Published November 2016

This proposal guidance is in effect for general and science theme research proposals submitted during the 2017 fiscal year. Separate guidance for joint facility proposals or research campaigns is available from the published Call.

EMSL awards the majority of resources to proposals responding to the annual calls/cycles. If you're responding to one of these, we encourage you to submit your proposal early to allow time before the deadline to make any edits or corrections noted by EMSL staff during the screening process.

Before beginning a proposal, please take a minute to review Tips for Writing a Successful Proposal. These tips are a collection of comments or suggestions that have been made over the years by our proposal reviewers. As always, however, a key component to developing your proposal will be discussions with the appropriate Capability Lead(s) based on your research goals and resource needs. Capabilities and contact information are detailed on EMSL's capability web pages.

Proposal Package Guidance

An EMSL user proposal requires detailed information for a thorough peer and management review. The Proposal Planning document (.pdf) will walk you through the information needed to complete the web-based proposal form via the User Portal and help you track your progress. Conforming to the instructions provided below is required and will be strictly enforced. Proposals that are not consistent with these instructions will be returned without review.

Please Note: *While anyone can write and submit the proposal on behalf of the research team, postdocs and students* ***may not serve as primary authors****.*

Document Formatting

- Pagination is required
- 11 point fonts (or larger for headings), Times New Roman (recommended)
- 1 inch margins
- No more than 5 lines of text within a vertical space of one inch
- Single-spaced (recommended); double-spaced is accepted but must meet established page limits
- Single-column format for text
- Adobe (.pdf) file format

Captions, symbols, special characters, can have a font of less than 11 points.

Project Description

Describe your research plan for using EMSL resources (***maximum*** of 4 pages). Visual materials, including charts, graphs, maps, photographs and other pictorial presentations must be included in

the 4-page limit. A separate abstract will be required as part of the online proposal form, and will be provided to the reviewers as part of your proposal package. The abstract submitted on the web-based proposal form does **not** count against your 4-page limit and ***should not be repeated*** in your Project Description. The abstract will be posted, as submitted, on EMSL's website if your proposal is accepted.

Remember to write the Project Description at a level appropriate for someone familiar with the general area of your research, but not necessarily an expert on the specific topic. To assist in targeting your research description to meet all required proposal elements, be sure to read the EMSL Proposal Review Criteria, which includes potential considerations within each criterion, and the scoring descriptions.

The Project Description must include the following sections:

- **Title**. The project title must be brief, scientifically or technically valid, intelligible to a scientifically or technically literate reader, and suitable for use in the public press.

- **Specific Aims** (generally 250 words or less). State the specific objectives of the research proposed (e.g., to test a stated hypothesis, create a novel design, solve a specific problem, challenge an existing paradigm or clinical practice, address a critical barrier to progress in the field, or develop new technology), providing concise and unambiguous details.

- **Mission Relevance** (2-3 sentences). Clearly explain how your research addresses specific mission areas and advances the science pertinent to DOE's Office of Biological and Environmental Research and/or describe the value/impact of its economic or societal importance. Just stating there is a linkage is not enough; you need to describe it in detail and show what your project will add to their portfolio.

- **Background/Introduction** (approximately 400 words or less). State the scientific question(s) being addressed, and the anticipated importance or significance of results to be obtained, especially as related to EMSL's mission.

- **Approach or Work Plan** (approximately 1200 - 1500 words). Describe the work to be conducted at EMSL in the first year of the project, along with any preliminary, background measurements, or tests completed that validate the approach (include references where relevant and attach the full citations as an addendum). Be sure to state which team member will be doing which portion of the work plan and demonstrate why your project requires EMSL resources and cannot be done anywhere else. Be specific and if your research includes samples, provide a description, along with any unique characteristics (e.g., transgenic biological material, dilute solution or environmental samples containing explosives, soil or ground waters collected from Hanford, etc.), and an estimated timeline for when your samples will be ready. Poor justification can affect the overall science and resource scores.

- **Computing Approach (required if compute cycles requested, additional one-page maximum)**. The Computing Approach does **not** count against the 4-page limit, but **is *required if compute cycles are requested***. There is no upper limit on node-hours that can be

requested, but the amount of time requested ***must be justified in this section and tied to the scientific aims.*** Poor justification of the computing need for the project can affect the science and resource scores. If you have any questions regarding these requirements, please contact the Capability Lead for MSC Scientific Consulting.

- ***Software.***
  The PI should specify the computational method or approach, software to be used, and provide a strong justification for the hours requested. Specifically, the following details should be included:
  - Software codes you will be running (NWChem, VASP, etc.). If applicable, reference a web-link (e.g. to github or other source code repository).
  - Indicate if the software is already on Cascade (http://www.emsl.pnl.gov/MSC/UserGuide/compute_jobs/available_science_applications.html).

    If it is not, but you have used it on other supercomputers, provide information about the computing system used. For example, indicate the typical run (XX nodes, using YY cores, running for ZZ days or hours), processor speed, and memory per node.
- ***Computing Resources Requested.***
  Provide details for your computing request (see table below), including the total number of node-hours requested for the first year of the proposal, data archive storage needs, and the number of simulations/analyses you plan to run with each code on Cascade. Provide some indication of the expected average number of node-hours needed per simulation/analysis.

  Note: Allocations are awarded in units of wall-clock time expressed in node-hours. Each Cascade node contains 16 processor cores. Consequently 150,000 Cascade node-hours are equal to 2,400,000 processor core-hours. Cascade can deliver a total of 12,000,000 node-hours per year.

Total Compute Hour Request for first year of proposal: 375,000					
Total Data Archive Request for first year of proposal: 3 GB					
Software Details	***Estimated # of jobs***	***Average node hours per job***	***Total Node Hours***	***Project Team Expertise***	***EMSL Support Requested*** *Specific needs (e.g., compiling code, libraries needed, help running jobs, etc.)*
NWChem	50	1,500	75,000	New user	Name of MSC staff member with whom this request has been discussed
TETHYS	20	15,000	300,000	Expert user	Support for porting existing codes onto Cascade

CVs and Additional Information

As part of the proposal package, please include the following information as appendices *in the order listed below:*

1. **Appendix 1: References Lists**
   Reference information is required, but should not be embedded in the text. Instead, attach the list as Appendix 1. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. If the document is available electronically, the website address also should be identified. Proposers must be especially careful to follow accepted scholarly practices in providing citations for source materials relied upon when preparing any section of the proposal. While there is no established page limitation for the references, this section must include bibliographic citations only and *must not be used to provide parenthetical information outside of the 4-page Project Description.*

2. **Appendix 2: CV's (required)**
   Attach abbreviated CV's **(2-page maximum each)** for the PI and each of the key investigators that would support the review of the team's qualifications for the research proposed (Criterion 2).

3. **Appendix 3: Experimental EMSL Resources (required).**
   Include a table of experimental resources requested for the **first year** of your project (instruments **and** EMSL staff support), including the number of samples (if applicable), estimated date(s) of sample shipment, instrument units requested (see note below), the expertise on each resource to be provided by your team members (including duration of EMSL stay), and EMSL staff support being requested. "Units Requested" can be instrument hours or products.

   Note: If you are unsure how to fill out the table, contact the instrument scientist or Capability Lead listed on the website ***at least two weeks prior to published deadlines***. They'll work with you regarding the specific needs for your research aims. Failure to complete the table correctly can affect your proposal's resource score.

Experimental Resources	**# of Samples**	**Estimated sample shipment date to EMSL**	**Units Requested (specify unit)**	**Project Team Expertise per Resource**	**EMSL Support Requested**
XPS Quantera	15	November 2016	720 hours	Will send postdoc to operate but needs training	Analysis of data
Microfabrication Clean Room	NA	Will send design specifications by January 2017	10 glass/silicon micromodels	NA	Micromodels to be fabricated by EMSL staff
X-Ray Diffraction, Microbeam	50	December 2016	100 hours	None	Operator and analysis

Environmental TEM	5	January 2017	100 hours	Expert operator	Sample prep and analysis
LTQ	15	March 2017	100 hours	Analysis	Operator and AMT tags

4. **Appendix 4: Active Collaborator List (required)**
   To help EMSL avoid conflicts of interest on our Proposal Review Panels, please attach a list of active collaborations (see example below) that the PI and co-PI(s) have had in the past 2 years. In addition to research projects, collaborations might include co-authors *with whom you've actively interacted*, co-editors, advisors or advisees or financial affiliations with an institution or individual.

   Participation in very large collaborative efforts with an individual does not necessarily constitute a conflict of interest. Identify those who would have a personal interest in this proposal or whose unbiased judgment would be questioned by a reasonable person familiar with your relationship. You may substitute a list from a recent NSF, DOE, or other proposal that meets the spirit of this request, and lists in excess of 100 collaborators (per investigator) can be shortened to include only the closest collaborators. Please use your best judgment in these cases.

CONFLICT OF INTEREST LIST				
Name	**Key Co-Author**	**Collaborator**	**Advisee/Advisor (Specify)**	**Other (Specify Nature)**
Agarie, Jeremy	X	X		
Antony, Mark	X		Advisor	
Barnes, Jeremy	X	X		
Blaxter, Johan	X			Co-owner private company
Cushman, Joan	X			
Jones, Maurice		X	Advisee	

5. **Appendix 5: Suggested Reviewers or Reviewers Not to Include (optional)**
   Proposers may include a list of suggested reviewers who they believe are especially well qualified to review the proposal and who are not recent collaborators/co-authors. Proposers also may designate persons they would prefer not review the proposal, indicating why. These suggestions are optional and the decision whether or not to use the suggestions remains with EMSL management.