

Carnegie Mellon University



Anton End User Agreement (“Agreement”) Ver. 1.9, 10/30/2023

Your signature on this document serves as acknowledgement that you have read and understand your responsibilities as a User and hereby agree to comply with them. As noted below, you must also have an authorized signatory of your institution execute this document if you do not have full authority to agree to these terms and to fulfill all of the obligations described in this document.

1) Introduction

This Agreement outlines the terms of use and obligations for each user (“User”) of the Anton 2 system resources through Carnegie Mellon University (“CMU”). This Anton supercomputer system is on loan to CMU from D. E. Shaw Research, LLC (“DESRES”) for use as outlined in grant no. R01GM116961 from the National Institutes of Health (“NIH Award”) to CMU through the Biomedical Applications Group at the Pittsburgh Supercomputing Center (“PSC”).

All computational resource provider sites have legal and other obligations to protect shared resources as well as the intellectual property of users. Users share this responsibility by observing the rules of acceptable use that are outlined in this document. Resources for this Anton project include hardware, software, network connections, and storage systems owned and/or maintained by PSC. The Anton supercomputer and the other resources described in the prior sentence and provided for use of the Users under this Agreement are collectively called “Anton” and/or “Anton resources.” Each resource is finite and shared by the community of awarded research users. Responsible conduct on the part of each User is essential to ensure equitable and secure access for all. Failure to use Anton resources properly may result in one or more of the consequences outlined in Section 9, including but not limited to loss of access to Anton, legal actions taken by the Anton Parties (as defined below in Section 2) pursuant to this Agreement, or other possible civil and/or criminal penalties.

2) Disclaimers and Limitation of Liabilities

ANY AND ALL INFORMATION, MATERIALS, SERVICES, INTELLECTUAL PROPERTY AND OTHER PROPERTY AND RIGHTS PROVIDED AND/OR MADE AVAILABLE BY CMU PURSUANT TO THIS AGREEMENT (INCLUDING BUT NOT LIMITED TO USE OF ANTON) ARE PROVIDED AND/OR MADE AVAILABLE ON AN "AS IS" BASIS. NEITHER CMU (INCLUDING ITS INTERNAL UNITS PSC AND NSRBC), DESRES, OTHERS INVOLVED WITH THE NIH AWARD AND/OR ANTON USE (INCLUDING BUT NOT LIMITED TO THE NATIONAL RESEARCH COUNCIL, BOARD OF LIFE SCIENCES AT THE NATIONAL ACADEMIES OF SCIENCE IN WASHINGTON, D.C.) NOR THEIR RESPECTIVE TRUSTEES, DIRECTORS, OFFICERS, EMPLOYEES, ATTORNEYS, AGENTS, SUCCESSORS AND ASSIGNS (COLLECTIVELY, THE "**ANTON PARTIES**") MAKE ANY WARRANTIES OF ANY KIND, EITHER EXPRESS OR IMPLIED, AS TO ANY MATTER, AND ALL SUCH WARRANTIES (INCLUDING BUT NOT LIMITED TO WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE) ARE EXPRESSLY DISCLAIMED. WITHOUT LIMITING THE GENERALITY OF THE FOREGOING, NONE OF THE ANTON PARTIES MAKES ANY WARRANTY OF ANY KIND RELATING TO EXCLUSIVITY, ERROR-FREE OPERATION, RESULTS TO BE OBTAINED FROM USE, FREEDOM FROM PATENT, TRADEMARK AND/OR COPYRIGHT INFRINGEMENT. USERS AND THEIR RESPECTIVE INSTITUTIONS ARE PROHIBITED FROM MAKING ANY EXPRESS OR IMPLIED WARRANTY TO ANY THIRD PARTY ON BEHALF OF ANY ANTON PARTIES RELATING TO ANY MATTER, INCLUDING THE APPLICATION OF OR THE RESULTS TO BE OBTAINED FROM THE INFORMATION, MATERIALS, SERVICES, INTELLECTUAL PROPERTY OR OTHER PROPERTY RIGHTS PROVIDED AND/OR MADE AVAILABLE TO USERS PURSUANT TO THIS AGREEMENT (INCLUDING BUT NOT LIMITED TO THE ANTON).

TO THE MAXIMUM EXTENT ALLOWED UNDER LAW, NONE OF THE ANTON PARTIES SHALL BE RESPONSIBLE OR LIABLE, ON A CONTINGENT BASIS OR OTHERWISE, FOR ANY INJURY OR DAMAGES, WHETHER CAUSED BY THE NEGLIGENCE OF THE ANTON PARTIES OR FOR ANY REASON WHATSOEVER (INCLUDING ANY BREACH OF THIS AGREEMENT), TO USERS, THEIR INSTITUTIONS OR ANY THIRD PARTY, AND THE ANTON PARTIES SHALL NOT BE LIABLE FOR ANY LOSS OF PROFITS OR FOR ANY INCIDENTAL, INDIRECT, SPECIAL OR CONSEQUENTIAL DAMAGES, IN EACH CASE ARISING OUT OF OR RELATING TO THIS AGREEMENT OR IN CONNECTION WITH THEIR USE OF ANTON, EVEN IF THE ANTON PARTIES HAVE BEEN ADVISED OF THE POSSIBILITY OF SUCH DAMAGES OR HAVE OR GAIN KNOWLEDGE OF THE EXISTENCE OF SUCH DAMAGES.

3) Indemnification

Use of Anton is the sole risk of Users, and each User agrees that their use of Anton must be consistent with any and all applicable laws and regulations and the requirements of this Agreement. To the maximum extent allowable under law, each User (and their institution, to the extent it is signing this Agreement) hereby agrees to defend, indemnify and hold harmless the Anton Parties from and against any liability, damage, loss or expense (including reasonable attorneys' fees and expenses) incurred by or imposed upon any or all of the Anton Parties in connection with any claim, suit, action or demand ("**Claims**") arising out of or relating to: (a) any bodily injury, death and/or property damage (including that incurred by User and/or Users' respective institution(s)) arising in connection with use of Anton; (b) any information, product, process or other material made and/or derived from the work performed by User using Anton; (c) the terms of this Agreement, including but not limited to failure of User to comply with any requirements or obligations hereunder; and/or (d) their use of Anton. The foregoing indemnity applies to Claims under any theory of liability (including without limitation, actions in the form of tort, warranty, or strict liability, or violation of any law and regardless of whether such action has any factual basis).

4) Account, Password, and Certificate Management

PSC will provide the User's Principal Investigator (PI) and his/her research group with the accounts necessary to access the Anton system, provided that such individuals have executed this Agreement and that any User who is not the PI has been approved by the PI and established as a User as provided in Section 5 below. Each User account is assigned for one User only and must not be shared with others.

Passwords and certificates are the keys to an account. Each User agrees to: (a) never share a password out loud, or write it down where it could be found and/or associated with the account; (b) never use tools which openly expose passwords or certificates on the network (such as telnet); (c) make sure that file and directory permissions prevent others from reading or copying the private key portion of certificates, which is the equivalent of a password; (d) not store User's password(s) in unencrypted or encrypted files.

Each User shall create passwords that are difficult to guess and that cannot be found in a dictionary. Birthdays, family names, and single words are examples of easily-guessed passwords. Each User agrees to change User's password periodically, even if User has no reason to believe that anyone else has it.

PSC support staff will never ask for a User's password, and will never send a password via e-mail, set a password to a requested string of characters, or perform any other activity which could reveal a password to others. If a support person insists that a User share the User's password, do NOT do so and report the incident to GRANTS@psc.edu.

It is every User's responsibility to use passwords and security tools properly. If any User believes his/her account has been compromised or if the User becomes aware of suspicious activity, User agrees to take the following actions:

- notify GRANTS@psc.edu immediately

- not to modify files found in User's account
- not to execute unknown programs User might find
- if possible, not to use User's account until the issue is resolved

Some indications that a compromise has occurred include:

- files in User's home directory or project areas which User did not create
- unexplained alteration or deletion of User files
- discrepancies between the allocation balance and what User thinks has been used

5) User IDs and Accounts for PI's Research Team

Additional Anton users on the PI's research team must be authorized by the PI in writing. Each authorized User will be given an individual User ID and account on the production Anton machine. Use of such individual accounts will be charged against the PI's research allocation. The PI's billing statements will show the usage and charges incurred by each account on the award.

The PI may submit user authorization via email to GRANTS@psc.edu, and should include the following information:

- 1) Actual name
- 2) Department and organization
- 3) Address (Full U.S. mail address)
- 4) Phone number(s)
- 5) Email address
- 6) Academic status
- 7) Requested user ID

PI may not add additional Users and/or substitute another individual for any User unless PI has obtained CMU's prior written consent through the PSC and unless such new Users have signed CMU's then-current form of this Agreement. In addition, PI agrees that (s)he will use reasonable efforts to notify CMU through PSC in writing immediately if any User during the term of PI's award allocation leaves the research team and/or is no longer working on the project for which Anton time was awarded; however, in such cases, PI understands and agrees that (s)he is fully responsible for any and all activities of User as provided in this Agreement (including but not limited to use of node time and usage under PI's award) unless and until CMU receives PI's notice that such User is no longer affiliated with the project and CMU terminates User's access to Anton. Each User agrees that (s)he shall not, under any circumstances, allow other parties access to and/or use of Anton.

In the event that a User authorization should be removed from an award, the PI must notify PSC as soon as possible. This information may also be sent by email to GRANTS@psc.edu.

6) Unauthorized Use and Access

Each User understands and agrees that (s)he may use Anton only for the purposes defined in the PI's approved allocation request under which User is participating, the terms of which are incorporated into this Agreement by reference. In the event of a conflict between the terms of the allocation request and the terms of this Agreement, the terms of this Agreement shall prevail. In the event the allocation is extended or subsequent access is granted, such allocation and access must be used solely for specific approved research purposes—nothing else. Users must operate within sanctioned parameters regardless of what may be technically possible.

7) Unacceptable Behavior

Below are examples of unacceptable behavior. Each User agrees not to engage in such behavior.

- Using, or attempting to use, Anton resources without authorization or for purposes other than those stated in the PI's approved allocation request
- Attempting to copy or reverse engineer any Anton resources (including but not limited to any DESRES property, including all Anton hardware and software for Molecular Dynamics simulations)
- Tampering with or obstructing the operation of and/or access to Anton resources and/or attempting to circumvent system security
- Tampering with and/or obstructing access to a User's data
- Reading, changing, distributing, or copying others' data or software without authorization
- Using Anton resources to attempt to gain unauthorized access to other computational sites
- Activities in violation of any and all applicable local, state, and/or federal laws, regulations, and/or ordinances, and/or those of other countries
- Activities that violate the intellectual property rights and/or privacy rights of a third party
- Sharing passwords, and/or attempting to "crack" or guess other Users' passwords
- Obtaining passwords by other means, such as password capturing programs

8) Reporting Suspicious Activity

All Users must immediately report exposed or compromised passwords, keys, passphrases, or certificates, as well as any suspicious activity on an account. All suspicious activity must be reported to GRANTS@psc.edu, whether or not compromise of an account or system is suspected.

9) Consequences

Failure to abide by this agreement may result in a variety of penalties, including:

- Temporary account suspension or permanent revocation without notice if there is suspicion of account or system compromise, or malicious or illegal activity.
- Loss of current allocation and the inability to obtain future allocations.
- Abusive activity may be reported to Users' home institution(s) for administrative review and/or action.
- Civil litigation may be pursued to recoup costs incurred from unauthorized use of resources or incident response due to a system compromise or malicious activity.
- Criminal penalties could result from violations of federal, state, or local laws. Incidents may be reported to the appropriate authorities for investigation and/or prosecution.

10) Publications and Acknowledgements

All work performed under an Anton award must be intended for publication in open literature. No proprietary or otherwise restricted publication may be based on work done under an Anton award.

All publications that include Anton simulation results and/or analysis must acknowledge use of the machine and other resources, including relevant staff support, at the PSC, and support for the machine's use through the relevant NIH grants awarded to CMU through the PSC.

11) Reports

The PI must provide a brief written report (2-5 pages) to the PSC no later than 3 months after the expiration date of the relevant allocation award, summarizing the scientific research performed and the results obtained with Anton. CMU is hereby granted a nonexclusive, worldwide, perpetual, irrevocable right and license to use, copy and disseminate the report for the purposes of its NIH Award, including but not limited to providing copies to the granting institution (National Institute of General Medical Sciences) or other agencies. If CMU would like to use the report for other purposes, CMU will obtain the prior permission from the award PI.

12) Award Dates and Access to Anton Node Hours

Due to the nature of this specialized machine and associated projects, the PI and all Users working under an award allocation must finish their simulations on Anton during their award period. Any remaining Anton node hours will not be carried forward and will expire. Thus, it is crucial that PIs start using their allocation immediately once their award becomes effective.

13) Termination of Access

This Agreement will remain in effect for the duration of the award allocation unless sooner terminated. CMU may terminate this Agreement upon written notice to User in the event of the termination of CMU's agreement with DESRES for use of Anton and/or

the termination of CMU's NIH Award. Any User may provide written notice to CMU if the User does not want to continue to access and use Anton. In addition to the termination rights listed above, CMU reserves the right at any time to terminate a User's access where CMU determines in its sole discretion that the User and/or the User's conduct poses a risk to CMU or others and/or violates the terms of this Agreement or the parameters of the applicable Anton allocation award.

Upon termination or expiration of this Agreement (or upon the removal of the User from this Agreement or the end of User's award allocation, if earlier), the User's right to access Anton immediately ceases. Any property of any User and/or of User's institution left on Anton and/or any other CMU systems as of such date may be disposed of by CMU in its discretion and without accounting to the User and/or the User's institution (unless CMU has agreed in writing in advance to other arrangements). Any provisions which by their nature should naturally survive termination or expiration will do so (including but not limited to the disclaimers and indemnification provisions, as well as the reporting and data sharing obligations).

14) Intellectual Property and Data Sharing

The PSC subscribes to NIH and NSF rules associated with intellectual property. All Users are required to follow all laws that pertain to any intellectual property that is in their care.

For more information on NIH policies, see:

<https://grants.nih.gov/policy/intell-property.htm>

For more information on NSF policies, see: <https://www.nsf.gov/od/ogc/intelprop.jsp>

In accordance with stipulations set forth in the NIH Award, all data generated during the project must be made available as a shared public resource on PSC's data storage system. During the actual research and data acquisition/analysis phase, Users are not obligated to make such items publicly available and may keep their results and associated material privately on the storage system. After publication, data must become publicly accessible. "Published" data refers to all raw simulation input files and trajectories generated on Anton. In addition, investigators are highly encouraged to document their data, metadata, and analysis, also making this information publicly available after publication. In all cases, the PI and all associated Users must allow their Anton data to be made publicly accessible on PSC's data storage facility either after:

- (i) an initial publication reporting the scientific results obtained on Anton, or
- (ii) 12 months after the expiration date of the award allocation under which User was using Anton, whichever comes first.

15) Proper Acquisition and Licensing of Software

All User-supplied analysis software applied to Anton simulation results must have been appropriately acquired and properly licensed. Possession or use of illegally copied software is prohibited. Likewise Users shall not duplicate copyright-protected software or materials, except as permitted by the owner of the copyright. Some software installed on PSC resources may require special authorization in order to be used. Users must abide by the requirements for protecting it from misuse.

16) Conflicting External Requirements & User's Authority

Users and their institutions are subject to relevant laws and regulations, have organizational policies, and may be parties to various contractual arrangements. It is the responsibility of Users (and their institution(s), where applicable) to manage these external requirements in a manner that will not prevent compliance with this Agreement. By signing this Agreement, User represents that (s)he has the full authority and ability to comply with the terms of this Agreement, including but not limited to the right to grant the licenses to the reports and to commit to the publication of data as described above. In the event that User's institution holds certain rights (for example, if the institution will hold the copyright in the reports) User will be responsible for either obtaining the institution's countersignature on this Agreement and/or obtaining sufficient authorization from the institution to enable User to execute this Agreement and agree to such terms on the institution's behalf. If User is not sure whether (s)he needs the countersignature of someone else at his/her institution, User should contact the legal department of User's institution for guidance.

17) Support/Diagnostic Access by Anton Parties

Authorized PSC site personnel will provide first-line user support and may review User files for the purposes of aiding an individual or providing diagnostic investigation of Anton resources. User activity may be monitored as allowed under policy and law for the protection of data and resources. Any or all files on Anton resources may be intercepted, monitored, recorded, copied, audited, inspected, and disclosed to authorized site or law enforcement personnel, as well as authorized officials of other agencies, both foreign and domestic. By using Anton resources, Users acknowledge and consent to this activity at the discretion of authorized site personnel.

If necessary, additional authorized personnel from Anton Parties may assist with support and/or diagnostics by reviewing User files with authorized PSC personnel, and by using Anton resources, Users acknowledge and consent to this activity. In all cases, access to user data and communications will not normally be performed without explicit authorization and/or advance notice unless exigent circumstances exist. Post-incident notification will be provided in such cases except to the extent prohibited by law.

18) Use of Names

With respect to this Agreement, Users may not make use of DESRES, CMU, PSC and/or any other trademarks or service marks in connection with any press releases, publicity, promotion or other dissemination to multiple third parties without prior written consent from DESRES and/or CMU. CMU may identify the Users as users of Anton to the extent necessary to further its educational and research mission and/or to fulfill CMU's obligations under the terms of the NIH Award.

19) Disputes

This Agreement shall be governed by the laws of the Commonwealth of Pennsylvania without regard to its conflicts of laws provisions. All claims and/or controversies of every kind and nature arising out of or relating to this Agreement, including any questions concerning its existence, negotiation, validity, meaning, performance, non-performance, breach, continuance or termination shall be settled exclusively in the United States District Court for the Western District of Pennsylvania or, if such Court does not have jurisdiction, in any court of general jurisdiction in Allegheny County, Pennsylvania, and the parties consent to the exclusive jurisdiction of such courts and waive any objection which such parties may have to the laying of venue in any such courts. However, notwithstanding anything to the contrary in the foregoing, this provision shall not apply to any state institution to the extent the state institution is prohibited by law from accepting Pennsylvania law and/or venue.

20) Export Control

As an institution of higher learning, CMU performs fundamental research that is exempt from export control licensing under applicable export control laws. In addition, as noted above, results from using Anton are expected to be published. As a result, User shall not use export-controlled information or materials on Anton or elsewhere on CMU's premises except to the extent it has received CMU's prior written consent through the process detailed below. To the extent any User wishes to request that CMU consider allowing User to bring and/or use export-controlled information or materials on Anton and/or onto CMU's premises pursuant to this Agreement, they must submit an advance written request to CMU's Office of Sponsored Programs detailing the nature and exportcontrolled category of such proposed information/materials, which request may be granted or denied by CMU in its sole discretion.

21) Notices

Any notice to the other party under this Agreement must be in writing, signed by the party giving it, and provided by either electronic mail, registered mail, certified mail, and/or reputable overnight courier (such as UPS, FedEx, etc.) to the addresses listed on the signature page to this Agreement. Either party may update the contact information by providing written notice to the other party as required by this Section.

22) Miscellaneous; Entire Agreement

This Agreement is binding upon and shall inure to the benefit of the parties hereto, their representatives, successors and assigns. No failure or successive failures on the part of any party, its successors or assigns, to enforce any covenant or agreement, and no waiver or successive waivers on its or their part of any condition of this Agreement, shall operate as a discharge of such covenant, agreement, or condition, or render the same invalid, or impair the right of either party, its successors and assigns, to enforce the same in the event of any subsequent breach or breaches by the other party, its successors or assigns. This Agreement (including the relevant allocation application) constitutes the entire agreement among the parties and supersedes all previous agreements and understandings relating to the subject matter of this Agreement. The Agreement may not be altered, amended, or modified except by a written instrument signed by the duly authorized representatives of each party. This Agreement may be executed in counterparts. Unless explicitly accepted in this Agreement or in a document specifically entitled as an amendment to this Agreement, terms appearing in purchase orders shall be of no effect other than evidencing Institution's and User's intent to be bound to this Agreement. This Agreement is made in favor of, and for the express benefit of, CMU and the other Anton Parties. Except as provided in the prior sentence, there are no other third party beneficiaries.

Intending to be legally bound, this Agreement is effective for Pls as of the earlier of: (a) the date the User signs this Agreement; or (b) the date that the User is allowed access to Anton.

USER

ACCEPTED AND AGREED BY USER FOR THE BENEFIT OF CMU AND THE OTHER ANTON PARTIES:

• By: _____

Note: BY SIGNING THIS AGREEMENT WITHOUT ADDITIONAL SIGNATURE FROM USER'S INSTITUTION, USER REPRESENTS THAT (S)HE HAS THE FULL AUTHORITY TO SIGN THIS DOCUMENT AND ABIDE BY THESE OBLIGATIONS. IF USER DOES NOT HAVE THE FULL AUTHORITY WITHOUT ADDITIONAL INSTITUTIONAL COUNTERSIGNATURE, USER MUST OBTAIN THE COUNTERSIGNATURE OF AN AUTHORIZED REPRESENTATIVE OF USER'S INSTITUTION.

Printed Name:

Date:

INSTITUTION

INSTITUTION CONFIRMS THAT USER MAY ACCESS AND USE ANTON IN ACCORDANCE WITH THESE AGREEMENT TERMS. TO THE EXTENT THAT USER DOES NOT HAVE AUTHORITY TO GRANT THE RIGHTS AND PERFORM THE

RESPONSIBILITIES DESCRIBED IN THIS AGREEMENT, INSTITUTION HEREBY GRANTS SUCH RIGHTS AND AGREES TO PERFORM SUCH RESPONSIBILITIES IN FAVOR OF, AND FOR THE BENEFIT OF, CMU AND THE OTHER ANTON PARTIES.

By: _____ **Printed**

Name:

Title:

Name of Institution:

Date:

Address for notices:

ANY NOTICES OR REQUESTS FOR PERMISSIONS TO BE GIVEN TO PSC UNDER THIS AGREEMENT SHALL BE SENT AS FOLLOWS:

Addresses for notices:

Philip Blood, PhD
Scientific Director
Pittsburgh Supercomputing Center
300 S. Craig St.
Pittsburgh, PA 15213
412-268-4960 Telephone
412-268-5832 Fax

David Moses, PhD
Executive Director
Pittsburgh Supercomputing Center 300
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412-268-4960 Telephone
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