

**Advanced Biomedical Computing Center (ABCC)**  
**Application for System Access**

**General Information**

All applications will require a Principal Investigator (PI) to sponsor the group or project. A Project as defined by this application may represent an entire laboratory or organization, or it may represent a specific project within an organization. The PI will need to fill out the initial application form for the group or project by checking the box marked "Applying as P.I. of a Project or Laboratory". Applications for other scientists that are associated with the project or group should also be submitted at that time. As part of the approval process, a project will be established and a Project ID will be assigned. As more investigators are added to your lab or project they may easily be registered any time thereafter. While each associated investigator will need to include their application with the one submitted by the PI, only the PI will need to supply the Activity or Project Abstract (justification for system use). The PI and each associate will receive a unique system USERNAME and password upon approval. In addition, each system user will be assigned a unique User Authentication Code. While this code is not required for accessing any of the computer systems, you will need to retain it for verification when contacting ABCC systems managers for information regarding your account or when requesting a new or reset password. Your User Authentication Code should be kept confidential. A copy of the approved application and a small documentation package will be returned to each successful applicant. Students should not be listed as Principal Investigators.

**Supercomputer Time Allocation**

All awarded supercomputer time will be allocated to the Project Account ID that is established by the PI's application. All investigators that are associated with the project or lab will share the total time allocation. The ABCC will provide each PI with monthly reports showing how supercomputer resources were used by the research staff. It will be up to the PI to manage the use of those resources. The Project Account ID will be required at system login on the supercomputer and as part of the required information with NQS (batch) job submissions. The combination of the USERNAME and the Project Account ID will be verified and used in accounting for all system usage on the PVP supercomputers. Access to the other superscalar servers will not require any Project Account ID during login or batch job submission.

**Submitting Applications**

Applications can be submitted at any time. Please type or print clearly. Applications for general access will be processed on a weekly basis, however, applications for supercomputer time exceeding 40 hours per year will only be reviewed once every calendar quarter. Quarterly application deadlines will be February 15, May 15, August 15, and November 15.

**Acknowledgement Requirements**

All publications should acknowledge the contribution of the NCI Advanced Biomedical Computing Center. (e.g. "We acknowledge the National Cancer Institute for allocation of computing time and staff support at the Advanced Biomedical Computing Center of the Frederick Cancer Research and Development Center.")

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**Password Selection**

Each system user will be assigned a unique **Username** to be used when accessing the ABCC systems. An initial password will also be provided. The initial password will only be valid for a single login session and will need to be changed immediately. Please choose a password that is not easily compromised. In general, your password should **not** be made up of common words that could be found in the dictionary (including foreign languages and the forward and backwards representations of each); they should **not** use any part of your Username; and they should **not** be made from proper names (either people or things). A good password **should** include a combination of letters and numbers, and if upper and lower case characters are permitted, both should be included. One popular method of password selection is to use the first (or last) letter of an obscure phrase with mixed case letters, special characters, and numbers.

**Obtaining and Submitting Applications**

Additional applications are available via any of the following methods:

1. By anonymous ftp to: ftp.ncifcrf.gov > /pub/BSC.application
2. Through the use of the GCG Fetch program: >  

```
$ analysis  
$ gcg  
$ fetch bsc.application
```
3. by U.S. Mail, or FAX
4. or by coming to the administrative office of building 430.

Completed and signed applications may be FAXed directly to Dr. Jacob Maizel's office: (301)846-5598, or sent via U.S. Mail to:

Dr. Jacob V. Maizel, Jr.  
Chief, Laboratory of Experimental & Computational Biology  
NCI/FCRDC, Bldg. 469, Rm. 151  
P.O. Box B  
Frederick, MD 21702-1201

**Note! Accounts are NOT to be shared. Each system user must have an authorized username and account. The ABCC cannot be responsible for information that is lost due to the sharing of system accounts.**

## Conditions of Use of ABCC Resources

1. Accounts are NOT to be shared.
2. ABCC instructions regarding security and password protection must be followed.
3. Project descriptions from this form may be used in ABCC reports.
4. Results and abstracts from research publications will be provided to the ABCC on a regular basis (at least semi-annually).
5. Users will notify ABCC systems administrators immediately upon change in organizational affiliation, mailing address, telephone number, or employment status.

## Instructions

Check all appropriate boxes at the top of the form and **obtain required signatures**. If completing Parts B or C, please don't forget to attach required C.V.'s and bibliographies. All shaded areas are reserved for NCI and ABCC use only.

A copy of the approved application and a small documentation package will be returned to each applicant. Please be sure to note the assigned Username, User Authentication Code, and Project Account ID. These should be kept confidential within the project or group.

### Part A

- Items 1-10: Self Explanatory
- Items 11a-c: List the Principal Investigator (PI) for the project or group in addition to current collaborators. The collaborator list is used for scientific reference only and does not imply that these individuals are authorized to access the ABCC facilities. The application for the project or group **must also include an abstract** describing the research being performed. Additional associates need not include this information.
- Item 12: Describe needs and/or benefits that will be provided by the ABCC systems.
- Items 13-15: Self Explanatory
- Item 16: Describe any special assistance that may be required of the ABCC staff (e.g. consulting, basic system training, special documentation, etc.).
- Item 17: Check all appropriate research categories.

### Part B

- Item 18: Describe current experience with supercomputers to include accounts on other systems and the operating systems that you have used.
- Item 19: Describe supercomputer computational requirements as they apply to your research (e.g. need to perform molecular mechanics/dynamics calculations, quantum chemistry, software packages needed, etc.).
- Item 20: Describe any specific supercomputer support requirements dictated by your research (e.g. consultation on molecular modeling programs, special assistance from ABCC staff, large disk storage requirements, graphics needs, etc.).
- Item 21: All applications requesting more than 5 hours of time require a C.V. and bibliography.

### **Part C**

- Item 22: Total estimated time in CPU hours required for the project or group.
- Item 23a-e: Comprehensive description of the research being performed by your project or group.
- Item 24: List the single job CPU time required of the most frequently used programs or software packages. An example would be the regular use of such programs as GAUSSIAN, CHARMM, DISCOVER, etc. and the typical run time for a single job (e.g. GAUSSIAN 92 - 4 CPU hours).
- Item 25: Describe any optimization efforts that have been applied to software that has been written by you or members of your group. Commercial or ABCC supplied software need not be addressed.
- Item 26: All applications requesting more than 5 hours of time require C.V.'s and bibliographies.

Advanced Biomedical Computing Center  
Application Form

*Do Not Write in Italicized Areas*

**Duplicate as Needed**

**Application Type:**      New Account      Renewal      Extension (more time needed)

**Check:**      Use of resources other than supercomputer (e.g. Sequence Analysis, E-Mail, etc.)

**Complete A only (Items 1-17)**

Up to 40 hours of supercomputer time

**PI must complete A & B (Items 1-21)**

Greater than 40 hours of supercomputer time

**PI must complete A, B, & C (Items 1-26)**

Applying under existing account

**Specify Project Account ID \_\_\_\_\_**

**Check:**      Applying as P.I. of a Project or Laboratory

**(Must be checked to be awarded Cray time)**

Applying as member of a Project or Laboratory

*Project Account ID (ABCC assigned)*      \_\_\_\_\_

*User Auth Code (ABCC assigned)*      \_\_\_\_\_

*Username (ABCC assigned)*      \_\_\_\_\_

**Check:**      **I have read and understand “Conditions of Use of the ABCC.”**

1. Name:      Dr.      Ms.      Mr.      \_\_\_\_\_  
(First Name      Middle Initial      Last or Family Name)
2. Position, Title:      \_\_\_\_\_
3. Organization Affiliation:      \_\_\_\_\_
4. Institution/Department:      \_\_\_\_\_
5. Address: (Bldg & Room #)      \_\_\_\_\_
6. Street:      \_\_\_\_\_
7. City, State, Zip Code:      \_\_\_\_\_
8. Electronic Mail Address:      \_\_\_\_\_
9. Telephone Number:      \_\_\_\_\_
10. FAX Telephone Number:      \_\_\_\_\_

**ABCC Application - Part A**

11. Activity/Project Name: \_\_\_\_\_

a. Principal Investigator: \_\_\_\_\_

b. Collaborators: \_\_\_\_\_  
\_\_\_\_\_

c. **Abstract:** **Required for all applications** - please attach sheet

12. Justification/Need for ABCC Access: \_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_

13. Proposed Access Method: (e.g. Internet, Local Area Network, Dial-in, NIHnet, etc.)  
\_\_\_\_\_

14. Estimate of Use: Continuous or Occasional (Please check one)

15. Special Requirements (Memory, Disks, Archival Storage, etc.): \_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_

16. Assistance Required: \_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_

17. Primary Research Categories (Check):

- |                              |                                       |
|------------------------------|---------------------------------------|
| D: Drug Design               | X: Crystallography                    |
| M: Molecular modeling        | S: Sequence, protein or nucleic acids |
| Q: Quantum calculations      | N: Neuro-modeling                     |
| I: Image Processing          | C: Cell modeling                      |
| R: RNA secondary structure   | T: Statistics                         |
| U: Mathematical modeling     | P: Physical Chemistry                 |
| A: Macro-Molecular Structure | O: Other _____                        |

Applicant Signature: \_\_\_\_\_ Date: \_\_\_\_\_

PI Approval: \_\_\_\_\_ Date: \_\_\_\_\_

*Chairman NCI*  
*TAG, Approval:* \_\_\_\_\_ *Date:* \_\_\_\_\_

**ABCC Application - Part B**

18. Familiarity with Supercomputers (e.g. Operating Systems, etc.): \_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_

19. Computational Requirement: \_\_\_\_\_  
\_\_\_\_\_

19. Support Required: \_\_\_\_\_  
\_\_\_\_\_

21. **Please Attach** - C.V. and Bibliography **for each collaborator and/or associate** that will be authorized to work on this project.

22. Time (CPU Hours) Requested: \_\_\_\_\_  
(Total time required for the project or group)

23. Project Description:  
Applications for large amounts of time require a thoughtful, concise project description, which must include the following topics:

- a. Objective/goal - What is the overall scientific goal or objective of the calculation? Be specific enough to show how the proposed calculations will help reach that objective.
- b. Computational Methodology/Algorithm - What programs or algorithms will be used? Describe the types of programs and algorithms and also give the specific names of programs and algorithms.
- c. Preliminary Results or Progress to Date - This is important for all applications, but is absolutely essential for all renewals and all requests for additional time.
- d. Relations to Experimental Data - What experimental data will be used in these calculations? What experiments, if any, will be done to test the calculated results? Who will do these experiments?
- e. Significance - What's the scientific or medical significance of this work? (Relation or connection this calculation has with an experimental study or data)

**Applications will be rejected if these questions are not answered carefully enough for the committee to make an informed scientific decision.**

24. Estimated Time for a Typical Single Calculation (CPU Hours): \_\_\_\_\_  
(Estimate for those computations that are performed most often by members of your group)

24. Please describe efforts to vectorize or optimize and any improvements obtained.  
\_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_

26. **Please Attach** - C.V. and Bibliography **for each collaborator and/or associate** that will be authorized to work on this project