

MSC Computationally Intensive Research Applications Electronic Proposal Guide

Deadline for receipt of complete proposals for CIRA is Friday, 5:00 PM (PDT), May 1, 2009

A **Letter-of-Intent** is no longer required. We recommend the Team Leader review the EMSL Call for Proposals (<http://www.emsl.pnl.gov>) before submitting their team's proposal to the EMSL User Portal. Please contact the MSC (mscf@emsl.pnl.gov) or 509-371-6448) with any questions on the call for proposals or this form.

ONLY THE FIRST YEAR'S WORTH OF RESEARCH NEEDS TO BE SUBMITTED FOR REVIEW.

Proposal Submission Requirements. The Team Leader (or delegate) is required to submit the CIR proposal for their team. All proposals are required to be submitted electronically via the EMSL User Portal. No paper proposals will be accepted. All parts of the electronic proposal form must be completed and submitted together at the same time for a proposal to be considered complete. Incomplete proposals will not be accepted or reviewed. All proposals must follow the format specified below. Proposals that do not follow the instructions, omit required information, or deviate from the proposal format will be considered as incomplete proposals, and will not be accepted or reviewed. Once a proposal is submitted, it cannot be modified by the author. If changes need to be made, please contact the MSC (see first paragraph).

Before entering the EUS, PIs should gather information regarding team members' names, affiliations and other information (described below) for entry into the form. Part of the EUS includes the capability to attach large sections of your proposal as Adobe PDF files or as Microsoft Word files. **The complete proposal must be submitted via the EMSL User Portal at <http://eus.emsl.pnl.gov/Portal>.** An acknowledgment for receipt of a complete proposal will be sent by e-mail to the Team Leader. Each research participant entered into the EUS will receive an EMSL user ID number if they don't already have one from a previous proposal.

The following information will be needed for each participant on the proposal:

- Prefix (Dr. or Mr. or Ms.)
- First Name
- Full Middle Name (use NMN if no middle name)
- Last Name
- Suffix (if necessary)
- Primary Citizenship
- Secondary Citizenship (optional)
- Profession (*i.e.*, Professional, Student, Postdoc, Research Scientist, Faculty/staff, Retired)
- Telephone number
- Facsimile number (optional)
- Email address
- Institution Name
- Type of Institution (*i.e.*, Academic, National Lab, *etc.*)
- Department (optional)
- Business Address
- Country
- State
- City
- Postal Code
- Curriculum Vitae (for PI and up to six principal participants, to be added as Attachments)

The EMSL Usage System (EUS) is designed as a central web-based utility for establishing and tracking collaborations with the EMSL and is entered by logging into the EMSL User Portal. As you go through the EUS, the first web page will have general information and list open or saved proposals. For a new CIR proposal applications, click on the “Create New Proposal” button in the upper right. The actual proposal submission section is divided into four parts:

- **Participants** – needs to be repeated for each team member,
- **Details** – research details are attached here including computer time needed,
- **Logistics** – questions about funding and materials.
- **Submit Proposal**

The first participant should be the Primary Author who is also referred to as the Team Leader or Principal Investigator. The Principal Investigator should not be a Post-doc or graduate student. The second section includes details of the research, a place to attach the bulk of the proposal, and anticipated computational needs. The third section contains questions about funding, materials to be used, and any additional comments. MSC Computationally Intensive Research projects are generally non-proprietary in nature with results to be published in the open literature. Users engaged in proprietary research at EMSL are obligated to pay full cost recovery for their use of EMSL.

If you need to save your work and return later to complete it, use the “Save” button at the top of the page. [To return to the saved proposal if you have closed your browser, go to <http://eus.emsl.pnl.gov/Portal> and log in again. Select from the list of saved proposals the proposal you want to return to.]

A step-by-step description of what data needs to be entered into the EUS starts below. Please review the requirements and have information and documents ready **before you begin**. The Adobe PDF or Microsoft Word files should be prepared ahead of time for quick attachment. **Please follow the maximum page limits for each section. All sections listed below under “Attachments:” must be included for the proposal to be complete.**

Before you enter the EMSL User Portal, you may need to agree to the Terms and Conditions for Using EMSL. The URL for the User Portal is <http://eus.emsl.pnl.gov/Portal>. After reading the terms and conditions, and you agree with the terms and conditions, select “I Agree” to enter the EUS.

Participants

Research Team Leader:

Please enter the information listed below for the Team Leader first. A separate window will open asking you to “create new user” or select “returning EMSL user.” If a new user, enter required information (see below); if a returning EMSL user enter their last name and choose the person you want from the list. If the person you want is not listed, click “Create a New User” at the bottom right of the Add Participant box. Then enter their name and the rest of the information listed below. You will also be asked if the team member plans on visiting the EMSL. Please respond accordingly. Once you have added the primary author (team leader), select “Add Participant” to enter information for each additional team member. Postdoctoral and graduate students only need to be included if they will need computer accounts.

After all participants have been added, click on Details next to the #2.

Proposal Participant

Prefix:

First Name:

Full Middle Name: (no initials; if no middle name, use "NMN")

Last Name:

Suffix: (if necessary)

Primary Citizenship

Secondary Citizenship (if necessary)

Profession (*i.e.*, Professional, Student, Grad Student, Postdoc, Research Scientist, Faculty/staff):

Telephone number:

Facsimile number: (optional)

Email address:

Institution Information

Institution Name:

Type of Institution: (Select from the pop-up window)

Department: (if applicable)

Business Address:

Country: (Select from the pop-up window)

City

Postal Code

Details

Proposal Details

Primary Research Area:

Choose the research area most closely associated with your proposal. These areas are most in line with the DOE's research directives. If none of these listed are appropriate, select "Other" and specify it in the next field.

- Biological and Life Sciences (excludes medical applications)
- Chemistry (excludes materials chemistry)
- Earth Sciences
- Engineering
- Environmental Sciences
- Materials Sciences (incl. condensed matter phys. & materials chem..)
- Medical Applications
- Optics
- Physics (excludes condensed matter physics)
- Polymers
- Other - Specify

Title:

The title for the proposal should be short and concise.

Proposal Abstract [Maximum 2 paragraphs]:

This should be about 500 words in length, briefly describing *what will be done in general terms since this abstract will be publically displayed on our Web pages if approved*. This can be cut and pasted from a previously prepared Word document. **Do not duplicate in the main body text.**

Proposed Research (.doc or .pdf):

This is where the bulk of the proposal will be entered. This should be entered as a single document for research planned for the first year. The “Additional files” section should contain the Appendix and CVs. They will all be attached to the EUS proposal sent for external peer review. A description of each section follows. The maximum length for each text section is shown in brackets. Font size and type should be 11 or 12 for “Times New Roman” or 12 for Garamond. Margins can range from one inch to half an inch on top, sides and bottom.

1. Project Definition [Maximum 1 page]:

Define project and objectives including background and relevance to the environmental problems and research needs facing the U.S. Department of Energy and the Nation. What is the “Computationally Intensive” aspect of the project? Into which EMSL Science Theme(s) does the research fit or would benefit? Why is this research worth doing?

2. Proposed First Year of Work [Maximum 2 pages]:

Describe the proposed work in enough detail to justify resource allocation. Describe the computational methods/approach that will be used. Give expected outcomes/results from the project and their impact on DOE environmental mission goals ([Click Here for goals](#)). Include a project work plan for the first year’s work. This section **MUST** contain enough information for a reviewer familiar with this type of research to answer these questions: What is the scientific merit and quality of the proposed research and is there potential to contribute significantly to highly cited publications?

3. References:

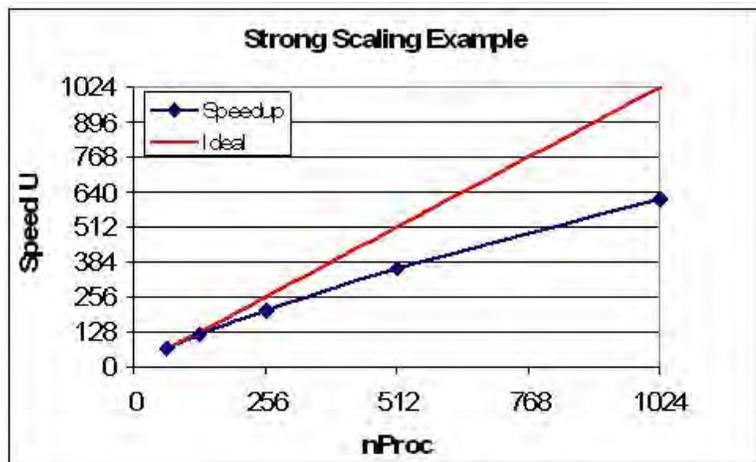
Include the appropriate reference citations for the proposed research.

Additional files (.doc, .pdf, or graphics only):

This is where the rest of the details required for the Computationally Intensive Research applications must go. It consists of an Appendix with several sections given below and CVs for the PI and a co-PIs. They will all be attached to the EUS proposal sent for external peer review. A description of each section follows. The maximum length for each text section is shown in brackets. Font size and type should be 11 or 12 for “Times New Roman” or 12 for Garamond. Margins can range from one inch to half an inch on top, sides and bottom.

1. Software [Maximum 1 page]:

List the software program(s) to be used. If they are not currently supported codes ([Click Here for list](#)), then benchmark data must be included in terms of speedup factor *versus* number of nodes (see example below). The plots can be from Chinook or another distributed memory type cluster. If the code is not parallel (or does not efficiently scale), estimate how much computer time will be required to develop an efficient, scalable parallel implementation of the code. If software development/porting efforts are planned, identify the length of time anticipated for that work and the amount of assistance from MSC consulting staff that may be needed. The EMSL does not guarantee availability of any third-party software for a project or user. Users may install their own copy of third party software with the exception of any Gaussian, Inc. software.



nProc	Speedup	Ideal
64	64.00	64.00
128	115.20	128.00
256	204.80	256.00
512	358.40	512.00
1024	614.40	1024.00

Strong Scaling Example

2. Proposed MSC Computational Resources [Maximum 1 page]:

Estimate the MSC computational resources (in node-hours) required for the proposed work for the first year. Chinook has 2 quad-core processors per node. Be as specific as possible (*e.g.*, 64 nodes x 250 wall-clock hours = 16,000 node-hours) and state the basis for your estimate (*e.g.*, runs of previous jobs on MPP2, Chinook or other parallel computers). Remember your code may not be able to use all 8 processor-cores on a node effectively. We plan to have benchmarks available for NWChem on Chinook. For other code, use your best estimate. *The requested computational resources specified here must sum to match those given in the **Logistics** section of the proposal.*

3. Proposed MSC Archival Storage Requirements [Half page Maximum]:

Describe the type and amount of storage needed for the first year. Distinguish between short-term and long-term disk storage. Identify what, if any, types of data in the NWf database your project will make freely accessible to other EMSL researchers and/or publicly available. *The storage resources specified here must be consistent with those given in the **Logistics** section of the proposal.*

4. Curriculum Vitae for Team Leader and Team Members [Maximum 2 pages each].

Include curriculum vitae for the Team Leader plus up to five of the team members. Not all team members need to have a vitae. The vitae should include recent publications relevant to the proposed research. The CVs should include team members with the skill and publication record to convince reviewers of the likelihood for success.

Preferred Start Date:

Choose a date (month, day, and year) when you expect to begin work. The earliest date is October 1, 2009 since this is when we plan to have computational resources available.

Preferred End Date:

Choose a date (month, day, and year) when you expect to complete the work. For a 3-year proposal this would be September 30, 2012.

Proposal Type:

From the pull down list, choose “Current Call...” then click on “Capability” and select “Computationally Intensive Research.”

Is this proposal associated with a National Science Foundation Supplemental Funding Request?

Yes No

Select yes if it is, otherwise select no. Pretty straight forward.

Will you desire the assistance of EMSL staff in obtaining and interpreting the results?

Yes No

Select yes if you anticipate the assistance of EMSL staff, otherwise select no. We are here to help.

PNNL Staff Contact:

If you have discussed this proposal with a PNNL Staff member, please enter his/her name.

EMSL Resources

Since you will be primarily using Chinook, the HP Linux cluster, click on “Add Requested Resource.” Click on the orange + sign next to “Computing.” The list will open up revealing five options. Click on the orange + sign next to “Super Computing.” Finally you will see the Chinook cluster. Click on the green + sign. You can select “Data File Storage” if you will be needing archival storage on the NWfs system. When done, click on the red X in the upper right corner.

Usage:

Click the mouse on the field with the numeral “1” and enter the total number of node-hours requested for the first year. (Allocation awards are expected to be on the order of 350,000-2,000,000 node-hours for a one-year period). For example: “750000” then, hit enter. These amounts should correspond to the time estimates in Section 2 (Proposed MSC Computational Resources) of the additional files (Appendix). Repeat this for any other facility and instrument you will need.

If you make a mistake, just click on the red – sign by the word “Clear.”

When you have completed entering all the data, click “Logistics” next to the #3.

Logistics

Finally, we ask a few questions regarding funding agencies and whether you will need additional equipment or if you intend to bring any equipment or materials to the EMSL as part of this proposal.

Proposal Funding

Funding Agency (Agencies):

Use the pick list provided to select all the agencies from which team members are funded. If “other”, then please specify. Multiple selections can be made by holding down the Ctrl key while clicking with mouse.

Work Package #:

If the Primary Author (Team Leader) is a PNNL employee, include a work package number.

Materials & Equipment

This section probably will all be answered with a No response. But we need to ask for your response. It is possible that you will be including experimental components in the proposal that require one or more of the following:

Will your research involve the use of human blood, tissues, DNA, cells, cell lines, or human biological samples in any form?

Yes No

Does this work involve the use of live animals?

Yes No

Will you be bringing or sending any *chemicals* to the EMSL facility?

Yes No

Will you be bringing or sending any *samples* to the EMSL facility?

Yes No

If you intend to bring any equipment to EMSL as part of this proposed research, please list it in the **User Equipment:** field. If you are bringing a laptop that will need to connect to the PNNL network, please list them as well.

Comments

If you have any additional needs or comments regarding the proposal or the process, please enter them in the **Comment:** field.

When you are finished, select “Submit Proposal” next to the #4.

Remember, once the proposal is submitted, you can no longer modify it. Modifications can be made by the Facility coordinator or EMSL Host if necessary. Just send an e-mail to emsl@emsl.pnl.gov with any modifications.

Congratulations! You are now finished.