exploratory research and method development, which have fewer established procedures and require the flexibility to make frequent changes as the methods and analyses are refined. Concerns that a QMS would restrict their autonomy, flexibility, or creativity were raised by staff in a number of USGS laboratories. Moreover, the current QMS implementation plan is unrealistic, given resource and time constraints. Few large research organizations have attempted to establish a QMS under these conditions.

The USGS has an additional option (institution-defined best practices) that would achieve its quality goals, retain laboratory abilities to experiment and innovate, and reduce resource needs. For laboratories focused primarily on supporting research, the USGS

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should establish expectations for maintaining and demonstrating data quality, and allow each laboratory principal investigator to develop data quality procedures that meet those expectations. Because institution-defined best practices are less expensive to implement than a QMS, more resources could be directed to laboratories that carry out substantial production activities requiring a QMS.

For both approaches, ample time is needed to

- Communicate with staff, including explaining the quality goals of the organization and gaining staff input and feedback on system design and implementation;
- Provide staff training, including meetings with quality assurance experts;
- Establish mechanisms to recognize, support, and reward the substantial time and resources invested by laboratory scientists and quality assurance experts to meet USGS data quality goals;
- Develop QMS champions who would help lead the necessary culture change; and
- Learn from implementation experiences and continually improve the system.

This flexible approach that incorporates institution-defined best practices for research activities and QMS for production activities would better meet the quality goals of the USGS and the diverse needs of its laboratories, foster staff buy-in, and cultivate an enduring quality culture across the agency.

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Appendix

Biographical Sketches of Committee Members

WILLIAM A. HOPKINS, Chair, is a professor in the Department of Fish and Wildlife Conservation and director of the Global Change Center at Virginia Polytechnic Institute and State University. His research focuses on physiological ecology and wildlife ecotoxicology with the goal of understanding how wildlife responds physiologically and behaviorally to anthropogenic disturbances. He is particularly intrigued by tradeoffs among physiological processes such as reproduction, thermoregulation, and immune function and how global changes may force animals to reprioritize their investments of time and energy. Dr. Hopkins has participated in a diverse range of advisory activities including several National Academies of Sciences, Engineering, and Medicine and Environmental Protection Agency (EPA) study committees on ecological and human health effects of coal mining, disposal of coal combustion residues in mines, aquifer storage of water to support everglades restoration, and ecological effects of diverse environmental pollutants. He has also worked with industry stakeholders and the U.S. Fish and Wildlife Service on five Natural Resource Damage Assessments, and a U.S. Fish and Wildlife Service-sponsored assessment of whether the hellbender salamander should be protected as an Endangered Species. He received a B.S. in biology from Mercer University, an M.S. in zoology from Auburn University, and a Ph.D. in ecology, evolution, and organismal biology from the University of South Carolina.

SUSAN L. BRANTLEY (NAS) is Distinguished Professor of Geosciences and director of the Earth and Environmental Systems Institute at the Pennsylvania State University. Her research interests are in aqueous geochemistry, geochemical kinetics, and microbial biogeochemistry with a focus on chemical, biological, and physical processes associated with the circulation of aqueous fluids in shallow hydrogeologic settings. Dr. Brantley has received numerous awards for her research including the Arthur L. Day Medal from the Geological Society of America and the Wollaston Medal from the Geological Society of London. She is also a fellow of the American Geophysical Union, European Association of Geochemistry, Geochemical Society, Geological Society of America, and the International Association of GeoChemistry. Dr. Brantley has participated in a variety of advisory committee activities and is a current member of the Nuclear Waste Technical Review Board, a past chair of the Department of Energy's Earth Science Council, and a past member of National Academies of Sciences, Engineering, and Medicine committees on unconventional hydrocarbons, nuclear waste, and Earth surface processes. She received a B.A. in chemistry and an M.A. and Ph.D. in geological and geophysical sciences, all from Princeton University. She is a member of the National Academy of Sciences.

REBECCA DAVIES is the director of Quality Central and an associate professor in the Veterinary Diagnostic Laboratory (VDL) and the Department of Veterinary Population Medicine at the University of Minnesota College of Veterinary Medicine. Her interests include the establishment and adoption of a research quality assurance standard for nonregulated research, the development of sustainable models for incorporating quality assurance monitoring programs into academic research programs, research on research, and the use of laboratory error data and quality assessment metrics to drive improvements in laboratory and research settings. Since 2009, Dr. Davies has led the VDL effort to meet the American Association of Veterinary Laboratory Diagnostician's laboratory accreditation requirements. Dr. Davies serves on that association's laboratory accreditation committee and is an active member of the Society for Quality Assurance and the Research Quality Association. She is also a member of the Association of Biomolecular Resource Facilities' Committee for Core Rigor and Reproducibility and of the Asian and Pacific Rim Research Integrity Network's Education and Training Working Group. Dr. Davies received her Ph.D. in comparative animal physiology from the University of Minnesota.

DON DePAOLO (NAS) is Chancellors Professor, Emeritus, in the Department of Earth and Planetary Science at the University of California, Berkeley, and Senior Advisor at Lawrence Berkeley National Laboratory (LBNL). Previously, he held several management positions at LBNL, including director of the Earth Sciences Division and associate laboratory director of Energy Sciences. He currently directs two research centers: the Center for Isotope Geochemistry and the Center for Nanoscale Control of Geologic CO_2. Dr. DePaolo's research focuses on the use of naturally occurring isotopes to explore a variety of earth science questions related to mantle dynamics and magma chamber processes as well as tracking fluids moving through groundwater systems to trace contaminates. He is the recipient of numerous awards, including the J.B. MacElwane Award and H.H. Hess Medal from the American Geophysical Union, the Arthur L. Day Medal from the Geological Society of America, and the Harold Urey Medal from the European Association of Geochemistry. He is a fellow of these societies as well as the American Association for the Advancement of Science, the California Academy of Sciences, and the American Academy of Arts and Sciences. Dr. DePaolo has served on

National Academies committees on strengthening the EPA laboratory enterprise, grand research questions in the solid-earth sciences, and future roles, challenges, and opportunities for the U.S. Geological Survey (USGS). He received a B.S. with honors in geology from the State University of New York, Binghamton, and a Ph.D. in geology (minor in chemistry) from the California Institute of Technology. He is a member of the National Academy of Sciences.

ANDY EATON has spent 38 years at Eurofins Eaton Analytical LLC (formerly MWH Labs), a multistate certified water testing laboratory, serving at various times as technical director, marketing director, and laboratory director. He is a Board-Certified Environmental Scientist with more than 40 years of experience in water–quality–related environmental problems such as those associated with contaminants such as pharmaceuticals, arsenic, perchlorate, chromium, perfluoroalkyl substances, dioxane, and bromate. His work has focused on the development of analytical methods, data quality assurance, and detection, quantitation, and monitoring. He also carries out studies supporting EPA rules for unregulated contaminant monitoring. Dr. Eaton serves on the Joint Editorial Board for "Standard Methods for the Examination of Water and Wastewater," a comprehensive reference with best practices for water analysts. He is a recipient of the George W. Fuller Award and the Charlie Carter Award, which recognize distinguished service and leadership in water supply or environmental measurement and monitoring. He received a B.A. in earth sciences from Antioch College and a Ph.D. from Harvard University, in geology, with a focus on marine geochemistry.

ROBERT FLEISCHER is senior scientist and head of the Center for Conservation Genomics at the Smithsonian Conservation Biology Institute. His primary fields of interest are evolutionary and conservation biology, with a focus on population and evolutionary genetics, systematics, and molecular and behavioral ecology, mostly on free-ranging bird and mammal species, and their pathogens. Most of his recent projects use genomic, transcriptomic, and microbiome methods. Dr. Fleischer has served on a number of advisory committees on systematics and threatened birds. He is a fellow of the American Association for the Advancement of Science and the American Ornithologists' Union, and received that society's Brewster Medal for exceptional work on Western Hemisphere birds. Dr. Fleischer received a B.A. in biology from the University of California, Santa Barbara, and a Ph.D. in evolutionary biology from the University of Kansas.

MADELINE GOTKOWITZ is Research Division Chief at the Montana Bureau of Mines and Geology, located at Montana Tech of the University of Montana. Her research interests include physical hydrogeology (e.g., surface water–groundwater interactions and flow across aquitards), geologic sources of naturally occurring contaminants (e.g., arsenic, chromium, and radium) in Wisconsin's aquifers, and the spatial and temporal distribution of wastewater constituents in groundwater (e.g., enteric viruses, artificial sweeteners, and personal care products).

The groundwater contaminant work relies heavily on analytical data collected by the USGS and other laboratories. Dr. Gotkowitz is a former president and current member of the City of Madison, Wisconsin's Water Utility Board. She received a B.A. in environmental science from Smith College, an M.S. in hydrology from New Mexico Tech, and a Ph.D. in environmental science from the University of Wisconsin, Madison.

DENNIS (CHUNGING) JIANG is a senior research scientist and petroleum geochemist at the Geological Survey of Canada. From 2006 to 2012, he worked as a geochemist and manager of the geochemistry laboratory at Geosolutions of Unconventional Systems and Heavy Oil Recovery, Inc. (GUSHOR). Dr. Jiang's research interests focus on petroleum systems in Canadian sedimentary basins including geochemical analyses to characterize crude oils and determine their source rocks and methodology development to assess shale petroleum resources and to characterize reservoirs. Among his responsibilities at GUSHOR and other private companies was quality assessment and quality control of laboratory data. Dr. Jiang holds patents on a method for determining a value of a property of oil extracted from a sample, a method and apparatus for obtaining heavy oil samples from a reservoir sample, and preconditioning an oilfield reservoir. He received a B.Sc. in chemistry from Shandong University in China, an M.Sc. in petroleum geology from the Research Institute of Petroleum Exploration and Development in China, and a Ph.D. in organic geochemistry from the Curtin University of Technology in Australia.

DAMIAN SHEA is a professor of environmental chemistry and toxicology at North Carolina State University and president and founder of Statera Environmental, Inc., an environmental technology and consulting company. He has been studying the detection, sources, fate, and effects of chemicals in the environment for more than 30 years. He combines knowledge and experience in chemistry, toxicology, risk assessment, and social sciences with the ultimate goal of improving our ability to assess, communicate, and mitigate the risks of chemicals to human and ecological health. In a previous position at Battelle, he was instrumental in developing the quality assurance and quality control program for the Exxon Valdez Oil Spill that continues to serve as the basis for oil spill monitoring programs today. Dr. Shea has served on numerous expert panels including a U.S. Bureau of Ocean Energy Management panel on offshore oil exploration in the Arctic and an EPA bioaccumulation subcommittee to review EPA's revisions to national water quality criteria. He is a member of the American Chemical Society, Society for Environmental Toxicology and Chemistry, Society of Toxicology, and International Society of Exposure Science. He received a Ph.D. in environmental chemistry from the University of Maryland.

WENLU ZHU is a professor in the Department of Geology at the University of Maryland, College Park. Her research focuses on the coupling between rock deformation and fluid flow in Earth's crust and mantle. She measures mechanical and transport properties and characterizes rock structure at various scales in three and four dimensions. Her work on damage accumulation and fracture propagation in sedimentary rocks has application to fault slip and earthquake nucleation. Dr. Zhu received the 2007 Basic Research Award from the American Rock Mechanics Association and is currently the president-elect of the Mineral and Rock Physics Section in the American Geophysical Union. She received a B.S. and an M.S. in geophysics from Peking University in China and a Ph.D. in geophysics from the State University of New York at Stony Brook.