ADVICE ON THE MISSION, OPERATION, AND FUTURE PLANS OF THE ENVIRONMENTAL MOLECULAR SCIENCES LABORATORY

Prepared by a Subcommittee of the
Biological and Environmental Research Advisory Committee

October 7, 2005

EXECUTIVE SUMMARY

In November 2004, Dr. Raymond Orbach, Director of the Office of Science, U.S. Department of Energy (DOE), asked the Biological and Environmental Research Advisory Committee (BERAC) to provide advice on the mission, operation, and future plans of the Environmental Molecular Sciences Laboratory (EMSL) that is located at the Pacific Northwest National Laboratory (PNNL) in Richland, Washington. The EMSL operations budget is provided by the Environmental Remediation Sciences Division (ERSD) of the Office of Biological and Environmental Research (BER), one of the program offices in the Office of Science. The research conducted within EMSL is supported by at least three of the BER divisions, by other parts of DOE, and by other federal agencies. The specific questions asked in Dr. Orbach's charge letter are:

- Does the relationship and management structure among EMSL, PNNL and ERSD foster the highest quality of science at EMSL?
- Is the science conducted at EMSL cutting edge? If so, is it appropriate for a BER-supported user facility?
- Is EMSL appropriately structured to support a full range of DOE and national science research priorities?
- Is the user model for allocating resources for all EMSL facilities appropriate? Does EMSL attract the best mix of users?
- Could changes be made to increase the impact of EMSL on DOE science goals?
- Given a flat budget for ERSD, what priority should EMSL have within the Division's portfolio?
- Does the EMSL have a well-defined plan to refresh capital equipment, and is it appropriate? What short- and long-term strategies should be considered in this context? Does EMSL appropriately manage the acquisition, use and retirement of instruments?
- How does EMSL manage general user access to equipment purchased with non-ERSD funds? How does this impact EMSL operation as an ERSD-supported user facility?

An *ad hoc* subcommittee, chaired by a member of BERAC, was established to respond to this charge. The BERAC subcommittee met on May 17 – 19, 2005, at EMSL.

Background

EMSL opened its doors in October 1997, with its operating dollars and associated capital equipment funds coming from BER/ERSD. In order to stimulate the initiation of research using EMSL capabilities, 50 percent of the time available on experimental resources housed within EMSL was allocated to scientists located within the EMSL organization, and the remainder was allocated to visiting, externally-based scientists. The one exception to this 50 percent split of time allocation was the high-performance computer; all time on this machine was allocated, and continues to be allocated, based on peer review of scientific applications that require high performance computing.

In 2001, ERSD conducted a peer review of the entire EMSL and, following this review, PNNL management made the decision to move those EMSL scientists who did not charge a significant

fraction of their time to user support out of the formal EMSL reporting structure and into the Fundamental Science Directorate of PNNL. In Fiscal Year (FY) 2004, BER directed PNNL/EMSL to terminate the 50/50 allocation model and to use the operating dollars in support of the EMSL role as a national scientific user facility. Those scientists who were reassigned to the Fundamental Science Directorate maintained their research laboratories and offices within EMSL. Currently, the bulk of the operating dollars provided by ERSD to the EMSL is used to support user operations for EMSL as a national scientific user facility. The building infrastructure supported by the operating dollars supports both the user facility and those PNNL scientists who, while not reporting to the EMSL director, conduct their research within EMSL, but who may or may not be designated as formal users of the national facility.

Two other background issues are of particular importance to the conclusions drawn by the BERAC subcommittee. First, since EMSL opened, there have been three directors of the Pacific Northwest National Laboratory and four directors of EMSL itself. Hence, there has not been a consistent statement of the EMSL mission, nor has there been continuity in developing robust processes for the management of EMSL. Second, during its full seven years of operation, the EMSL operations budget has increased from approximately $29M to approximately $40M. This increase is predominately due to additional dedicated funds in support of the EMSL supercomputer. Excluding the fixed costs associated with the supercomputer, the remaining budget has remained relatively constant. As a result of inflation and increased space and labor costs, the "buying power" of the remaining operations budget is less than 84 percent of what it was in FY 1998.

General Observations

Although the charge to which the BERAC subcommittee responded was focused on scientific issues, it became very clear that the scientific effort and scientific staff are strongly affected by administrative issues within the EMSL. Consequently, the report contains comments on observations and recommendations related to administrative and management issues not explicitly within the scope of the charge.

First and foremost, it does not appear that BER leadership, EMSL leadership, and PNNL leadership share a coherent vision as to what the EMSL mission is. There are two aspects to this. The first is whether or not the primary, if not sole, responsibility of EMSL is to serve as a national scientific user facility. ***In the context of this report, there is the explicit assumption that the EMSL's primary function is that of a national scientific user facility. Should there be concurrence that this is not the primary Laboratory function, then some of the conclusions in this report may have to be revisited.*** The second aspect of the necessary future articulation of the EMSL mission is the extent to which research conducted within the EMSL must have an obvious environmental connection. EMSL is a unique national resource. Certainly, if a critical and pressing national need having nothing to do with "the environment" emerged, and this need could be uniquely met using EMSL facilities, not allowing EMSL to respond would be detrimental to the Nation's interests.

Although it is too early in her tenure to assess the impact that the newly appointed EMSL Director, Dr. Allison Campbell, will have on the overall performance of the Laboratory,

interactions with the subcommittee during the review meetings suggest that she is committed to ensuring that EMSL perform – both in science and in service – at the highest level possible. The commitment on the part of Dr. Leonard Peters, PNNL Director, to keep her in this position for a minimum of five years is a very positive step that will provide a much-needed continuity in the management of EMSL. Dr. Campbell is faced with significant challenges, as she inherits a legacy of administrative issues that need immediate attention to promote EMSL's future success. In particular, the relative inexperience of the facility technical leads/managers and the potential conflict with internal priorities of PNNL as a whole will need to be addressed. The present situation, involving her recent promotion to this position, should be looked upon as an excellent opportunity to make needed changes.

Critical issues that need to be addressed include the roles of the EMSL User Advisory Committee and the EMSL Scientific Advisory Committee. These roles must be clearly articulated, and they must be distinct from each other. The User Advisory Committee should serve as the conduit for dialogue between the broad user community and the EMSL administration, and its membership should be selected by the users, not by the EMSL director. User satisfaction, user requests, user advice, and user suggestions should all be areas for discussion by this committee. The Scientific Advisory Committee should be responsible for advice about the broad vision and broad future of EMSL, including prioritization of scientific foci and their integration with national needs. This committee should be visionary and help EMSL anticipate the scientific capabilities that it will need to acquire in the longer-term future, not in the short-term.

There appears to be a very strong need for a well-posed and well-documented "Strategic Plan." This document must be more than a planning document, as it must serve as the primary tool and guide for planning, operations, external communications, and means to acquire general guidance (e.g., from ERSD, from the advisory committees). The Strategic Plan should set and articulate the vision for the EMSL, it should contain specific goals for attaining this vision, and it should provide the rationale for these goals. These goals should be measurable. It should define the organizational structure and institutional pathways for attaining the specific goals, including individual responsibilities. It should provide a funding analysis, including a cash-flow tree indicating the flow of financial resources associated with each goal.

The presence of non-DOE funding for EMSL, when appropriately chosen and coordinated to ensure alignment with DOE interests, is a potential means of leveraging DOE operations funding and thus can be a very valuable resource for EMSL. At this time, the acquisition of such resources appears to be haphazard and primarily through "take it or leave it" opportunities. Clearly, unanticipated opportunities for funding do arise, and advantage should be taken of these when possible. In addition, however, a more systematic procedure for developing such funding sources should be explored.

EMSL recently developed two initiatives that are, in principle, guided by the desire to engage multiple investigators in research activities addressing complex problems that will only be solved by multi-disciplinary interactions. These are the Grand Challenges and the Collaborative Access Teams (CATs). The BERAC subcommittee does not encourage the continuation of the Grand Challenges and CATs, as they are currently constituted. The BERAC subcommittee does,

however, encourage the development of, and focus on, research themes. Cross-disciplinary research, multiple technique approaches, and multiple-thread investigations (attacking a problem from multiple directions) should all be encouraged.

With regard to the question of expansion of EMSL capabilities, potential instrumentation upgrades and acquisitions specific to a given facility are discussed in the context of that facility. A general consideration that must be addressed is a growing recognition of the value that radiological capabilities would bring to the overall breadth of environmental studies that could be conducted within EMSL. The location of such capabilities – whether they should be resident in the existing EMSL facility, should be in an annex to the EMSL building, or should be in other PNNL buildings – is not an issue that was discussed to any significant degree by the BERAC subcommittee, as the myriad issues associated with developing this capability are beyond the scope of the charge. On a purely scientific basis, the subcommittee does encourage discussion between BER, PNNL, and EMSL about this possibility. One specific issue related to radiological capabilities is that phosphorus-32 is an important and ubiquitous tracer in cell biology, and its use should be allowed within EMSL. The subcommittee was led to believe that phosphorus-32 is precluded from studies in the EMSL because of an inadvertent error in the permitting of the building; it is strongly urged that this be corrected as soon as possible.

One additional observation is critical. Many of the issues raised by the 2001 ERSD-convened review panel were again identified as concerns by the BERAC subcommittee. In particular, these include inadequacies in the function of the User Advisory Committee; the need to enhance efforts to identify, promote, and increase the scientific impact of EMSL user research and to market EMSL capabilities; the need for focused strategic planning; the need for EMSL and PNNL leadership to work with BER to find the resources to keep instrumentation/capabilities at state-of-the-art; and the need to work with BER and the Office of Science to strengthen the DOE relevance of research performed at EMSL. It is hoped that the findings of the 2005 BERAC subcommittee review will be given serious consideration by all parties involved.

With regard to the specific questions posed by Dr. Orbach, the answers that follow are summary observations made as a result of the review of the six EMSL facilities.

Does the relationship and management structure among EMSL, PNNL and ERSD foster the highest quality of science at EMSL?

Although the review committee is encouraged by the apparently strengthened interactions between the EMSL director and the PNNL director, the highest quality of science will not be achieved until there is agreement between EMSL, PNNL, and ERSD as to the mission of EMSL. ERSD should play a more active role than is currently the case in helping to ensure that EMSL satisfies its mission. Further, it appears that a major issue that needs resolution is the relative amount of activity within EMSL that is associated with PNNL-initiated research. A properly constituted and active Scientific Advisory Committee may provide invaluable assistance in prioritizing medium- and long-term objectives that address both PNNL research needs and those of the broader community.

Is the science conducted at EMSL cutting edge? If so, is it appropriate for a BER-supported user facility?

In general, the science conducted in the EMSL is of very high quality, and a significant amount is, indeed, cutting edge. It is appropriate for BER to support this Laboratory that is a national resource.

Is EMSL appropriately structured to support a full range of DOE and national science research priorities?

No single laboratory can support a "full range" of DOE and national science research priorities. However, EMSL does support a significant range of research priorities. Greater impact might be achieved if more of the projects conducted within the EMSL took advantage of capabilities in more than one of the six facilities.

Is the user model for allocating resources for all EMSL facilities appropriate? Does EMSL attract the best mix of users?

There is no consistent model for attracting users to EMSL or for allocating time within a given EMSL facility. It is strongly recommended that each facility develop and implement a transparent process for soliciting and reviewing proposals for the use of that facility, and there should be consistencies across the six facilities. There should be clear criteria for assessing scientific merit, alignment with EMSL resources, and relationship to national research needs. Further, proposals that request time on instrumentation in more than one facility should be encouraged. In those facilities for which there is not currently an open, transparent solicitation, users are essentially solicited by word of mouth. It is reasonable to assume that many highly qualified scientists who could take advantage of EMSL are not being reached by this process, and, hence, the best mix of users is not being attracted to this important resource.

Could changes be made to increase the impact of EMSL on DOE science goals?

The first change that must be made is that there must be agreement between EMSL, PNNL, and ERSD as to the mission of EMSL. A strategic plan should be established to support that vision, and clear goals appropriate to that vision must be defined and monitored for each of the facilities. There must be a transparent process for soliciting and reviewing proposals at all facilities, and cross-cutting research must be encouraged. The addition of radiological capabilities would also strengthen the impact on some of DOE's environmental goals.

Given a flat budget for ERSD, what priority should EMSL have within the Division's portfolio?

The EMSL is a unique national resource, and it should have a very high priority within the Division's portfolio. Whether it is through ERSD (or other BER funds), or through cooperation with other funding agencies, the operating budget for EMSL must be increased. In addition to the issue of refreshing capital equipment, there simply is not sufficient fiscal support for the technical staff members who provide direct, hands-on support for the users of many of the very

sophisticated pieces of equipment. Thus, there is research capacity within EMSL that has lain idle.

Does the EMSL have a well-defined plan to refresh capital equipment, and is it appropriate? What short- and long-term strategies should be considered in this context? Does EMSL appropriately manage the acquisition, use and retirement of instruments?

While EMSL has taken steps, some of which are quite creative, to refresh capital equipment in the short-term, there is no long-term plan (except in the case of the supercomputer facility). This must be achieved in collaboration with ERSD and, possibly, in collaboration with other funding agencies. Refreshment of capital equipment must be prioritized, and a reconstituted Scientific Advisory Committee should become active in the prioritization process. Prioritization may result in the decommissioning of some equipment in order to maintain the quality of the most creative programs and those most critical to DOE and other national needs.

How does EMSL manage general user access to equipment purchased with non-ERSD funds? How does this impact EMSL operation as an ERSD-supported user facility?

A significant amount of equipment housed within EMSL was purchased with funds other than those provided by ERSD through the operations budget. In most cases, EMSL users are granted at least limited access to this equipment, and, hence, there can be benefits to the overall operation. It should be noted, however, that both the acquisition and the use of such equipment is on an *ad hoc* basis, and it is strongly recommended that a plan be established for acquiring and managing such equipment, including processes for making such equipment available to the broad user community.

TABLE OF ACRONYMS

BER	Office of Biological and Environmental Research
BERAC	Biological and Environmental Research Advisory Committee
BSL-3	Biosafety Level Three
CAT	Collaborative Access Team
CISD	Computing and Information Sciences Division
CPCSF	Chemistry and Physics of Complex Systems Facility
DOE	U.S. Department of Energy
EMSL	Environmental Molecular Sciences Laboratory
EPR	Electron Paramagnetic Resonance
ERSD	Environmental Remediation Sciences Division
ESBGCF	Environmental Spectroscopy and Biogeochemistry Facility
FY	Fiscal Year
HFMRF	High Field Magnetic Resonance Facility
HPMSF	High Performance Mass Spectrometry Facility
IDL	Instrument Development Laboratory
INSF	Interfacial and Nanoscale Science Facility
MHz	Megahertz
MSCF	Molecular Science Computing Facility
NMR	Nuclear Magnetic Resonance
PNNL	Pacific Northwest National Laboratory
TEM	Transmission Electron Microscope/Microscopy
WSU	Washington State University
XPS	X-ray Photo-Electron Spectroscopy

REPORT
BY A SUBCOMMITTEE OF THE
BIOLOGICAL AND ENVIRONMENTAL RESEARCH ADVISORY COMMITTEE
CHARGED WITH PROVIDING ADVICE ON THE
MISSION, OPERATION, AND FUTURE PLANS OF THE
ENVIRONMENTAL MOLECULAR SCIENCES LABORATORY

Introduction

In November 2004, Dr. Raymond Orbach, Director of the Office of Science, U.S. Department of Energy (DOE), asked the Biological and Environmental Research Advisory Committee (BERAC) to provide advice on the mission, operation, and future plans of the Environmental Molecular Sciences Laboratory (EMSL) that is located at the Pacific Northwest National Laboratory (PNNL) in Richland, Washington. The EMSL operations budget is provided by the Environmental Remediation Sciences Division (ERSD) of the Office of Biological and Environmental Research (BER), one of the program offices in the Office of Science. The research conducted within EMSL is supported by at least three of the BER divisions, by other parts of DOE, and by other federal agencies. The full charge letter is found in Appendix A. The specific questions asked in Dr. Orbach's charge letter are:

- Does the relationship and management structure among EMSL, PNNL and ERSD foster the highest quality of science at EMSL?
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- How does EMSL manage general user access to equipment purchased with non-ERSD funds? How does this impact EMSL operation as an ERSD-supported user facility?

An *ad hoc* subcommittee, chaired by a member of BERAC, was established to respond to this charge. The full membership of that subcommittee is found in Appendix B.

In reviewing the charge letter and the questions contained therein, BERAC felt that some of the questions contained implicit issues related to administrative and fiscal policies and processes that are outside of the scope of expertise that BERAC or the *ad hoc* subcommittee could provide. In response to this concern, Dr. Aristides Patrinos, Associate Director of the Office of Biological and Environmental Research, asked that the Office of Project Assessment within the Office of Science conduct an administrative review of EMSL. The charge letter from Dr. Patrinos is found

in Appendix C. Ultimately, the decision was made that the two reviews, one by BERAC and one by the Office of Project Assessment, would be conducted simultaneously, with several joint plenary and executive sessions being held.

The BERAC subcommittee and the committee convened by the Office of Project Assessment met on May 17 – 19, 2005, at EMSL. The interwoven agenda for these simultaneously held meetings is found in Appendix D. This BERAC report represents the deliberations conducted during the BERAC subcommittee meeting and subsequent document exchange.

Background

EMSL opened its doors in October 1997, with its operating dollars and associated capital equipment funds coming from BER/ERSD. In order to stimulate the initiation of research using EMSL capabilities, 50 percent of the time available on experimental resources housed within EMSL was allocated to scientists located within the EMSL organization, and the remainder was allocated to visiting, externally-based scientists. The one exception to this 50 percent split of time allocation was the high-performance computer; all time on this machine was allocated, and continues to be allocated, based on peer review of applications for high performance computing.

In 2001, ERSD conducted a peer review of the entire EMSL. Following this review, PNNL management made the decision to move those EMSL scientists who did not charge a significant fraction of their time to user support out of the formal EMSL reporting structure and into the Fundamental Science Directorate of PNNL. In Fiscal Year (FY) 2004, BER directed PNNL/EMSL to terminate the 50/50 allocation model and to use the operating dollars in support of the EMSL role as a national scientific user facility. Those scientists who were reassigned to the Fundamental Science Directorate maintained their research laboratories and offices within EMSL. Currently, the bulk of the operating dollars provided by ERSD to EMSL is used to support user operations for EMSL as a national scientific user facility. The building infrastructure supported by the operating dollars supports both the user facility and those PNNL scientists who, while not reporting to the EMSL director, conduct their research within EMSL. These PNNL scientists may or may not be designated as formal users of the national facility.

Two other background issues are of particular importance to the conclusions drawn by the BERAC subcommittee. First, since EMSL opened, there have been three directors of the Pacific Northwest National Laboratory and four directors of EMSL itself. Hence, there has not been a consistent statement of the EMSL mission, nor as there been continuity in developing robust processes for the management of EMSL. Second, during its full seven years of operation, the EMSL operations budget has increased from approximately $29M to approximately $40M. This increase is predominately due to additional dedicated funds in support of the EMSL supercomputer. Excluding the fixed costs associated with the supercomputer, the remaining budget has remained relatively constant. As a result of inflation and increased space and labor costs, the "buying power" of the remaining operations budget is less than 84 percent of what it was in FY 1998.

General Observations

Although the charge to which the BERAC subcommittee responded was focused on scientific issues, it became very clear that the scientific effort and scientific staff are strongly affected by administrative issues within the EMSL. Consequently, it is appropriate in this report to comment on observations and recommendations related to administrative and management issues not explicitly within the scope of the charge.

First and foremost, it does not appear that BER leadership, EMSL leadership, and PNNL leadership share a coherent vision as to what the EMSL mission is. There are two aspects to this. The first is whether or not the primary, if not sole, responsibility of EMSL is to serve as a national scientific user facility. ***In the context of this report, there is the explicit assumption that the EMSL's primary function is that of a national scientific user facility. Should there be concurrence that this is not the primary Laboratory function, then some of the conclusions in this report may have to be revisited.*** The second aspect of the necessary future articulation of the EMSL mission is the extent to which research conducted within the EMSL must have an obvious environmental connection. Presaging a conclusion discussed later in this report, EMSL is a unique national resource. Certainly, if a critical and pressing national need having nothing to do with "the environment" emerged, and this need could be uniquely met using EMSL facilities, not allowing EMSL to respond would be detrimental to the Nation's interests. Acknowledging that it is the management of BER, EMSL, and PNNL that must together develop a coherent mission statement for EMSL, this subcommittee suggests the following as a starting point for the dialogue:

> *. . . EMSL is a national user facility employing cutting-edge experimental and computational capabilities to support the needs of DOE and the nation, with a primary focus on the broad area of environmental molecular science.*

If EMSL is, indeed, to be a national scientific user facility, there need to be agreed-upon guidelines as to how much time in each facility is allocated to outside users. However, before such guidelines can be established, a robust definition of "user" must be developed. As part of the discussions about such a definition, there needs to be agreement as to whether or not PNNL (non-EMSL) scientists are outside users and whether their usage of the facilities is counted in the "outside user allocation."

Although it is too early in her tenure to assess the impact that the newly appointed EMSL Director, Dr. Allison Campbell, will have on the overall performance of the Laboratory, interactions with the subcommittee during the review meetings suggest that she is committed to ensuring that EMSL perform – both in science and in service – at the highest level possible. The commitment on the part of Dr. Leonard Peters, PNNL Director, to keep her in this position for a minimum of five years is a very positive step that will provide a much-needed continuity in the management of EMSL. Dr. Campbell is faced with significant challenges, as she inherits a legacy of administrative issues that need immediate attention if EMSL is to maintain its standing as a unique national scientific user facility. In particular, the relative inexperience of the facility technical leads/managers and the potential for conflict with internal priorities of PNNL as a whole will need to be addressed. The present situation, with Dr. Campbell's recent promotion to the directorship, should be looked upon as an excellent opportunity to address these challenges.

Critical issues that need to be addressed include the roles of the EMSL User Advisory Committee and the EMSL Scientific Advisory Committee. These roles must be clearly articulated, and they must be distinct from each other. The User Advisory Committee should serve as the conduit for dialogue between the broad user community and the EMSL administration, and its membership should be selected by the users, not by the EMSL director. Because of the breadth of users, it may be appropriate to have subcommittees of the User Advisory Committee, each of which focuses on a specific suite of capabilities (that may or may not be coincident with the six EMSL facilities), with a parent committee that deals with issues that span the entire EMSL. User satisfaction, user requests, user advice, and user suggestions should all be areas for discussion by this committee. To date, there has been a very low response by users to requests for completion of user satisfaction surveys. As a team, the User Advisory Committee and EMSL management must be creative in developing a successful survey mechanism. User survey responses are critical in establishing a record as to the performance of EMSL as a national user facility. If robust, survey data need to be taken seriously, should be used as guidance for the improvement of operations and, when appropriate and with proper caveats, should be given some consideration during staff performance evaluations.

The Scientific Advisory Committee, with members recognized as leaders in their respective fields of science and engineering, should be responsible for advice about the broad vision and broad future of EMSL, including prioritization of scientific foci in light of national needs. This committee should be visionary and help EMSL anticipate the scientific capabilities that it will need to acquire in the longer-term future, not in the short-term. It should serve as a sounding board for the strategic plan that EMSL must create to define its path forward.

If these committees are to be meaningful, it is critical that there be frequent and substantive communication between the committees and the EMSL director. At a minimum, the parties should communicate at least quarterly by electronic correspondence, and the committees should meet, at EMSL, at least once per year. If necessary to address pressing issues, additional conference calls or written correspondence may be necessary. Further, term limits should be set for members of both committees to ensure that fresh ideas are continuously incorporated into committee deliberations.

There is some concern that administrative actions or processes have been initiated before they were completely developed or explicitly defined. The two advisory committees, as currently structured, are examples of this, as are the Collaborative Access Teams that are discussed later in this document. *Ad hoc* internal committees are other examples. Implementing functions prematurely should be strongly discouraged, as they impact operational efficiency, staff morale, and the EMSL external image.

The presence of non-DOE funding for EMSL, when appropriately chosen and coordinated to ensure alignment with DOE interests, is a potential means of leveraging DOE operations funding and thus can be a very valuable resource for EMSL. At this time, the acquisition of such resources appears to be haphazard and primarily through “take it or leave it” opportunities. Clearly, unanticipated opportunities for funding do arise, and advantage should be taken of these when possible. In addition, however, a more systematic procedure for developing such funding sources should be explored.

If there is a decision by BER, in consultation with EMSL, that it would be appropriate and advantageous to foster work supported by other federal agencies at EMSL, then BER must take the lead in developing an "Interagency Coordination Plan" that is well-researched, definitive, and clearly articulated. In particular, the negotiations with the other agencies must be the responsibility of BER. Given that each agency has a different mode of doing business, it is important that explicit planning be performed in advance of implementation so that EMSL does not become embroiled in interagency disagreement. This Interagency Coordination Plan should ensure (i) that the projects supported by other agencies sustain and enhance the EMSL mission, and thus, by inference, are in keeping with BER missions; (ii) that BER is appropriately integrated into the selection and administration processes associated with these projects or is, at a minimum, in agreement with the procedures to be used; (iii) that the selection processes by EMSL and the external agency are conducted in a consistent and seamless manner that encourages participation by the most highly qualified investigators; and (iv) that there is optimal allocation of EMSL resources which necessarily requires efficient scheduling and access. If such a plan is, indeed, developed, it is critical that it impose minimal additional constraints and complexities on EMSL administration, although it should be appropriately linked to the EMSL Strategic Plan (*vide infra*).

There appears to be a very strong need for a well-posed "Strategic Plan" that has both substance and credibility. This must be a living document, updated periodically as part of the cyclical EMSL planning and evaluation processes. It must be more than a planning document, as it must serve as the primary tool and guide for planning, operations, external communications, and interactions with advisory bodies (e.g., ERSD, the advisory committees). The Strategic Plan should set and articulate the vision for EMSL, it should contain specific goals for attaining this vision, and it should provide the rationale for these goals. These goals should be measurable. It should define the organizational structure and institutional pathways for attaining the specific goals, including individual responsibilities. It should provide a funding analysis, including a cash-flow tree indicating the flow of financial resources associated with each goal. Some of these elements may be included, to a greater or lesser extent, in the EMSL Operations Manual, and the Operations Manual should be readily available to anyone who reads the Strategic Plan.

The Strategic Plan must communicate the vision, the goals, and the working structure of EMSL to a variety of concerned entities, including:

- BER, BERAC, and the senior leadership of the Office of Science. The principal client is a potential skeptic that needs to be convinced that EMSL is working in alignment with the best interests of both EMSL and BER.
- EMSL and PNNL staff. This is particularly important for coordination purposes, for communicating accountability, and for making sure that everyone is working with a shared vision.
- The external community, especially potential facility users. This group also contains skeptics, who must be convinced that EMSL is more than a self-serving organization. This group needs to have definitive guidance on the specific policies, mechanisms, and pathways for gaining access to EMSL facilities.
- EMSL review committees, which also contain skeptics.

EMSL has recently developed two initiatives that are, in principle, guided by the desire to engage multiple investigators in research activities addressing complex problems that will only be solved by multi-disciplinary interactions. The Grand Challenges are defined as "complex, large-scale scientific and engineering problems with broad scientific and environmental or economic impacts whose solution can be advanced by applying high-performance scientific techniques and resources. EMSL Grand Challenges differ from typical proposals in that they are multi-institution (from universities, other laboratories, and industry), multi-group teams that use multiple facilities within EMSL." The Collaborative Access Teams (CATs) "are teams of scientists from PNNL and industry, universities, and other laboratories who will work together using EMSL's facilities and equipment to rigorously focus on one area of high-impact research, such as oxide chemistry or structural biology. Results of this focused team concept will help solve larger scientific problems, while bringing new science capability to EMSL and providing opportunities for expanding EMSL's user base."

The BERAC subcommittee does not encourage the continuation of the Grand Challenges and CATs, as they are currently constituted. As interpreted by the subcommittee, the primary driver for the CATs is the desire to maintain the access to EMSL facilities that many PNNL staff members had before they were formally removed from the EMSL reporting structure. This is simply not appropriate. The primary motivation for the establishment of the Grand Challenges does appear to be the desire to ensure that EMSL resources are used to address high profile, complex scientific questions, and it is the subcommittee's understanding that these were encouraged by BER. However, the implementation of the Grand Challenges raises several concerns. It appears that the principal investigators drive the science and control the budget. This has significant potential for sacrificing the freedom and creativity of junior scientists and for inhibiting the development and application of critical, independent thought. The funding paradigm for the Grand Challenges raises several issues. PNNL is contributing internal research and development dollars towards these, which again raises the question as to what should be the relationship between PNNL and EMSL. Further, the period of time for which funding is available is too short to allow reasonable progress to be made in addressing the questions asked in defining the two existing Grand Challenges. Additional concerns are expressed elsewhere in this document.

The BERAC subcommittee does, however, encourage the development of, and focus on, research themes. Cross-disciplinary research, multiple technique approaches, and multiple-thread investigations (attacking a problem from multiple directions) should all be encouraged. As an example of an approach that might be considered, the BERAC subcommittee offers the following suggestion. Please note, however, that this is meant only to be illustrative of a type of approach that will foster focused collaborations without imposing top-down management of scientific ideas.

> Identify thematic questions by soliciting input from a reconstituted Science Advisory Committee. With an awareness of thematic research calls from various funding agencies that support the environmentally-focused research programs of some of EMSL's external users, issue a solicitation for use of EMSL resources that bring EMSL strengths to these important research areas for which individual, non-integrated projects have been funded. As part of the solicitation of proposals, (i) encourage

the use of multiple facilities in EMSL, including the concept of a single proposal being submitted by a group of users; (ii) request a separate section that indicates what complementary research activity would potentially catapult the value of the proposed studies to a greater realm; if such complementary research is in the pool of applications received, EMSL should support both projects. ERSD should provide "glue" funds to integrate the projects.

With regard to the question of expansion of EMSL capabilities, potential instrumentation upgrades and acquisitions specific to a given facility are discussed in the context of that facility. A general consideration that must be addressed is a growing recognition of the value that radiological capabilities would bring to the overall breadth of environmental studies that could be conducted within EMSL. The location of such capabilities – whether they should be resident in the existing EMSL facility, should be in an annex to the EMSL building, or should be in other PNNL buildings – is not an issue that was discussed to any significant degree by the BERAC subcommittee, as the myriad issues associated with developing these capabilities are beyond the scope of the charge. On a purely scientific basis, the subcommittee does encourage discussion between BER, PNNL, and EMSL about this possibility. One specific issue related to radiological capabilities is that phosphorus-32 is an important and ubiquitous tracer in cell biology, and its use should be allowed within EMSL. The subcommittee was led to believe that phosphorus-32 is precluded from studies in the EMSL because of an inadvertent error in the permitting of the building; it is strongly urged that this be corrected as soon as possible.

One additional observation is critical. Many of the issues raised by the 2001 ERSD-convened review panel were again identified as concerns by the BERAC subcommittee. In particular, these include inadequacies in the function of the User Advisory Committee; the need to enhance efforts to identify, promote, and increase the scientific impact of EMSL user research and to market EMSL capabilities; the need for focused strategic planning; the need for EMSL and PNNL leadership to work with BER to find the resources to keep instrumentation/capabilities at state-of-the-art; and the need to work with BER and the Office of Science to strengthen the DOE relevance of research performed at EMSL. It is hoped that the findings of the 2005 BERAC subcommittee review will be given serious consideration by all parties involved.

REVIEW OF THE SIX EMSL FACILITIES

As part of the review processes, each of the twelve scientific experts on the BERAC subcommittee reviewed one of the six EMSL facilities. What follows are the general observations of the two-member teams that reviewed each facility and facility-specific answers to the questions in the charge letter. In order to preserve the full sense of the reviewers' comments, the method of presentation for the discussion of each of the six facilities is not uniform.

The Chemistry and Physics of Complex Systems Facility

In general, the reviewers that focused specifically on the Chemistry and Physics of Complex Systems Facility (CPCSF) were highly impressed with the capability, the scientific productivity, the enthusiasm, and the dedication of the scientific staff. Several individual observations made during the review process are listed immediately below:

- In collaboration with external users, the research being conducted by CPCSF staff scientists is high quality and cutting-edge. It ranges from the study of fundamental properties of water, surfaces, and particles to applied research that directly addresses the needs of DOE.
- In FY 2005, the EMSL operating budget provides only 21 percent of the overall budget for CPCSF. The rest of the budget is provided from non-EMSL sources, such as research grants awarded to CPCSF scientific staff and to external users. Based on information provided to the reviewers, it appears that the majority of the technical staff members required to support the 12 different laboratories of CPCSF are supported by the EMSL operating budget at less than 55 percent full time equivalence.
- CPCSF provides a broad spectrum of instrumentation that offers many unique capabilities for studying questions related to the presumed environmental mission of EMSL. Many of these capabilities have been developed at EMSL and are not commercially available.
- Due to the uniqueness of many of the instruments developed at EMSL, the use of instrumentation at EMSL is highly dependent on participation and availability of the EMSL staff scientists responsible for that instrumentation.
- Not all of the equipment in the 12 CPCSF laboratories is fully utilized; in many cases, this is because there are not sufficient EMSL operations funds to support staff capable of training and supervising users. There does not appear to be a program in place to train user groups for long-term use on the EMSL instrumentation; this necessarily makes it difficult to make full use of the instrumentation.
- There does not appear to be a strong incentive to engage a broad spectrum of users in many of the capabilities in CPCSF.
- Although a few of the projects centered in CPCSF incorporate capabilities from other facilities within the EMSL, the majority of the projects performed within CPCSF involve only a single type of instrumentation. CPCSF does not issue a broad solicitation for projects that use its capabilities, and it may be that most of the users of the facility are not aware of the full array of analytical capabilities within the EMSL.

- It is not apparent that there is a procedure for prioritizing equipment purchases that is geared toward programmatic goals of EMSL.

Recommendations generated based on these observations are summarized below:

- Mechanisms should be established that provide training opportunities for users that will allow more comprehensive use of the equipment and that will promote long-term collaborations between knowledgeable user groups.
- CPCSF should issue annual calls for user proposals that are consistent with the EMSL mission, and the review of proposals should be conducted by an external peer review process.
- One of the review criteria for proposals should include the integration of equipment available at EMSL.
- Once EMSL goals are established, equipment needs should be prioritized in a manner consistent with those goals.

The two Grand Challenge projects presented at the review reflect high quality and innovative science, and EMSL and the associated scientists should be commended for these efforts. These are basically pilot projects, however, in the sense that similar ventures cannot be sustained in the future unless several elements are modified. First, these two projects are being conducted using, primarily, a combination of EMSL operating funds and Laboratory (PNNL) Directed Research and Development funds; this is not a viable long-term financial model. If they are forthcoming, future Grand Challenge efforts should be based on a more extensive funding paradigm that encourages greater participation by external scientists, open calls for participation, and larger funding amounts. Issuing a BER solicitation in conjunction with coordinated calls by external agencies as described above is a possible approach to be considered.

Second, the two Grand Challenge examples described during the BERAC review were, or will be, conducted over relatively short time spans. Any future Grand Challenge activity should be for a more prolonged period, on the order of a minimum of five years. Finally, the presented efforts were "single-thread" projects in the sense that they dealt with essentially single-pathway processes. Many potential future Grand Challenge endeavors can be expected to be multi-threaded. For example, a Grand Challenge to produce a comprehensive working model of heterogeneous tropospheric chemistry would necessitate examination of multiple reaction pathways and mechanisms, many of which are highly complex and would require high-level input from a diversity of scientists. EMSL should recognize and accommodate this feature in any future Grand Challenge that may be forthcoming.

With regard to the specific questions posed by Dr. Orbach, the answers that follow are focused on observations by the reviewers of the CPCS Facility.

Does the relationship and management structure among EMSL, PNNL, and ERSD foster the highest quality of science at EMSL?

There appears to be excellent collaboration between EMSL and PNNL for developing projects that are consistent with DOE goals. Much of the funding for EMSL staff is provided by these

collaborations. However, it is not clear that there is a relationship with ERSD or an advisory board that can provide the link between ERSD and EMSL.

The choice of Dr. Campbell as the EMSL Director and PNNL's commitment to keep her in that position for five years reflect high level attention to EMSL. This is emphasized by the PNNL director's decision to elevate EMSL to a level reporting directly to him. During the BERAC subcommittee review, Dr. Michael Kuperberg, Acting Director of ERSD, stated that ERSD intends to play a more prominent role in articulating goals, investment philosophy, and research directions for the EMSL. In view of the large ERSD investment in EMSL, this is totally appropriate. This committee strongly supports this action.

Is the science conducted at EMSL cutting edge? If so, is it appropriate for a BER supported user facility?

Based on the review of the science conducted in CPCSF, there is no question that EMSL is conducting cutting-edge science that is appropriate for a BER user facility. The scientific impact of this work is evident in the large number and high quality of resulting publications. In FY 2003 and FY 2004, the group reported 153 publications and 197 presentations, including two articles in *Science*. From 2000 to 2004, the research has been featured on nine journal covers.

Is EMSL appropriately structured to support a full range of DOE and national science research priorities?

The phrase "full range" implies a great deal, and if interpreted in its largest sense the answer is no. But that is not a reasonable expectation. EMSL is not presently configured, for example, to conduct radionuclide or biological-hazard research. EMSL is, however, structured to support a very wide range of research addressing DOE and national priorities. In particular, the facilities in CPCSF are excellent, and, in many cases, they are unmatched in their ability to address DOE and national science research priorities.

Is the user model for allocating resources for all EMSL facilities appropriate? Does EMSL attract the best mix of users?

The user model is not well-defined, and it needs enhanced and clarified definition. In CPCSF, the current mix of users is impressive, but it could be further enhanced by interagency collaboration, as described elsewhere in this document.

There did not appear to be an open or transparent approach for soliciting and reviewing user proposals, nor are the user proposals externally peer-reviewed. The review process typically involves solicitation of a user by the technical staff associated with a CPCSF capability, followed by submission of the user form. The review is conducted by the technical staff member associated with the capability and the technical lead for CPCSF. There is no history of a procedure to develop Calls for Proposals which could provide a better mix of users to the facility. Based on the documentation provided in the "ERS Resource Usage Report" (the software that tracks use of major pieces of equipment), there is very little external use of many of the instruments. Some of the instrumentation is utilized in large part by PNNL staff or Collaborative Access Teams.

Could changes be made to increase the impact of EMSL on DOE science goals?

Yes, significant changes are required to provide a set of coherent research themes that more clearly address DOE science goals. The research themes should be formulated in collaboration with BER and a Scientific Advisory Committee that includes prominent scientists and engineers from the community. These research themes should influence the solicitation for, and selection of, projects to be conducted, and they should also influence equipment upgrades and purchases.

Given a flat budget for ERSD, what priority should EMSL have within the Division's portfolio?

EMSL should have a high priority within the Division's portfolio. EMSL constitutes a major BER investment, and this investment should be protected and sustained, given the noted scientific productivity of the laboratory. Given the quality of current work and the potential for the future, EMSL should be viewed as a critical resource from which DOE as a whole, and BER and ERSD in specific, can profit.

Within CPCSF itself, a number of instruments are not adequately staffed to allow the level of training and supervision required for full usage of the equipment. Much of the instrumentation in CPCSF has been specially designed and fabricated to meet the unique sample analysis requirements associated with the goals of the research being conducted. This presents a unique challenge to the staff for providing a mechanism for users to develop and maintain competency on the instrumentation. There is a significant need for funding to be directed toward providing the technical staff necessary to obtain the true vision of EMSL as a user facility.

Does EMSL have a well defined plan to refresh capital equipment, and is it appropriate? What short- and long-term strategies should be considered in this context? Does EMSL appropriately manage the acquisition, use and retirement of instruments?

The EMSL management has been fairly aggressive in trying to manage resources to enable capital equipment to be refreshed. However, the $2M annual capital equipment allocation is too small, and short-term strategies, including applying operating funds to augment capital equipment acquisition, may be necessary. Longer-term strategies in the projected funding environment may require that upgrades and replacement be focused on a limited ensemble of the EMSL equipment, rather than on the full range of current capability. This, of course, would be painful and would decrease both the broad utility of the EMSL and the quantity of high quality scientific research being conducted thereat. If, upon review of this report and other appropriate discussions, it is determined that EMSL should, indeed, be of high priority within the ERSD portfolio, then additional funding may preclude draconian decisions. The potential to acquire necessary funding must be borne in mind when considering the possible expansion of EMSL capabilities to new areas, such as radionuclide and biohazard research.

Within CPCSF, there appears to be a significant and continuous effort to enhance the capabilities in order to provide facilities that remain at the cutting edge of molecular science. A significant portion of the funding for new equipment purchased within CPCSF comes from non-EMSL sources. In many cases, these external funds are used to leverage EMSL funds. This is an

adequate short-term strategy. However, the long-term strategies for equipment needs should be based on the long-term goals and priorities established for EMSL and on a thorough, and ongoing, analysis of data on the actual usage of different instrumentation.

How does EMSL manage general user access to equipment purchased with non-ERSD needs? How does this impact EMSL operation as an ERSD-supported user facility?

The CPCSF reviewers felt that there is a general belief that access to any equipment is available to all users. However, it was not clear that the process for users to obtain access to the instruments is fair and inclusive for all potential users, nor is it necessarily based on the best scientific use of the instrumentation. External user access to equipment is one of the major concerns facing the CPCSF. Many of the instruments require a significant amount of technical support, and this support places an extremely large burden on the technical consultants associated with each instrument. Again, based on the documentation provided in the "ERS Resource Usage Report", there is very little external use of many of the instruments in part because of the lack of funds allocated to EMSL support of the technical consultant.

Much of the equipment in the metal CPCS cluster facility was purchased by Washington State University (WSU), and most of the resident researchers are postdoctoral fellows in the research group of Prof. Lai-Sheng Wang, a WSU faculty member who has a joint appointment at PNNL. The primary reason that the equipment is housed within EMSL, rather than on the WSU campus in Pullman, is that the Tri-Cities Graduate Center is located in Richland and is operated by WSU. This metal cluster facility is a joint endeavor between WSU and PNNL. WSU profits from this arrangement because, in addition to enhancing the scientific productivity of the local Graduate Center, it is immersed in the EMSL environment with its array of additional analytical equipment and scientific expertise. PNNL views its contribution to this facility as part of its university outreach activities. PNNL and EMSL profit from this arrangement because of the facility's scientific productivity, the availability of the associated analytical equipment, and the opportunity for close interaction with the WSU scientific staff. This laboratory is highly productive in performing high-quality research which is generally supportive of DOE's mission. It definitely is an asset to EMSL and to ERSD.

There are also concerns that the potential emphasis on CATs and Grand Challenges is an inappropriate diversion of funds from EMSL operations.

The High Performance Mass Spectrometry Facility

As appears to be the case with the other facilities within the EMSL, the quality of the scientific research conducted within the High Performance Mass Spectrometry Facility (HPMSF) is quite high. Review of this facility illuminated some concerns that are unique to it, and others that are applicable to all of EMSL.

EMSL and its individual facilities need to do a better job of publicizing their existence and their accomplishments. It should be noted that the oral presentations made during the review meeting did not do an adequate job of highlighting the more exciting of the many scientific accomplishments. It is not clear that adequate thought has been given to the importance of "selling EMSL" by way of both publicizing capabilities and, of equal importance, formulating clear, compelling statements as to the importance of the scientific studies that have been, and can be, conducted at EMSL. Similarly, tours of the Laboratory, whether to reviewers such as the BERAC subcommittee, to potential users, or to political supporters must include the "wow! factor" in presentations.

While the HPMSF staff members make efforts to promote themselves to biologists and biochemists, more should still be done to develop a wider user base. Staff members should increase their efforts to present work at conferences that are frequented by the potential user base and to publish in journals read by a broad spectrum of scientists, in addition to publishing in mass spectrometry journals. It is likely that the staffs of other EMSL facilities also need to do a better job of promoting EMSL to their natural, potential user bases.

The reviewers were not impressed with the prototype Grand Challenges, which did not seem to be particularly "grand." It would be preferable to see EMSL focusing its support on individual investigators or on self-assembled groups of investigators. It is the bottom-up approach, not the top-down approach, that has driven scientific innovation. There is also a significant concern that the Grand Challenge approach discriminates against junior investigators. Interdisciplinary research should, however, be encouraged, such as by Calls for Proposals that span several EMSL facilities. In these times of limited budget, it is not clear that EMSL can afford to support Grand Challenges with operations funds. EMSL should only provide access to facilities and not provide direct research funding. EMSL should remain what it is designed to be – a user facility – and it should not try to in any way turn itself into a funding agency. The approximately $1,500,000 that EMSL might provide as a Grand Challenge is really only equivalent to a single proposal that might be supported by the National Institutes of Health; and this provides neither sufficient money nor sufficient time to address a "grand" scientific problem.

The Collaborative Access Teams (CATs) appear to be primarily a mechanism for insuring that PNNL researchers who reside in the EMSL building have access to the EMSL facilities. While CATs help to formalize the mechanism for PNNL researchers to use EMSL facilities, these researchers would still be using EMSL facilities even if CATs did not exist. Thus, the benefits of CATs are not clear.

Under the auspices of BER, a review of EMSL was conducted in 2001. Many of the major concerns from 2001 are still concerns in 2005. A major concern of the 2001 panel was the limited funds from DOE (only $2M per year) for instrument acquisitions and upgrades. Yet,

four years later, the DOE funding to EMSL remains essentially the same as it was in 2001. The 2001 panel also spoke of the need for better promotion of EMSL, for more Calls for Proposals and attraction of users, and for a better organized user committee. These are all still needed in 2005. The fact that many of the issues brought up in the 2001 review seem to have not been addressed by personnel at DOE and EMSL is worrisome. It is hoped that the findings of the 2005 review will be given more serious consideration.

There is currently little research that spans multiple EMSL facilities. The computational facility has few users who also work with the experimental facilities, and there are few users who work with more than one experimental facility. A major reason appears to be that such cross-disciplinary research is not encouraged by the current proposal process (where it exists). By way of illustration, if a user wants samples analyzed by both mass spectrometry and nuclear magnetic resonance, he/she must submit two proposals and hope that each is accepted by the appropriate facility. A mechanism for submitting and reviewing proposals that span two or more facilities would be beneficial to users and increase the amount of interdisciplinary research performed at EMSL.

Within a given facility, however, there does appear to be scientific integration across disciplines. A major strength of HPMSF is the scientific integration of personnel – mass spectrometrists, biologists, and informaticists – within the facility. The excellent Proteomics Research Information Storage and Management system of data analysis, which was developed by HPMSF personnel, is an example of the strength of this integration. There is also close collaboration with biologists at PNNL, who are among the HPMSF user base. Integration of experimental and computational techniques within the HPMSF appears to stem from collaborations with a PNNL scientist, Dr. Richard Smith, whose research group is housed within the EMSL but not as part of the EMSL user facility. Computational techniques that arise from collaboration with Dr. Smith do not appear to involve the EMSL high performance computational facility.

There is also strong interaction between HPMSF and EMSL's Instrument Development Laboratory (IDL). For example, an innovative mobile liquid chromatography system has been developed by HPMSF in conjunction with the IDL and is now used by other groups at EMSL. The presence of the IDL is a strong point that greatly assists in keeping EMSL's instrumentation at the cutting edge.

Sample turnaround times should be shortened by either increasing the instrumentation and/or staff of HPMSF (which may not be feasible in these times of flat budget) or prioritizing and becoming more selective about the samples accepted.

With regard to the specific questions posed by Dr. Orbach, the answers that follow are focused on observations made by the reviewers of HPMSF.

Does the relationship and management structure among EMSL, PNNL and ERSD foster the highest quality of science at EMSL?

The recent elevation of the EMSL director to the Associate Lab Director level in the PNNL hierarchy is a very positive step that should benefit EMSL by making its operation a higher priority at PNNL. The PNNL Director, Dr. Leonard Peters, appears to be supportive of EMSL;

this is a positive sign. BER personnel have exhibited a rather hands-off approach to EMSL management. While a hands-on approach may not be desirable, better communication of goals, results, and needs could only benefit EMSL, PNNL, and ERSD.

Although the reviewers were not privy to the reasons for the decision by EMSL and PNNL management to remove senior scientists from the EMSL management umbrella, the removal of some of the more senior scientific expertise from a facility such as HPMSF and the absence of such scientists in the operations and planning activities diminishes the overall effectiveness of EMSL. It is possible that there could be at least partial compensation for this if there were more significant roles for the Scientific Advisory Committee and the User Advisory Committee than is currently the case.

Is the science conducted at EMSL cutting edge? If so, is it appropriate for a BER-supported user facility?

HPMSF is at the very forefront of the field of proteomics – mass spectrometry research and development. HPMSF has amassed a very impressive array of instrumentation and supporting equipment/resources; indeed, this facility represents a one-of-a-kind national resource. It should also be noted that the research team was assembled from a group of very highly qualified research scientists having expertise in mass spectrometry, ion chemistry, analytical chemistry, and bioinformatics and computation, and it is important to note that several highly trained, qualified biologists/biochemists have been added to the team to facilitate research aimed at proteomics. In addition, over the past three – five years, the research activities have expanded to include collaborations with leading biologists, biochemists, and chemists from EMSL, PNNL, and academic, government, and industrial laboratories. The group has been highly innovative in terms of uniquely combining instrument development, research applications, and technology transfer within the framework of a user facility. This operational model has lead to advances in the field as well as provided to the EMSL user community research capabilities that are far in advance of commercialization of the hardware**.**

HPMSF plans to expand its capabilities through the addition of a 12-Tesla Ion Cyclotron Resonance instrument that will enable studies of post-translational modifications of proteins. While it does not appear that there is currently a user base driving this acquisition, it can be anticipated that the demand for such capabilities will be high in the not-too-distant future. These plans represent the continuing efforts of HPMSF to remain at the cutting edge.

While only a small fraction of the work conducted in HPMSF is directly relevant to environmental questions, the research performed therein addresses scientific issues that are important to other aspects of the DOE and BER missions and to other critical national scientific needs. Thus, the work performed in HPMSF is appropriate for a BER-supported user facility.

Is EMSL appropriately structured to support a full range of DOE and national science research priorities?

EMSL is currently equipped to support a wide range of DOE and national science research priorities, although they are not presently equipped to support the full range. For example, HPMSF is focused on proteomics, but it does not contain mass spectrometry instruments that might readily allow the analysis of catalysts, synthetic polymers, semi-conductors, etc. That is, it is a specialized facility. It is worth noting that several instrument vendors now offer hardware originally developed at EMSL as commercial products, and other researchers in EMSL/PNNL also have exported the hardware to their own laboratories.

There is also the question of whether one scientific facility, such as EMSL, should be structured to support the full range of DOE and national science research priorities. EMSL should focus on what it does best and not try to dilute its impact by being all things to all people. However, there are some areas, such as the ability to work with radiological and Biosafety Level Three (BSL-3) samples, that cannot currently be performed at EMSL but which are high priority both to the DOE and to the nation. BSL-3 capabilities are necessary for work with infectious agents that may cause serious and potentially lethal diseases as a result of exposure by inhalation. The technology used in HPMSF is well suited for important studies of BSL-3 agents and microbial proteomics; hence, it could be used in direct support of homeland security activities. The addition of BSL-3 facilities to EMSL should be considered, however it is premature to do so unless there is high level agreement that EMSL should, at a minimum, conduct homeland security research in this area or, at a maximum, be the central laboratory for developing homeland security applications of high performance mass spectrometry. Similarly, the overall value of applying such mass spectrometry techniques to radiological samples needs to be explored.

Is the user model for allocating resources for all EMSL facilities appropriate? Does EMSL attract the best mix of users?

There does not appear to be a robust definition of a user, nor is there consistency across the six major EMSL facilities in allocating resources to users, whatever that definition may be.

In these times of flat budget, the various EMSL facilities must attempt to maximize the output obtained from current resources. HPMSF does an excellent job of this by increasing the sample load, while not increasing the number of staff significantly, through the development of standardized methods of experimental analysis and automation of data analysis procedures. Robotics are also being applied for sample preparation procedures.

In terms of attracting users, there is no standardized procedure used by all the EMSL facilities for soliciting research projects. Serious consideration should be given to uniform proposal submission dates and review processes, and clear presentation and publicity about these processes would garner more (and more competitive) proposal submissions and would likely lead to a broader user base. Several of the facilities have had no specific Calls for Proposals even though EMSL has been in operation for eight years. HPMSF has not yet issued a formal Call for Proposals, although the review committee was informed that such a solicitation would be issued in the coming months. Some Calls for Proposals should be specific, while others may

be more general. Calls for Proposals that span several EMSL facilities should be encouraged.

Many users originally learn about the High Performance Mass Spectrometry Facility when EMSL and PNNL employees discuss their research at conferences attended by biologists and biochemists. These people submit proposals to the facility. Some proposals also come in through the general EMSL Call for Proposals. The proposals are evaluated by an internal review. Most proposals are accepted; indeed, there are no clear criteria as to what is required for a proposal to be accepted. The proposals that are rejected usually involved experiments that can not readily be performed at HPMSF because of its specialization as a facility geared towards proteomics. It is not clear how accessible the facility is to a broad spectrum of users, since many of HPMSF users have long-standing relationships with the facility, and a significant number are PNNL scientists.

Could changes be made to increase the impact of EMSL on DOE science goals?

Although DOE and BER have articulated their scientific goals through the DOE Strategic Plan and the Office of Science Strategic Plan, it is not clear that sufficient thought has been given to how EMSL will help the Department achieve these goals. In particular, as noted elsewhere in this report (*vide supra*), until BER, PNNL, and EMSL agree on the articulation of the EMSL mission, EMSL will not have the full impact that it can on the DOE science goals. In particular, the role of environmental science in the EMSL mission should be considered. A closer interaction and more communication between EMSL and DOE will be necessary before the impact of EMSL on DOE science goals can be increased. Further, an increased level of funding, especially for maintaining the inventory of instrumentation and supporting equipment, would increase capabilities as well as afford opportunities for new research ventures. The research problems at the forefront of national issues are highly dynamic and the research tools required to address these problems must also be dynamic. At the current funding level and in times of 'flat' budget, it will be difficult to maintain state-of-the-art capabilities.

If environmental studies are considered to be an important part of the EMSL mission, this is something that should be considered when evaluating proposals. For example, HPMSF currently has only a few projects that would be considered as "environmental." If environmental studies are considered by DOE to be an important part of the EMSL mission, then HPMSF may wish to give a higher priority to proposals that have environmental components.

Given a flat budget for ERSD, what priority should EMSL have within the Division's portfolio?

Centralized research facilities that are staffed with highly capable scientists and support staff are essential for maintaining cutting-edge research capabilities, especially in lean years. Consequently, facilities such as EMSL represent critical national resources. EMSL is further justified on the basis of growing concerns related to climate change and human-industrial impact on the environment, research into which will continue to require development of cutting-edge analytical techniques.

It is critical that the EMSL budget be increased so that instrumentation can be kept at state-of-the-art levels and additional staff can be hired to assist users and allow the instrumentation to

operate at maximum capacity. $2M per year in capital funds is simply not adequate to keep the EMSL instrumentation at state-of-the-art. EMSL must be given top priority in the Division's portfolio even if it means that other research areas for ERSD must have decreased funding.

Does the EMSL have a well-defined plan to refresh capital equipment, and is it appropriate? What short- and long-term strategies should be considered in this context? Does EMSL appropriately manage the acquisition, use and retirement of instruments?

No well defined plan to refresh capital equipment was presented. A method of prioritizing instruments needs to be developed. The process of allocating equipment funds among the EMSL facilities should be more formalized. Facility managers should present written requests for new instrument acquisitions that would provide specific examples of potential uses for the proposed instrumentation. This proposal process should not be onerous, but it should allow the facility manager to formulate clearly the requests. If requests for the purchase of instruments were more substantial than "funds are needed to replace aging equipment," then the likelihood of funding being granted would increase. While the EMSL director should have the ultimate responsibility for requesting funds from the DOE for equipment that is of highest priority, consideration should be given to having the Scientific Advisory Committee (once appropriately constituted and charged, *vide supra*) review the requests from the different facilities.

Regarding management of the use of instruments, HPMSF appears to do an excellent job of instrument and sample management. There is a highly developed computerized tracking system for samples; this allows users to see the status of their submissions and allows maximum use to be made of each piece of instrumentation. In addition, there is essentially no idle instrument time for the major mass spectrometers. Instruments are working to full capacity and the current sample queue is about 530 samples, the majority dating from March 2005 or later. However, as the facility expands its user base through the anticipated proposal solicitation process, it will become necessary to be more selective about the types of projects that are accepted.

The processes used to determine which instruments should be retired appear to be adequate.

How does EMSL manage general user access to equipment purchased with non-ERSD* funds? *How does this impact EMSL operations as an ERSD-supported user facility?

Mass spectrometry equipment purchased with non-ERSD funds, but physically located at EMSL, becomes part of the EMSL contingent of instruments. Although the projects that paid for a given piece of instrumentation receive first priority for its use, the remainder of instrument time is available to other EMSL users. Thus, the suite of instruments available to users of this facility is greater than it would be if there were reliance on instruments purchased solely with funds provided to EMSL by BER. The same is true of some staff members who are funded primarily by grants to PNNL users, but who are also available to assist other EMSL users. In short, for HPMSF, the impact of non-ERSD funds on EMSL users is very positive. This non-ERSD funding has become essential for the facility's growth due to the years of flat-funding of EMSL by DOE. Without this funding, HPMSF would not be the world's premiere proteomics mass spectrometry facility.

The Molecular Science Computing Facility

In general, the reviewers were very impressed by the Molecular Science Computing Facility (MSCF). The facility is at the leading-edge of national supercomputer capabilities. Appropriate attention has been paid to ancillary capabilities like IO (Input/Output) and storage so that these do not restrict the usefulness of the supercomputer. The entire operation is well managed. One impressive statistic is that in the past year, efficiency of codes has increased from 9 percent to 13 percent of peak. 13 percent is quite respectable for machines of this type.

The presentation made to the reviewers states that the facility "focuses on providing the right hardware, software and consulting to teams of computational scientists for grand challenge science." (Please note that MSCF has a definition of "Grand Challenge projects" that differs from that used by EMSL as a whole.) This suggests that there is a single best hardware, which is unlikely. Since well under 10 percent of the usage of MCSF involves more than 512 processors on a single job, the facility could likely be run as four independent and possibly diverse 500 processors systems, instead of one coupled 2000 processor system. This would increase the number of research projects that could be efficiently performed. Larger jobs could be sent to other DOE labs, such as the high performance computing facility at the Oak Ridge National Laboratory or the National Energy Research Scientific Computing Center. Rather than buying or leasing a new, 2000 processor system every four years, buying one 500 processor system each year would take advantage of Moore's law, would not require that all funds for a computer upgrade be provided at once, would allow the acquisition of diverse architectures in different years as they become available, and would make it more likely that "the right hardware" would be available to the various projects. This change in acquisition procedure would, however, make it more difficult to administer the overall system.

There is a good process for determining need. Every four years, there is a call for "white papers" from prestigious biologists, chemists, and environmental scientists (including some former users of MSCF) on potential science themes that are consonant with the EMSL mission and that are appropriate for high performance computing. A two-day workshop is then held at which top scientific community representatives provide insight into the major scientific drivers of the next three to five years. This process leads to the production of the "Greenbook" that articulates the scientific drivers that will influence MSCF in the next three – five years. The document describes future challenges in the areas of biological and chemical sciences and environmental systems, the role that MSCF computing and expert staff resources will play, and how MSCF and its recommended upgraded computational resources will positively impact the environmental mission of DOE. These drivers are then translated into requirements for proposal solicitations.

The machine is healthily oversubscribed. Based on the presentation made to the reviewers, it appeared that, in FY 2005, 20M CPU hours were requested and 16M were allocated, which would imply very little oversubscription. However, upon probing by the reviewers, it turns out that only about 4.4M hours were available to respond to new requests for 8.2M hours, since over 10M hours were already committed for activities from previous Grand Challenge calls.

There is a clear, well-defined process for resource allocation. Mission relevance is enforced by tailoring the call for what are called Grand Challenge proposals that account for 80 percent of the

cycles allocated. These Grand Challenges have focused on major environmental problems, especially those with a molecular emphasis. (It is strongly recommended that term "Grand Challenge" be replaced with other wording, especially if the EMSL maintains the broader "Grand Challenge" program.)

There is close connection between the MSCF staff and the Grand Challenge users. Each Grand Challenge project has a designated staff member as a point of contact who keeps in close touch with the progress of the project. This also enables MSCF to remain informed as publications emerge from the work performed at the EMSL.

The quality of science being enabled by MSCF appears to be quite high. Several publications have been published in leading journals. By restricting the number of Grand Challenge projects, each project can be allocated sufficient computing time to make it competitive with what research groups could get at other facilities like the National Science Foundation supercomputing centers, the Department of Defense centers, and other DOE centers.

It was difficult to assess user satisfaction. While there were several supportive testimonials presented, responses to the previous user surveys included considerable grumbling about the machine often being down. This facility needs a more targeted user survey than the EMSL-wide survey, and such a survey is apparently being designed.

The reviewers asked the very pointed question as to why EMSL needs a supercomputer, as opposed to the need to keep resident expertise in applications software. The main answer was that the EMSL machine is optimized for EMSL science, as articulated in the Greenbook. Placing such a large facility within a BER facility guarantees that researchers supported by BER will have access to adequate computing power. Many such users would likely not receive adequate time on other computing resources. Moreover, access for small exploratory projects can be, and often is, enabled in a day. This is particularly valuable, since such access is, for many projects, the determining factor as to whether or not a more time-consuming project should be commenced. One user with whom the reviewers spoke said that he could not have performed his studies without NWChem (a computational chemistry package developed at EMSL) and that the authors of NWChem were willing to adapt the code for his purposes.

NWChem, ECCE (the extensible computational chemistry environment developed at EMSL) and Global Array tools appear to be very impressive software developments that enable efficient use of large distributed memory supercomputers for chemistry applications. (It should be noted that neither of the primary reviewers of the MSCF are computational chemists, and further advice as to the quality of these products might be valuable.) This is a major effort of the sort that university groups cannot muster. While it addresses all chemistry, it is clearly very relevant to the presumed environmental mission of EMSL.

There are some cross-cutting activities at the EMSL that foster cooperative capability development involving the supercomputer, e.g., Genomics:GTL, although such cross-cutting activities could be significantly enhanced. Projects within the Environmental Spectroscopy and Biogeochemistry Facility that use supercomputer time were specifically identified. In FY 2004, about 44 percent of the usage of the MSCF was by PNNL scientists. Specifically, 20 percent was by PNNL staff from outside of EMSL, 15 percent was by MCSF staff members who had

successfully competed through the proposal process for research cycles, and 9 percent was by staff members from other EMSL facilities who had also competed successfully through the proposal process. In total, between both external users and the full set of PNNL users, those computational Grand Challenge projects that also involved complementary projects using other EMSL facilities used 3M hours in FY 2004 and already used 4M hours in FY 2005 (out of a total of about 15M hours/year delivered). This is a greater usage of the MSCF than seems to have been reported through review of the other EMSL facilities.

In response to a specific inquiry, the reviewers found that there is considerable interaction with the Computing and Information Sciences Division (CISD) of PNNL in software development (NWChem, ECCE). CISD also handles networking, security, and managing desktops, and it supports research on High Performance Computing interprocessor communication, which has impact on NWChem.

Other observations were made that are broadly applicable to EMSL, not solely to MSCF. Clearly, the issue of upgrading equipment is an important one, and it is likely that there will not be sufficient capital funds to maintain all equipment at a state-of-the-art level. Equipment needs must be prioritized, and the mission and vision of EMSL, and how these relate to equipment, must be important factors in the prioritization process. The uniqueness of the equipment, or its limited availability at other facilities, should also be considered.

Senior scientific staff that will help the vision of EMSL mature over time need to be placed back into EMSL. The focus of the scientific staff should be to (1) drive the vision forward and (2) ensure that the users and research at EMSL are aligned with the BER/ERSD goals. The metric for EMSL success should not only be the user/facility publication record but also the success in providing solutions to scientific challenges that dramatically impact the environmental remediation of DOE facilities.

The EMSL-wide Grand Challenge approach, based on the two already underway, does not necessarily seem to be the best approach for focusing the work at EMSL. A better approach to driving the EMSL mission might be to develop EMSL-wide proposal calls that provide focus to the direction of EMSL. CATs are not obviously a means for driving the vision for EMSL.

With regard to the specific questions posed by Dr. Orbach, the answers that follow are focused on observations made by the reviewers of MSCF.

Does the relationship and management structure among EMSL, PNNL and ERSD foster the highest quality of science at EMSL.

As noted elsewhere in this report, there does not appear to be a clearly articulated mission/vision for EMSL that is shared by EMSL, PNNL, and ERSD. While the scientific studies conducted at EMSL are, for the most part, of very high quality, that lack of a coherent vision undoubtedly has adverse implications on the potential impacts of EMSL achievements.

Is the science conducted at EMSL cutting edge? If so, is it appropriate for a BER-supported user facility?

The research conducted in the MSCF is at the cutting edge of computing applications. Relative to other high performance computing facilities, the EMSL facility is unique in its focus on BER issues, providing an opportunity for access to supercomputing CPU hours related specifically to biological and environmental research. Access for such work would likely be minimal at other supercomputing facilities. While the facility is primarily focused on computational chemistry (particularly through its support of the NWChem software), the draft 2005 Greenbook suggests that the MSCF will be broadening its scope to attract users that are involved in larger scale atmospheric and subsurface flow and transport activities. This broadening of the user base will better align the facility with the ERSD/BER research needs and is strongly encouraged.

Is EMSL appropriately structured to support a full range of DOE and national science research priorities?

MSCF is structured as a user facility and relies on its users and the scientific community to identify its research priorities. Due to the uncertainty in the mission/vision for EMSL, the research priorities do not appear to be purposefully aligned with the other five facilities, EMSL as a whole, or DOE. Based on the Greenbook, it appears that the vision for MSCF and its research priorities are being developed without oversight or input from EMSL or BER management.

Is the user model for allocating resources for all EMSL facilities appropriate? Does EMSL attract the best mix of users?

The model developed for allocating resources at MSCF is based on a rigorous proposal review process conducted by reviewers both internal and external to EMSL. It is based on two types of allocations, Grand Challenges and pilot proposals. It appears that the time between proposal submission and allocation of resources for Grand Challenge proposals is long (six months) and an effort should be made to streamline the proposal review process. The review process for pilot projects can be as short as one day.

The mix of users, broken down by PNNL and external, based on jobs submitted to the computing facility is 45:55. PNNL users are a combination of EMSL and non-EMSL staff members. The fraction of external users is not unlike other user facilities. Unfortunately, however, there is no apparent guidance on what the appropriate ratio of external to internal users should be. Such a ratio needs to be established.

Could changes be made to increase the impact of EMSL on DOE science goals?

The methodology used for allocating CPU time to users (internal/external reviews) is excellent and ensures that MSCF is appropriately used for high-impact science. However, senior staff members are needed to guide the vision of the MSCF (and EMSL as a whole). While the external scientific community can be relied upon to review the scientific merit of proposals, there is a need for MSCF/EMSL staff to focus the EMSL research on DOE science goals. In essence,

EMSL needs a clearer vision for its facilities, and this vision needs to "trickle down" to its facility managers and be incorporated in the proposal calls.

Given a flat budget for ERSD, what priority should EMSL have within the Division's portfolio?

The flat budget for ERSD (and the implications for the EMSL budget) will require difficult decisions to be made by the EMSL and ERSD management. Sacrificing other projects supported by ERSD is probably not advisable. Instead, EMSL will need to find other funding sources (leveraging) and make difficult decisions with regards to essential versus secondary equipment/facilities. To date, it does not appear that EMSL has developed a plan for, or hierarchy of, the equipment in terms of value to the science community and its users. The EMSL vision for the future should drive this decision making process.

Does EMSL have a well-defined plan to refresh capital equipment and is it appropriate? What short-term and long-term strategies should be considered in this context? Does EMSL appropriately manage the acquisition, use and retirement of instruments?

MSCF has been successful at maintaining funding that is sufficient to remain competitive in the supercomputing arena. It is essential that it continue on this path. The reliance on the Greenbook survey to direct the purchase of future computing and storage capabilities is appropriate. However, as noted above, there may be a need to widen the scope of possibilities for refreshing the computational resources (*i.e*., several smaller clusters may be more appropriate than one large one given the user base and the vision for the future user base). Furthermore, it is important for EMSL management to be involved in the Greenbook survey to ensure that the visions for MSCF and EMSL are aligned.

How does EMSL manage general user access to equipment purchased with non-ERSD funds? How does this impact EMSL operation as an ERSD-supported user facility?

MSCF resources appear to be wholly purchased with ERSD funds. As such, there is no conflict with regards to access or influence from other non-EMSL groups. However, the proximity of EMSL to PNNL naturally results in a significant fraction of the MSCF CPU being allocated to PNNL staff. The 45 percent (EMSL plus PNNL) allocated to these users is not unlike other user facilities. As stated earlier, there may need to be a goal set for the fraction of users that should be external.

There is considerable interaction with CISD in software development (NWChem, ECCE). The fraction of NWChem/ECCE development funded by CISD vs. EMSL is unclear. One positive example for the use of external funds was the funding of a scientist with an atmospheric chemistry background (through user funds) to help in code development/debugging. This seems to be an effective application of outside funds.

The Interfacial and Nanoscale Science Facility

The Interfacial and Nanoscale Science Facility (INSF) contains a diverse set of instrumentation that provides a broad spectrum of capabilities for fabricating and analyzing nanoscale structures. Some of these are unique, particularly in the ability to combine various measurement techniques and tools on a single sample without exposure to external environments. The facility is comprised of a very diverse set of capabilities, with 27 laboratories and 23 major instruments. It is run by approximately 11 staff members, but there are only six full time equivalents providing technical operations support. This limits the availability of the instrumentation to outside users. Indeed, while some of the equipment is heavily used, other equipment cannot be used to capacity because the requisite staff support is not available.

The large capital equipment base is aging and/or falling behind the state-of-the-art, thus limiting the ability to support users adequately in the requested scientific endeavors. For example, the Time of Flight – Secondary Ion Mass Spectrometer is outdated and is unable to perform some of the needed measurements. With changes in research emphasis, new tools are necessary, such as a cryo-Transmission Electron Microscope (TEM) for analysis of biological samples. Anticipation of future scientific directions drives requirements for new, improved capabilities such as an aberration-corrected Transmission Electron Microscope with an environmental cell, a next generation high pressure catalysis system, a fine-focus accelerator microbeam line, a Focused Ion Beam-Scanning Electron Microscope, and high spatial resolution X-ray Photo-electron Spectroscopy (XPS). Some of the capital equipment, and many of the ongoing projects, are partially funded by non-BER sources. This can lead to conflicts over priorities, but it also represents an opportunity for effectively leveraging resources.

The scientific studies performed using the capabilities of INSF are of high quality, and many of the users are of high profile and well-established scientific reputations. Several very prominent scientists have chosen to spend sabbaticals at the EMSL in order to use INSF capabilities, and they remain users of the facility after having returned to their home institutions. A broad range of scientific inquiries are performed using the instrumentation at the facility, most under the general umbrella of interfacial and nanoscale science as applied to environmental problems. In FY 2004, the facility was involved with 315 user projects. This breadth of activities has both an upside and a downside. The studies have had positive impact over a wide range of areas, but the overall impact could be greater if research were focused into fewer areas. The majority of users (75 – 80 percent) are repeat users, approximately half are from academia, and approximately 40 percent are PNNL staff scientists who are not supported by EMSL operating funds and who must submit user proposals prior to accessing the equipment.

Some of the projects conducted in INSF do take advantage of capabilities in other EMSL facilities. In particular, there are projects involving the Chemistry and Physics of Complex Systems Facility and the Environmental Spectroscopy and Biogeochemistry Facility. While many projects have a theoretical or modeling component, it appears that few utilize the Molecular Sciences Computing Facility.

With regard to user access, there is no formal Call for Proposals. Solicitations are somewhat *ad hoc* and seem to rely on word-of-mouth or advertisement at conferences, workshops, and

seminars. Proposals are accepted for review at any time. They are usually reviewed by the relevant technical staff member contact within INSF, and, if minimal criteria are met, the proposals are accepted. There does not appear to be an overarching theme or focus for accepted proposals, and what prioritization exists appears to be from *ad hoc* discussions among facility staff members. Indeed, few proposals are rejected. Timeliness of access to the facility is instrument dependent – some instruments have heavy demand but quick turnaround (XPS), others (Molecular Beam Epitaxy, TEM) have longer lead time and turnaround. With better prioritization of activities across the facility, a better distribution of access to the instrumentation might be achieved.

External users and Grand Challenge projects have priority in the facility. However, in general, there appears to be a lack of longer-term goals or focus. This is also evident in the Grand Challenges; the Biogeochemistry project has no clear follow-on effort planned, and the Membrane Biology project does not have a well-defined project plan.

Based on these general observations, it is recommended that signature scientific areas for INSF be clearly defined, with a science roadmap for the facility established such that the research performed therein is focused towards achieving long-term scientific goals. This will require enhanced scientific leadership within the facility, bringing more senior expertise into a group of highly competent, but still junior, staff scientists. Metrics for monitoring progress towards those goals should be established and tracked. A capital equipment renewal/replacement strategy based upon the roadmap needs to be defined.

There should be a formal Call for Proposals that clearly identifies the science focus areas of interest/importance to INSF. There should be more formal reviews (including external reviewers) of “large” user proposals (e.g., those requiring several weeks of facility time) to prioritize the potential scientific quality and impact. User proposals should also be prioritized on the basis of their potential contribution to the science goals/roadmap for INSF. An improved process for obtaining feedback from users should be established.

A capability for the measurement and characterization of radiological samples should be developed.

With regard to the specific questions posed by Dr. Orbach, the answers that follow are focused on observations made by the reviewers of INSF.

Does the relationship and management structure among EMSL, PNNL and ERSD foster the highest quality of science at EMSL?

The current structure does not ensure the highest quality science in the long-term. There is no consistent, well-defined mission or vision for EMSL, and this also applies to INSF. Since the operating funds are not sufficient to provide full support for the staff scientists who work directly with users, much of the rest of their support comes from research project funds. This raises the question as to whether the research projects or the user facility take(s) the lead role. If there is a user facility, but less than half of its effort is devoted to supporting users, is it then appropriate to call it a "user facility," or is it a project facility that also happens to support users?

Confounding this is the formal separation of many of the research staff from EMSL, as occurred in recent years. Many of the staff members who remain in the EMSL, while technically highly qualified, are still rather junior in terms of experience and in terms of breadth of scientific vision. In most cases, the more senior scientific expertise resides in those PNNL staff members who are no longer formally within the EMSL organization. This absence of senior scientific leadership raises questions about EMSL's future ability to set strategic scientific directions, recruit additional high caliber staff scientists, and maintain high scientific output directed towards focused goals.

If there is not a well-defined mission or vision for EMSL that is shared by EMSL, PNNL, and ERSD, and if most of the scientific leadership resides in PNNL (not EMSL) staff, and if the interaction with users is primarily through EMSL staff, how do the science and user services roles come together in a common thrust to promote the highest quality research? The current structure does not necessarily lead to common science and user support goals, and it raises the question as to what should be the relative roles of quality and direction of science *vs.* user services. These ambiguities and the current structure do not seem to foster the highest quality science.

Currently, there appears to be little directed coupling between the research portfolio of ERSD and the projects utilizing the capabilities of EMSL. That portfolio could be used to facilitate the advancement of science areas that constitute the primary foci of EMSL. Such an approach could help enhance significantly both the overall quality of the science enabled by EMSL and the depth and impact of its scientific advances.

Is the science conducted at EMSL cutting edge? If so, is it appropriate for a BER-supported user facility?

The quality of science conducted at EMSL is high, and it is appropriate to BER. INSF has done an excellent job of establishing and maintaining collaborative research with distinguished users. Sabbaticals have been used effectively in these exchanges. The fact that many repeat users are of high standing in the scientific community speaks well of the overall quality of science performed. Many of these research areas are certainly appropriate for a BER user facility, but they lack an overall focus. Thus, the impact is diluted because of the broad spectrum of research performed and lack of defined thematic areas with specific goals.

Is EMSL appropriately structured to support a full range of DOE and national science research priorities?

EMSL is probably not ideally structured to provide full effectiveness. There seem to be few commonalities among the operations of the six facilities, the advisory committees are not used with full effectiveness, the priorities are not well defined, and the mechanisms for effectively emphasizing or measuring progress towards those priorities are not identified. Achievement of effective support will require establishing a clearly articulated set of goals, then establishing a structure that most effectively works to achieve those goals.

Is the user model for allocating resources for all EMSL facilities appropriate? Does EMSL attract the best mix of users?

It is not clear how the resources are allocated among EMSL facilities (other than a historical distribution that dates back to the opening of EMSL). What are the overarching science themes, and how do these relate to goals for users and user projects? How is movement towards those goals enabled by the resource allocations to the different facilities? The lack of a Call for Proposals and formal review process in many of the facilities, including INSF, likely predicates that the best mix of users is not attracted. Formal Calls for Proposals should be used as a mechanism for helping to focus research into the highest impact areas and to solicit the best ideas from users for research in those areas.

Could changes be made to increase the impact of EMSL on DOE science goals?

There are definitely changes that could increase the impact of EMSL on DOE science goals. Establishing strong, senior scientific leadership within EMSL would assist in the impact. Defining science roadmaps for the facility to establish goals would then allow a great deal more focus for the research portfolio. A clear definition of priorities for EMSL facilities would be of benefit, as would be the establishment of generally uniform procedures that govern access, use, and support.

Given a flat budget for ERSD, what priority should EMSL have within the Division's portfolio?

Since EMSL is the flagship facility of ERSD and already consumes 35-40 percent of its budget, it should have the highest priority within ERSD. Within EMSL, priorities will have to be made for most of the projects, with resources flowing toward those which rank highest.

Does the EMSL have a well-defined plan to refresh capital equipment, and is it appropriate? What short- and long-term strategies should be considered in this context? Does EMSL appropriately manage the acquisition, use and retirement of instruments?

The current capital equipment budget, $2M annually with an additional (approximately) $2M leveraged from other sources, is inadequate to maintain the facility. Even if the laboratory can maintain a 1:1 match of EMSL capital equipment funds with other funding, this will likely be insufficient to re-capitalize as needed. Given the current lack of long-term planning, science goals, and roadmaps, it is difficult to assess the plan and its appropriateness for acquisition, use, and retirement of equipment. It is obvious, however, that the current $4M/year is insufficient to replace an investment of over $120M seven years ago. The new EMSL leadership is working on these plans and goals, and the capital equipment plan should be checked against those as they become defined.

How does EMSL manage general user access to equipment purchased with non-ERSD funds? How does this impact EMSL operation as an ERSD-supported user facility?

First priority on equipment purchased fully by non-ERSD funds is given to projects sponsored by the funding source. If such equipment is not completely utilized by projects sponsored by the

funding agency, it is made available to other projects. For equipment that is purchased using funds from both ERSD and non-ERSD funds, it is not clear that there exists a documented procedure for handling potential conflicts over the use of that equipment. It appears that any such conflicts are worked out informally by the scientists desiring access to the equipment.

The fact that a significant portion of the EMSL equipment and staff are supported by non-ERSD funds definitely impacts the EMSL operation as a user facility. Although this is not a formally dictated level of outside support, it has been an almost inevitable method to augment funds since the current level of operation funding is inadequate to support either the staffing base necessary to run the user facilities or to provide the capital equipment needed for those facilities. Such cross directive funding is not *a priori* a bad thing, in fact it may have positive aspects, but when present in the current percentage it may detract from the primary mission of the EMSL funding (the user services role of the scientists). The non-ERSD supported activities may, in practical terms, have higher priority than external user requirements. Mechanisms should be in place to ensure that the outside funding aligns with the important missions of EMSL including that of a user facility. There should also be defined, appropriate processes and procedures to deal with conflicts over use of equipment or staff support for projects associated with these various funding sources.

The Environmental Spectroscopy and Biogeochemistry Facility

The Environmental Spectroscopy and Biogeochemistry Facility (ESBGCF) comprises a combination of instruments and equipment applicable to the study of chemical reactions in heterogeneous natural materials, with an emphasis on soil and subsurface systems. The facility staff, complemented with other PNNL staff, forms a multidisciplinary research team with expertise in chemistry, molecular modeling and simulation, mineral physics, geochemistry, microbiology, hydrology, and environmental engineering.

ESBGCF is able to make a unique contribution to forefront research in environmental biogeochemistry in several ways:

- Some advanced instrumental facilities are extremely rare, particularly for use with environmental samples (e.g., conversion electron Mössbauer spectrometer for surface analysis, applied field Mössbauer spectrometer (currently under development); dual source gamma spectrometer for fluid detection in the intermediate-scale porous medium flow cell).
- The facility offers a wide breadth of instrumentation, providing a "one-stop shop" (e.g., laser capabilities ranging from femtosecond to continuum; a variety of standard analytical equipment [e.g., Gas Chromatography/Mass Spectrometry (GC/MS), Ion Chromatography, Liquid Chromatography**,** Inductively Coupled Plasma Mass Spectrometry, Total Organic Carbon Analyzer, Atomic Force Microscopy] to support investigations using more advanced, less-commonly accessible instrumentation).
- The scientific consultants associated with the facility provide users with expertise over a wide range of fields (spectroscopy, geochemistry, molecular modeling, microbiology, hydrology, etc.), which allows inherently interdisciplinary questions to be addressed effectively.

ESBGCF has a strong user base including leading and distinguished researchers. Most often, users have come to the facility through prior collaborations or personal contacts with ESBGCF scientific consultants, although some new users have applied to use the facility with no prior contact.

The level of use of instruments in ESBGCF varies considerably. Some instruments can and do run full-time as automated instruments. Running other instruments may require direct supervision by a scientific consultant, and access to the instrument may be limited by the availability of staff time. For example, in FY04, the flow cell was fully utilized (61 percent on-site user, 28 percent capability development), but one Mössbauer spectrometer and the time-resolved laser fluorescence system were used at only 25 percent capacity. (Other Mössbauer spectrometers were more fully utilized.)

ESBGCF has been very productive and has supported projects that have led to publications in leading journals, such as *Environmental Science & Technology* and *Geochimica et Cosmochimica Acta*. For example, the ESBGCF capability in geochemical molecular modeling

resulted in 42 publications of which the most frequently cited is Rosso KM, and JR Rustad (2000) "Ab Initio Calculation of Homogeneous Outer Sphere Electron Transfer Rates: Application to M(OH2)(6)(3+/2+) Redox Couples" Journal of Physical Chemistry A 104(29): 6718-6725 (18 citations). Use of the Mössbauer spectrometers resulted in 15 publications of which the most frequently cited is Zachara JM, RK Kukkadapu, JK Fredrickson, YA Gorby, and SC Smith (2002) "Biomineralization of Poorly Crystalline Fe(III) Oxides by Dissimilatory Metal Reducing Bacteria (DMRB)" *Geomicrobiology Journal* 19: 179-207 (31 citations). And use of the laser-induced time-resolved fluorescence system resulted in 13 publications of which the most frequently cited is Ainsworth CC, D Friedrich, PL Gassman, Z Wang, and AG Joly (1998) "Characterization of salicylate-alumina surface complexes by polarized fluorescence spectroscopy" Geochimica et Cosmochimica Acta 62(4):595-612 (15 citations).

ESBGCF scientific consultants and users also present results obtained using the facility at national and international scientific conferences and other professional venues. This enhances the impact of work performed at EMSL on the scientific community.

A number of recommendations can be made based on these general observations:

- EMSL, and ESBGCF in particular, must attract a broader cohort of users. The overall EMSL proposal submission process that is posted on the EMSL website should include a question such as "How did you learn of EMSL and its capabilities?" ESBGCF should be more proactive in attracting new users to the facility. ESBGCF scientific consultants should be encouraged to give seminars at universities and presentations at technical meetings and to target these presentations so as to increase the visibility of ESBGC facilities among potential users, especially distinguished users. The (lack of) incentives for scientific consultants to broaden the user pool should be considered. Further, ESBGCF should work with the outreach office to inform faculty from undergraduate- and minority-serving institutions of ESBGCF capabilities.
- Limitations on increasing instrument use (either absolute physical limits or available staff time) should be examined and addressed for each ESBGCF instrument. Funding for bachelor's or master's level technical staff could relieve scientific consultants of the burden of routine instrument use and maintenance and should be explored as a cost-effective way to increase instrument utilization. Information about instrument utilization should be used in strategic planning for instrument replacement, upgrades, etc.
- ESBGCF (and EMSL generally) should focus on building world-class technological and engineering expertise. This would allow unique capabilities to be developed in-house through technological improvements to existing or commercial instruments. This approach might be a more cost-effective approach to building unique capabilities than purchasing the newest commercial instrumentation.
- Planning for instrument upgrades and acquisition should maximize cross-facility cooperation and minimize redundancy in capabilities between facilities when possible.
- The capabilities of ESBGCF would be enhanced by increasing the ability to accept and interrogate samples containing radioisotopes. An on-site radiological annex (or other means to achieve this objective) should be developed.
- ESBGCF should promote and leverage research in thematic areas consistent with its capabilities, expertise, and the EMSL mission. However, research by single investigators

and small teams should not be slighted. The exclusionary aspects of the Grand Challenges and CATs should be minimized.
- ESBGCF (and EMSL generally) should try to attract new users by advertising the opportunity to obtain "proof of concept" results. Submission of proposals for extramural funding based on this seed work (with EMSL access specified in the proposal and guaranteed by EMSL) should be encouraged.
- EMSL is a unique facility that meets critical national needs. Major increases in future support will be needed to sustain its cutting edge capabilities.

With regard to the specific questions posed by Dr. Orbach, the answers that follow are focused on observations made by the reviewers of ESBGCF.

Does the relationship and management structure among EMSL, PNNL, and ERSD foster the highest quality science at EMSL?

The management structure appears (to the naïve outsider) to be extraordinarily obscure and convoluted. Despite this, it appears that, from the perspective of researchers and technical leads, this structure is functional. In effect, EMSL works across "management lines." Advantages of this structure include:

- Access to expertise across disciplines, EMSL facilities, and at PNNL;
- Collaboration between geochemists, microbiologists, and spectroscopists within the ESBGC facility;
- Leveraging of funds for capital investment and salary support.

The ESBGC technical lead has good access to top administration, and the researchers do not appear to find the management structure intrusive.

Is the science at EMSL cutting edge?

Science conducted at ESBGCF is cutting edge in several aspects. The signature capabilities of ESBGCF are: Mössbauer spectroscopy, time-resolved laser fluorescence spectroscopy, and the gamma spectrometer instrumented intermediate-scale flow cell. These instruments/equipment are approaching uniqueness and offer users cutting-edge capabilities. ESBGCF also offers a unique range of expertise in support of user activities. For example, the collaboration of the scientific consultants on the intermediate scale flow cell with users extends from experimental design to performance of the flow experiments to simulation of results. In addition, the ESBGC facility provides a wide range of ancillary analytical instrumentation in support of its signature capabilities (e.g., GC/MS for analysis of organics being studied in the intermediate scale flow cell).

The Biogeochemistry Grand Challenge has benefited (and benefited from) ESBGCF. The Grand Challenge has driven new activities and applications (e.g., the application of Atomic Force Microscopy to image microorganisms on mineral surfaces and to examine electron transfer to cytochromes). However, there is a justifiable concern that the capabilities in ESBGCF (and within EMSL overall) are becoming obsolete over time. Capabilities must be kept at the cutting

edge. ESBGCF has a unique opportunity to build cutting-edge capabilities by making in-house technological improvements on commercial instruments.

Is EMSL appropriately structured to support a full range of DOE and national science research priorities?

The structure of EMSL is advantageous in that funding for both capital expenditures and staff support can be leveraged across several DOE programs. This allows instrumental capabilities and staff expertise to be leveraged across DOE programmatic and user activities. ESBGCF instruments are used by both users (external and PNNL) and by EMSL line staff in support of research activities that have been funded externally (mostly by DOE programs). The range of technical expertise available within ESBGCF (and EMSL generally) is well suited to addressing DOE and national science priorities.

There is some apparent redundancy in the portfolio of capabilities among different facilities (e.g, between ESBGCF and INSF). However, the different needs and applications within these facilities may necessitate some duplication of capabilities.

ESBGCF is a relatively small operation compared to some other facilities. User access to some instruments within ESBGCF is limited by funding for the support of scientific consultants.

Is the user model for allocating resources for all EMSL facilities appropriate? Does EMSL attract the best mix of users?

For ESBGCF, the majority of users come to the facility after personal contact by scientific consultants or as a result of previous collaborations. This has resulted in a strong user base and excellent collaborations between users and scientific consultants. However, the concern arises that this operating model is somewhat exclusionary. Also, submission of more proposals from a broader range of users might result in competitive selection of proposals that lead to more focused and higher-impact research. In addition, ESBGCF capabilities could be an extremely valuable resource to undergraduate- and minority-serving institutions (which are less well-equipped than Research I universities).

Could changes be made to increase the impact of EMSL on DOE science goals?

The scientific impact of EMSL activities could be increased by involving more high-impact researchers as EMSL users. In addition, greater visibility for EMSL scientific consultants would increase scientific impact. Scientific impact and impact on DOE and national needs could also be increased by improving technological capabilities. Increased ability to perform additional work with radioisotopes and radioactive materials would increase the impact of EMSL research on DOE and national needs.

EMSL senior management has stated its interest in shifting from single-investigator to team research. As noted in the general recommendations, above, the Grand Challenges and Collaborative Access Teams further shift resources away from individual investigators, and this is not strongly supported by the review team.

The impact of EMSL could also be increased by developing a role for EMSL in the initiation of new research ideas and directions. EMSL facilities could be used to provide "proof of concept" preliminary data that would allow users to obtain new extramural funding.

Given a flat budget for ERSD, what priority should EMSL have within the Division's portfolio?

Within ESBGCF, the flat budget environment is being addressed in several ways. Tactical investments are being made in improvements or upgrades that will increase efficiency of facility operation (e.g., implementation of a closed system cryostat and dual sample capabilities for the Mössbauer spectrometer). Maintenance has been made a focus, and the technical lead intends to plan strategically to optimize future upgrades and improvements in support of key research activities.

In the short-term, ESBGCF (and EMSL facilities generally) can be maintained and upgraded to a moderate extent under the current budgetary allocation. An increased focus on in-house technology development could be more cost-effective than upgrading to the newest commercially-available instrumentation. However, future development and acquisition of cutting-edge capabilities will require major investment.

Does EMSL have a well-defined plan to refresh capital equipment, and is it appropriate? What short- and long-term strategies should be considered in this context? Does EMSL appropriately manage the acquisition, use and retirement of instruments?

ESBGCF has identified specific needs for new instrumentation (specifically a Raman spectrometer and a confocal microscope) that are well aligned with the range of research activities being conducted in the facility. This does not, however, appear to emphasize increasing the cutting-edge capabilities within the facility (possibly because funding is seen as insufficient for this). Obsolete instrumentation has been retired from the ESBGC facility.

How does EMSL manage general user access to equipment purchased with non-ERSD funds? How does this impact EMSL operation as an ERSD-supported user facility?

There is substantial capital investment in ESBGCF instrumentation derived from non-ERSD sources. Although there is no formal management plan in place to assign access to such instrumentation, there do not appear to be any conflicts or problems with access. Rather, the leveraging of funds serves to expand the capabilities of the facility and allows better utilization of instrumentation.

The High Field Magnetic Resonance Facility

The review team considered the Grand Challenges and CAT's to be non-ideal methods for encouraging interdisciplinary science. Both were implemented with non-standard peer review mechanisms and appear to have possibly diverted resources (staff and instrument time) from operational needs within the High Field Magnetic Resonance Facility (HFMRF) since they appear to have been assigned higher priorities than other ongoing projects that might have greater intrinsic merit. The reviewers were unaware of any explicit efforts to compare the merit of Grand Challenges and CATs to the merit of the ongoing projects within each facility.

EMSL is strongly cautioned not to have management dictate scientific priorities (e.g., through the Grand Challenges and CATs), but to encourage individual investigators (including both internal and external users) to pursue activities with the highest intrinsic merit and scientific impact within its mission. The mechanisms for peer review should be made more consistent across all facilities, and access to EMSL facilities should granted on the basis of merit and overlap with the mission of EMSL (which itself must be more clearly defined, as noted above).

The review committee addressed the desirability of building an annex to EMSL to handle low level radionuclide containing samples and of conducting general biochemical/molecular genetics work using radioisotopes. The committee was informed that the current sublet spaces for similar purposes in the 300 area were to become unavailable by 2009. Anecdotal evidence for occasional requests for experiments involving radiological samples was provided.

Significant activity in the nuclear magnetic resonance (NMR) field using the 300 Area resources is detailed below. Because of the uniqueness of the resource potentially available to the broad national research community, it is strongly recommended that this activity be supported and expanded. However, there are several models of how this would be best continued. These include locating this resource (i) in a minimal radiological protection level annex to EMSL; and (ii) adjacent to a rebuilt central PNNL radiological chemistry resource with substantially greater resources for material preparation and sample handling, critical adjuncts to the provision of unique capabilities in this area.

The review team is strongly supportive of the need for existing and expanded NMR capabilities for radionuclides. The EMSL resource in this area needs to evaluate its needs for adjunct chemical preparation, and sample machining in a controlled radiological environment, and EMSL management needs to estimate costs of both physical plant construction and continuing lab safety/environment operations. The panel is insufficiently informed as to whether these needs would be best met by a local EMSL annex or by, e.g., association/sublet with new PNNL radiological labs. EMSL management should discuss with its Scientific Advisory Committee the needs for other radioisotope applications and the opportunity cost of the local annex initiative as compared to other EMSL initiatives.

Other general observations are that (i) HFMRF could do more to integrate NMR and Electron Paramagnetic Resonance (EPR) experiments with theory and/or other types of experiments; and (ii) a Scientific Advisory Committee is critical for the future of EMSL especially to avoid problems of overly local focus and restrictive scientific view.

With regard to the specific questions posed by Dr. Orbach, the answers that follow are focused on observations made by the reviewers of HFMRF.

Does the relationship and management structure among EMSL, PNNL and ERSD foster the highest quality of science at EMSL?

No, the current structure does not foster the highest quality of science at EMSL. EMSL, PNNL and ERSD have conflicting mission statements that lead to significant confusion about priorities on the part of both staff scientists and users. The inconsistently defined priorities for each facility have hindered the overall quality of science at EMSL in general and are discouraging to those staff groups that make genuine efforts towards the broader mission of a unique resource for national needs. Specifically, the High Field Magnetic Resonance Facility (HFMRF) is stretched thin in its efforts to provide a very wide range of services to users. The process by which project and capital investment priorities are identified has been a "moving target" that frustrates efforts to enhance world-class capabilities.

The priorities for HFMRF must be spelled out more clearly. Staff time, future capital investments, and usage of the facility must be made consistent with these priorities. It is beyond the scope of this review to recommend specific priorities, although it is recommended that these priorities be established in consultation with an external Scientific Advisory Committee.

Is the science conducted at EMSL cutting edge? If so, is it appropriate for a BER-supported user facility?

Yes, many capabilities at HFMRF are world class, either unique (not available anywhere else) or highly significant (available only at a small number of other facilities). It is certainly appropriate as a BER-supported user facility in its applications of high-powered technological solutions to mission-critical science.

The unique or significant capabilities are summarized below:

a. Ultra-high field, medium-bore magnet (900 MHz, 21.1 Tesla, 63 mm)

This magnet system enables unique types of analysis of solid materials, such as ^{87}Sr analysis relevant to Hanford tank wastes. These applications have yielded approximately 800-fold improvements in sensitivity relative to lower field instruments and older pulse sequence technologies.

The high field system is also advantageous for analysis of hydrogen storage materials such as ammonium boranes, in which the resolution and sensitivity of the ^{11}B signals is strongly dependent on magnetic field.

The biological applications on this system to protein structure determination, studies of intermolecular interactions in protein-protein or protein-nucleic acid complexes (in particular those of very high molecular weight) are highly significant, and represent state-

of-the-art applications whose methodology is likely to be of high utility to DOE's scientific missions.

b. 300 MHz NMR spectrometer housed in 300 Area

This instrument provides unique capabilities, not in the type of experiments that can be performed, but in the fact that samples with high levels of radioactivity can be prepared and analyzed. To our knowledge this is the only site in the world with the capabilities to perform magic-angle spinning experiments on ceramics containing ^{238}Pu and ^{239}Pu.

The capability to perform trace level analysis of radionuclides such as ^{99}Tc likewise is a unique capability that is likely to be more broadly applied to a range of mission-critical applications to national needs.

c. Custom probe construction

HFMRF has unique, world-class capabilities in NMR probe construction that enable the capabilities noted above (as well as on other instruments) to be leveraged most effectively.

Among many probes constructed at EMSL, a subset is identified here:

(1) Magic-angle spinning probes with slow spinning, turning and magic-angle flopping capabilities;
(2) Probes combining magnetic resonance imaging with microscopy in the same platform, offering a unique approach to addressing metabolomics problems;
(3) Extreme temperature probes, capable of studying zeolite materials (^{133}Cs, ^{23}Na) at high temperatures (~250 ^{o}C) and metalloproteins (e.g., containing ^{67}Zn) at cryogenic temperatures (~10 K);
(4) An instrument for preparing hyperpolarized ^{3}He of utility for lung imaging and biomarker development projects.

These capabilities to build instruments at EMSL and customize performance for specific applications are certainly among the greatest assets of HFMRF.

Is EMSL appropriately structured to support a full range of DOE and national science research priorities?

The infrastructure and staff currently at EMSL are very well structured to support DOE and national research priorities. However, the principal question that remains to be addressed is whether the facility should be attempting to support a "full range" of applications, or a more selective list of high impact priorities. The latter is recommended.

Is the user model for allocating resources for all EMSL facilities appropriate?

HFMRF is exemplary among EMSL facilities in the effectiveness of its user allocation model. Calls requesting proposals for use of the facility are issued twice a year and are well advertised

in the NMR community, and the demand exceeds the amount of available instrument time. External peer review is effectively utilized in the evaluation of user applications. However, the reviewers recognized that areas of potentially very high scientific impact were not being as effectively identified as might be possible in the call for usage. EMSL and HMFRF should be more aggressive in seeking out users who are likely to utilize the unique capabilities (and potential future capabilities that would also be unique) to enhance the scientific impact of its activities. The staff's success in providing resources and/or collaborations with world leaders in the field should be regarded as a major objective.

Could changes be made to increase the impact of EMSL on DOE science goals?

As recommended above, HFMRF should be more pro-active in seeking out users with specialties in other areas of science (beyond magnetic resonance) who might be able to leverage the instrumental capabilities to address highly important scientific problems. This includes applications throughout many areas of environmental molecular science, such as analysis of radionuclides.

Given a flat budget for ERSD, what priority should EMSL have within the Division's portfolio?

The reviewers certainly recognize the need for a clearer set of priorities with HFMRF and EMSL in general. Although the reviewers do not have sufficient information to make specific recommendations for HFMRF at this time, a few general comments and recommendations are in order. EMSL, BER, and DOE management must be aware that a cursory review of HFMRF might lead to inaccurate conclusions about the relative value of each instrument in the facility. This is a complex set of issues that is far beyond the scope of a short visit. Priorities should be established in consultation with an external, HFMRF Scientific Advisory Committee that includes a significant number of scientific leaders who are not currently HFMRF users. This committee should meet at least monthly by phone conference, and it should not be treated as a rubber stamp for yearly application.

HFMRF provided the reviewers with a list of significant upgrade areas ("Potential Investments"). All have intrinsic merit. HFMRF, in consultation with the user community, EMSL management, and the HFMRF Scientific Advisory Committee, should assign priority on the basis of augmentation/addition of unique capabilities; impact on ongoing user activities; and refreshment of existing resources. Note that the reviewers order these criteria from most to least important; *i.e.*, the reviewers view augmentation and/or addition of unique capabilities as the highest priority for long-term planning. Impact on ongoing user activities should also be considered as part of year-to-year planning. Refreshment of existing resources is addressed further below.

Does the EMSL have a well-defined plan to refresh capital equipment, and is it appropriate? What short- and long-term strategies should be considered in this context? Does EMSL appropriately manage the acquisition, use and retirement of instruments?

The panel considered the "refreshment strategy" to be non-ideal for promoting scientific activities with the highest impact. Refreshment or replacement of existing instrumentation with

identical models should in general be avoided. This is an inefficient use of resources. If the same capabilities are being maintained, these routine maintenance activities should be managed from the operational budget; sufficient funds must be allocated and HFMRF given appropriate liberty to respond to needs in a timely fashion. This short-term strategy should keep instruments operational as designed and add capabilities by in-house development as noted above.

How does EMSL manage general user access to equipment purchased with non-ERSD funds? How does this impact EMSL operation as an ERSD-supported user facility?

In consultation with ERSD, EMSL should develop a consistent model for how non-ERSD capital funded equipment is to be used. For example, the beamline model of 25 percent of general user accessibility should be considered.

SUMMARY ANSWERS TO THE QUESTIONS POSED IN THE CHARGE LETTER

Does the relationship and management structure among EMSL, PNNL and ERSD foster the highest quality of science at EMSL?

Although the review committee is encouraged by the apparently strengthened interactions between the EMSL director and the PNNL director, the highest quality of science will not be achieved until there is agreement between EMSL, PNNL, and ERSD as to the mission of EMSL. ERSD should play a more active role than is currently the case in helping to ensure that EMSL satisfies its mission. Further, it appears that a major issue that needs resolution is the relative amount of activity within EMSL that is associated with PNNL-initiated research. A properly constituted and active Scientific Advisory Committee may provide invaluable assistance in prioritizing medium- and long-term objectives that address both PNNL research needs and those of the broader community.

Is the science conducted at EMSL cutting edge? If so, is it appropriate for a BER-supported user facility?

In general, the science conducted in the EMSL is of very high quality, and a significant amount is, indeed, cutting edge. It is appropriate for BER to support this Laboratory that is a national resource.

Is EMSL appropriately structured to support a full range of DOE and national science research priorities?

No single laboratory can support a "full range" of DOE and national science research priorities. However, EMSL does support a significant range of research priorities. Greater impact might be achieved if more of the projects conducted within the EMSL took advantage of capabilities in more than one of the six facilities.

Is the user model for allocating resources for all EMSL facilities appropriate? Does EMSL attract the best mix of users?

There is no consistent model for attracting users to EMSL or for allocating time within a given EMSL facility. It is strongly recommended that each facility develop and implement a transparent process for soliciting and reviewing proposals for the use of that facility, and there should be consistencies across the six facilities. There should be clear criteria for assessing scientific merit, alignment with EMSL resources, and relationship to national research needs. Further, proposals that request time on instrumentation in more than one facility should be encouraged. In those facilities for which there is not currently an open, transparent solicitation, users are essentially solicited by word of mouth. It is reasonable to assume that many highly qualified scientists who could take advantage of EMSL are not being reached by this process, and, hence, the best mix of users is not being attracted to this important resource.

Could changes be made to increase the impact of EMSL on DOE science goals?

The first change that must be made is that there must be agreement between EMSL, PNNL, and ERSD as to the mission of EMSL. A strategic plan should be established to support that vision, and clear goals appropriate to that vision must be defined and monitored for each of the facilities. There must be a transparent process for soliciting and reviewing proposals at all facilities, and cross-cutting research must be encouraged. The addition of radiological capabilities would also strengthen the impact on some of DOE's environmental goals.

Given a flat budget for ERSD, what priority should EMSL have within the Division's portfolio?

The EMSL is a unique national resource, and it should have a very high priority within the Division's portfolio. Whether it is through ERSD (or other BER funds), or through cooperation with other funding agencies (*vide supra*), the operating budget for EMSL must be increased. In addition to the issue of refreshing capital equipment, there simply is not sufficient fiscal support for the technical staff members who provide direct, hands-on support for the users of many of the very sophisticated pieces of equipment. Thus, there is research capacity within EMSL that has lain idle.

Does the EMSL have a well-defined plan to refresh capital equipment, and is it appropriate? What short- and long-term strategies should be considered in this context? Does EMSL appropriately manage the acquisition, use and retirement of instruments?

While EMSL has taken steps, some of which are quite creative, to refresh capital equipment in the short-term, there is no long-term plan (except in the case of MSCF). This must be achieved in collaboration with ERSD and, possibly, in collaboration with other funding agencies. Refreshment of capital equipment must be prioritized, and a reconstituted Scientific Advisory Committee should become active in the prioritization process. Prioritization may result in the decommissioning of some equipment in order to maintain the quality of the most creative programs and those most critical to DOE and other national needs.

How does EMSL manage general user access to equipment purchased with non-ERSD funds? How does this impact EMSL operation as an ERSD-supported user facility?

A significant amount of equipment housed within EMSL was purchased with funds other than those provided by ERSD through the operations budget. In most cases, EMSL users are granted at least limited access to this equipment, and, hence, there can be benefits to the overall operation. It should be noted, however, that both the acquisition and the use of such equipment is on an *ad hoc* basis, and it is strongly recommended that a plan be established for acquiring and managing such equipment, including processes for making such equipment available to the broad user community.

APPENDIX A: Charge letter to BERAC from Dr. Orbach

Department of Energy
Office of Science
Washington, DC 20585

November 18, 2004

Office of the Director

Dr. Keith O. Hodgson
Director, Stanford Synchrotron Radiation Laboratory
Department of Chemistry
Stanford University
Stanford, CA 94305

Dear Dr. Hodgson: Keith

The William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), which is located at the Pacific Northwest National Laboratory (PNNL) in Richland, Washington, is the premier national scientific user facility within the Office of Biological & Environmental Research (OBER). The initial DOE investment in over 100 leading-edge instrumentation and computational capabilities for molecular-level environmental research within EMSL exceeded $100 million. Since opening in October 1997, the number of EMSL users has increased from approximately 700 to 2500 annually. The scientific success of the facility, the increasing cost of operations and the need to refresh cutting edge instrumentation necessitates an examination of the vision, structure and operation of this important facility. The current vision of EMSL as the "premier science facility of BER" requires focus to guide resource investments and to identify future avenues of emphasis within the context of projected flat funding across BER programs.

By this letter, I am charging the BERAC to provide advice to the Office of Science on the mission, operation and future plans of EMSL. I would like a review panel to consider and evaluate the following issues:

- Does the relationship and management structure among EMSL, PNNL and ERSD foster the highest quality of science at EMSL?
- Is the science conducted at EMSL cutting edge? If so, is it appropriate for a BER-supported user facility?
- Is EMSL appropriately structured to support a full range of DOE and national science research priorities?
- Is the user model for allocating resources for all EMSL facilities appropriate? Does EMSL attract the best mix of users?
- Could changes be made to increase the impact of EMSL on DOE science goals?
- Given a flat budget for ERSD, what priority should EMSL have within the Division's portfolio?

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- Does the EMSL have a well-defined plan to refresh capital equipment, and is it appropriate? What short- and long-term strategies should be considered in this context? Does EMSL appropriately manage the acquisition, use and retirement of instruments?
- How does EMSL manage general user access to equipment purchased with non-ERSD funds? How does this impact EMSL operation as an ERSD-supported user facility?

I request that BERAC report on its findings and recommendations at its Fall 2005 meeting.

Sincerely,

Raymond L. Orbach
Director

APPENDIX B: Roster of the BERAC Subcommittee

Michelle S. Broido, PhD (Chairman, Member of BERAC)
Associate Vice Chancellor for Basic Biomedical Research
University of Pittsburgh

Carolyn J. Cassady, PhD
Associate Professor of Chemistry
University of Alabama

David Cowburn, PhD
President and CEO
New York Structural Biology Center

Paul V. Dressendorfer, PhD
Biomolecular Interfaces and Systems Department
Sandia National Laboratories

Jeremy M. Hales, PhD
Owner and Principal
Envair

Janet G. Hering, PhD
Professor of Environmental Science and Engineering
California Institute of Technology

Inez Hua, PhD
Associate Professor of Civil Engineering
Purdue University

Lynn E. Katz, PhD
Associate Professor of Civil, Architectural, and Environmental Engineering
University of Texas

Chad M. Rienstra, PhD
Assistant Professor of Chemistry
University of Illinois at Urbana-Champaign

Ralph Z. Roskies, PhD
Professor of Physics
Scientific Director, Pittsburgh Supercomputing Center
University of Pittsburgh

David H. Russell, PhD
Director, Laboratory of Biological Mass Spectrometry
Department of Chemistry
Texas A&M University

Charles G. Wade, PhD
Manager, Materials Analysis and Characterization
IBM Almaden Research Center,

Mavrik Zavarin, PhD
Environmental Sciences Division
Lawrence Livermore National Laboratory

APPENDIX C: Lehman Charge Letter

DATE: February 4, 2005

REPLY TO
ATTN OF: SC-70

SUBJECT: Operations Review of the William R. Wiley Environmental Molecular Sciences Laboratory

TO: Mr. Daniel R. Lehman, Director, Office of Project Assessment, SC-81

The Biological and Environmental Research (BER) program supports the operation of the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), a national scientific user facility located at the Pacific Northwest National Laboratory (PNNL) in Richland, Washington. The EMSL is supported by BER to develop and provide advanced experimental and computational capabilities to the scientific community to conduct interdisciplinary, collaborative research in molecular-level environmental science.

This memorandum is to request that you organize and conduct a review of the EMSL to evaluate its present performance and cost of operations, staffing, and funding. This review will be conducted in conjunction with a programmatic review of EMSL being conducted by BERAC on May 17-19, 2005.

It is requested that your review committee evaluate the EMSL's operations and address the following questions:

1. Are EMSL and PNNL management roles and responsibilities effectively carried out and coordinated?
2. Is EMSL management effectively setting priorities, tracking progress, and resolving problems that impact laboratory operations?
3. Are there adequate resources to accomplish the BER mission at EMSL in the context of a flat budget (FY 2005 and outyears)? Are the EMSL processes for allocating and managing BER resources (manpower and funds) appropriate?
4. Is the BER mission at EMSL impacted by non-BER sources of Operations or CE funding?
5. Is there an ongoing program of self-assessment or external benchmarking aimed at continuously improving EMSL's management and operations?

I very much appreciate your assistance in this matter. The insights and recommendations of your review team will be important to our future management of EMSL. I look forward to receiving your Committee's formal report within 60 days of the review.

[SIGNED]

Aristides Patrinos
Associate Director
Office of Biological and Environmental Research
Office of Science

cc:
R. Orbach, SC-1
J. Decker, SC-2
L. Dever, SC-3
M. Kuperberg, SC-75
P. Bayer, SC-75
P. Kruger, PNSO
L. Peters, PNNL
A. Campbell, EMSL
M. Broido, University of Pittsburgh

APPENDIX D: Agenda

May 17, 2005		Location
7:00 a.m.	**Transportation to EMSL** *A&A Motorcoach pick-up outside of hotel; Brittney Drollinger, PNNL escort*	Red Lion Kennewick
7:30 a.m.	**Badging/Check In**	EMSL Lobby
7:30 a.m.	**Breakfast** *Paul Kruger, Jeff Day, Allison Campbell, Gordon Anderson, and Reviewers*	EMSL 1075/1077
8:00 a.m.	**Joint Executive Session** *Paul Kruger, Jeff Day and Reviewers*	EMSL 1077
9:00 a.m.	**Laboratory Welcome & Introductions:** Len Peters/Paul Kruger/Allison Campbell *Open Plenary Session*	EMSL 1077
9:15 a.m.	**Overview of DOE Office of Biological and Environmental Research Vision for EMSL**: Mike Kuperberg *Open Plenary Session*	EMSL 1077
9:45 a.m.	**Break**	
10:00 a.m.	**PNNL Vision for EMSL:** Len Peters	EMSL 1077
10:15 a.m.	**EMSL Overview:** Allison Campbell *Open Plenary Session*	EMSL 1077
11:15 a.m.	**EMSL Science:** Allison Campbell *Open Plenary Session*	EMSL 1077
12:15 p.m.	**Advisory Committees:** Len Spicer/Allison Campbell *Open Plenary Session*	EMSL 1077
12:30 p.m.	**Lunch** *Reviewers and Len Spicer*	EMSL 1075/1077
1:30 p.m.	**EMSL Tour** (Molecular Science Computing Facility/Graphics and Visualization Laboratory/1130, 1309, 1410, 1526, 1611, Instrument Development Laboratory)	
2:30 p.m.	**Lehman Subcommittee Breakout Sessions** • *TBD* • *TBD* • *TBD*	 EMSL 1075 EMSL 1029 EMSL 1036
2:30 p.m.	**Broido Subcommittee Plenary – Cross Cutting Science:** Gordon Anderson • EMSL Scientific Grand Challenges: John Zachara/Jim Fredrickson/Himadri Pakrasi • Structural Genomics Collaborative Access Team: Mike Kennedy *Open Plenary Session*	EMSL 1077

4:00 p.m.	**Broido Subcommittee Breakout Sessions**	
	• Chemistry and Physics of Complex Systems: Lynn Katz/Jake Hales	EMSL 1185
	• Environmental Spectroscopy and Biogeochemistry: Inez Hua/Janet Hering	EMSL 1585
	• Interfacial and Nanoscale Science: Paul Dressendorfer/Chuck Wade	EMSL 2185
	• High-Performance Mass Spectrometry: David Russell/Carolyn Cassady	EMSL 1385
	• High-Field Magnetic Resonance: David Cowburn/Chad Rienstra	EMSL 2385
	• Molecular Science Computing: Ralph Roskies/Mavrik Zavarin	Graphics Vis. Lab
5:00 p.m.	**Lehman Executive Session**	EMSL 1075
5:00 p.m.	**Broido Executive Session**	EMSL 1077
5:30 p.m.	**Joint Executive Session**	EMSL 1077
6:30 p.m.	**Adjourn**	
6:30 p.m.	**Wine Reception and Poster Session**	EMSL Lobby
	Reviewers, Len Peters, Len Spicer, Steve Colson, EMSL Management	
7:00 p.m.	**Dinner**	Dr. Bill's Bistro
	• Roy Gephart, "An Overview of Hanford Nuclear Waste History"	
	Reviewers, Len Peters, Len Spicer, Steve Colson, EMSL Management	
9:00 p.m.	**Transportation to Hotel**	Outside EMSL
	A&A Motorcoach to Red Lion Kennewick	

May 18, 2005		Location
7:30 a.m.	**Transportation to EMSL** *A&A Motorcoach pick-up outside of hotel*	Red Lion Kennewick
8:00 a.m.	**Breakfast**	EMSL 1075/1077
8:30 a.m.	**Joint Plenary – Refreshment of Scientific Capabilities:** Gordon Anderson *Open Plenary Session*	EMSL 1077
9:30 a.m.	**Broido Subcommittee Breakout Sessions**	*Facility Labs or*
	• Chemistry and Physics of Complex Systems: Lynn Katz/Jake Hales	EMSL 1185
	• Environmental Spectroscopy and Biogeochemistry: Inez Hua/Janet Hering	EMSL 1585
	• Interfacial and Nanoscale Science: Paul Dressendorfer/Chuck Wade	EMSL 2185
	• High-Performance Mass Spectrometry: David Russell/Carolyn Cassady	EMSL 1385
	• High-Field Magnetic Resonance: David Cowburn/Chad Rienstra	EMSL 2385
	• Molecular Science Computing: Ralph Roskies/Mavrik Zavarin	Graphics Vis Lab
9:30 a.m.	**Lehman Subcommittee Breakout Sessions**	TBD
	• TBD	
12:00 p.m.	**Lunch** *Reviewers, Allison Campbell, Gordon Anderson, Invited Researchers*	EMSL 1075/1077
1:00 p.m.	**Broido Subcommittee Breakout Sessions**	Facility Labs or
	• Chemistry and Physics of Complex Systems: Lynn Katz/Jake Hales	EMSL 1185
	• Environmental Spectroscopy and Biogeochemistry: Inez Hua/Janet Hering	EMSL 1585
	• Interfacial and Nanoscale Science: Paul Dressendorfer/Chuck Wade	EMSL 2185
	• High-Performance Mass Spectrometry: David Russell/Carolyn Cassady	EMSL 1385
	• High-Field Magnetic Resonance: David Cowburn/Chad Rienstra	EMSL 2385
	• Molecular Science Computing: Ralph Roskies/Mavrik Zavarin	Graphics Vis Lab
1:00 p.m.	**Lehman Subcommittee Breakout Sessions**	TBD
	• TBD	
3:00 p.m.	**Lehman Executive Session**	EMSL 1075
4:30 p.m.	**Broido Executive Session**	EMSL 1077
5:00 p.m.	**Joint Executive Session**	EMSL 1077
6:00 p.m.	**Adjourn**	
6:15 p.m.	**Transportation to Hotel** *A&A Motorcoach to Red Lion Kennewick*	Outside of EMSL

May 19, 2005		Location
7:00 a.m.	**Lehman Subcommittee Check Out of Hotel/Transportation to EMSL** *A&A Motorcoach pick-up outside of hotel* *Luggage can be stored in EMSL Director's suite*	Red Lion Kennewick
7:30 a.m.	**Breakfast** *Reviewers Only*	EMSL 1077
8:00 a.m.	**Lehman Breakout Sessions/Report Writing**	EMSL 1075/TBD
8:00 a.m.	**Broido Breakout Sessions/Report Writing**	EMSL 1077/TBD
9:00 a.m.	**Lehman Subcommittee Dry Run**	EMSL 1075
11:00 a.m.	**Lehman Subcommittee Closeout with Lab Management & Broido Subcommittee**	EMSL 1077
12:00 p.m.	**Lunch and Lehman Subcommittee Adjourn** *Reviewers Only*	EMSL 1077
1:00 p.m.	**Transportation to Airport for Lehman Subcommittee** *Van transportation to airport*	Outside EMSL
1:00 p.m.	**Broido Report Writing**	EMSL 1077
3:30 p.m.	**Broido Dry Run**	EMSL 1077
4:30 p.m.	**Broido Closeout with Lab Management** *Subcommittee, Len Peters, EMSL Management*	EMSL 1077
5:30 p.m.	**Broido Subcommittee Adjourn**	
5:45 p.m.	**Transportation to Hotel** *Van transportation to Red Lion Kennewick*	Outside EMSL
As needed	**Transportation to Airport for Broido Subcommittee** *Hotel Shuttle Service*	