# Writing a Successful Anton Proposal

Welcome! We'll begin at 3:05 ET.

PSC
PITTSBURGH SUPERCOMPUTING CENTER

Carnegie Mellon University

University of Pittsburgh

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# Agenda

In this webinar we will  explain:

- Who can apply for computer time on Anton
- How to write a successful proposal

# Anton 3 at PSC

- Anton is a special purpose supercomputer for molecular dynamics (MD) simulations of biological systems. It dramatically increases the speed of the MD simulations.
- Designed and built by D. E. Shaw Research (DESRES). Hosted by the Pittsburgh Supercomputing Center (PSC) with support from the NIH National Institute of General Medical Sciences.
- Made available without cost to researchers associated with US universities and other not-for-profit institutions.
- More information about Anton can be found at:

  https://www.psc.edu/resources/anton/

# Anton enables breakthrough science

- Simulating for a few days on Anton, a researcher is able to obtain results that would take years of continuous runtime on any other resource, reaching timescales of hundreds of microseconds.

- Utilized for diverse biomolecular research: nucleic acids, lipids, proteins, designed nanostructures composed of nucleic acids or proteins, force field development, generation of long trajectories for analysis with AI methods.

# Who and How

**Who can benefit from running on Anton?**

Researchers who need long-time scale (approaching millisecond-long) molecular dynamics simulations of biological systems (nucleic acids, proteins, lipids).

**How to get access to Anton?**

Submit a competitive proposal. Request for Proposals are issued once a year. RFP
**Deadline: October 21, 2025.**

Begin the submission process **a couple of days before the deadline**, because you will need to create an account at PSC. See here for more information: RFP

# Who can apply

## Who can apply:

- The principal investigator (PI) must be faculty or staff member at a U.S. academic or not-for-profit research institution.
- A graduate student  or postdoctoral researcher may not be a PI, but a qualified advisor may apply on their behalf.
- Each investigator can serve as a PI for only ONE application in a given allocation round.
- IMPORTANT: If a PI or co-PI is on another Anton proposal (as co-PI or PI, respectively), they must clearly demonstrate that the research efforts described in the two proposals are **distinct and independent** of each other.
- Researchers with no previous experience with Anton are encouraged to apply
- 25% of the total allocated time is reserved for PIs that have not previously had an allocation on an Anton system at PSC.

# Tips for a successful proposal

By allowing MD simulations over time scales approaching milliseconds, Anton fundamentally changes the types of questions biomedical researchers can address.

1. Explain how Anton will enable your group to achieve breakthrough scientific results that cannot be achieved in any other supercomputer.

2. Make sure your system meets the technical requirements to run on Anton.

3. Provide all requested info in all required proposal sections.

Contact PSC in case of doubts: anton-support@psc.edu

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# The proposal

- Proposals should be two to six pages in length, not including references.
- May submit up to two additional supporting documents (e.g., published papers) in PDF format on the submission page.
- Proposal must be self-contained. Reviewers are not required to refer to supporting documents or any other external documents when reviewing proposals.
- Grantsmanship is important

# Proposal Sections

- **The main proposal document must have these 7 sections:**

1. Summary of the project, including descriptive title of proposed research (400 words maximum for summary & title).
2. Name, address, email, and telephone number of the Principal Investigator and co-PIs.
3. Background information (1 page maximum): Include sufficient background information on the research field to allow reviewers to judge the scientific merit of the proposed research.
4. Scientific Objectives (2 pages maximum) explaining:
    - Why Anton is necessary for the planned project
    - Why the project could not be efficiently completed on conventional supercomputers
    - Scientific impact of their proposed project

# Section 4. Scientific Objectives

- Projects should focus exclusively on questions that will greatly take advantage of Anton 's unique capabilities.
- **Explain why achieving the scientific objectives requires access to Anton, and could not be efficiently achieved on any other high performance computing system, e.g.:**
  - Need for longer MD trajectories (approaching millisecond-long), that are not feasible on conventional systems.
  - Phenomena that cannot be observed with shorter simulations.

# Proposal Sections (Continued)

5. **Project Feasibility and Team Qualifications** (2 pages maximum): Address these five points (the Simulation Requirements outlined in the RFP):

1. Simulations must be standard MD in constant NVE, NVT (isothermal) or NPT (isothermal, isobaric). Consist of protein, DNA, RNA, lipids, water, and standard ions. Ligands, custom molecules OK.
2. Periodic boundary conditions and explicit solvent. Simulation cell must have only right angles, with a minimum of 50 A per side.
3. Force Field must be variants of standard, non-polarizable CHARMM or Amber biomolecular force fields).
4. Number of atoms (between 100,000 and 8,500,000 atoms, including solvent)
   The sweet spot: 500,000 to 6M
5. Simulations will not finish in less than 1 hour on Anton

- State whether the proposed system has already been built and equilibrated. If not, provide evidence that the proposed system can be successfully built and simulated.
- Describe the expertise and experience of the researcher.
- If there is a co-PI on a proposal, explain that the work described in the proposal will be conducted primarily in the PI's lab.

# Enhanced sampling

- Can apply a uniform constant electric field.
- Position restraints.
- Enhanced sampling as explained in the RFP and the previous lecture.

# Pre-equilibration of the system

- Systems need to be **pre-equilibrated** prior to running on Anton using the software described in the RFP (Desmond, Amber, CHARMM, Gromacs, or NAMD).
- For the easiest conversion to Anton, we strongly suggest using Desmond to equilibrate, especially if your system has custom molecules.
- Bridges-2 at PSC is part of NSF ACCESS. It is available for free for testing and equilibrating your MD simulations.

Information about Bridges-2
https://www.psc.edu/resources/bridges-2/

Getting started with ACCESS resources
https://allocations.access-ci.org/get-your-first-project

ACCESS Explore, Discover, or Accelerate allocations can be requested at any time.

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# Proposal Document (Continued)

6. Requested Resources (1 page maximum):

- Clearly state and provide justification for the number of Anton machine-days requested.

- Provide strong scientific arguments as to why the **length** and **number** of proposed simulation runs will be both sufficient and necessary to achieve the stated scientific objectives.

# Estimating the amount of simulation time to ask for:

| Chemical system | Number of atoms | ~ Performance (microseconds/machine-day) |
|---|---|---|
| F1-AtPase | 327,506 | 90.6 |
| STMV | 1,066,628 | 42.3 |
| Ribosome | 2,180,503 | 25.4 |
| STMV 2x2x1 | 4,266,512 | 10.0 |
| STMV 2x2x2 | 8,533,024 | 3.0 |

- 2.5-femtosecond time steps with long-range interactions evaluated at every third time step and thermostat applied every 48 time steps. Details in the RFP

# Example of estimating MD simulation units

- Example:
- STMV system 1,066,628 atoms  42.3 microseconds in one machine-day.

- Maximum that can be requested: 9.1 machine-days.

- Show these calculations in your proposal so it is easy to see how you made your estimates!

# Progress Report for PIs with previous allocations

**7. Progress Report: Separate document. Required only for PIs with previous allocations – 2 pages maximum**

- Describe how the PI's previous allocation was used. Summarize findings or results.
- **All information required to assess progress should be clearly communicated in the text of the progress report itself** and should not depend on reviewers reading supporting documents or any other external documents. (Progress Report should be self-contained.)
- Explain any significant digressions from the originally proposed resource usage plan for the prior period, if applicable.
- Describe reasons for underutilization of previous allocation, if applicable.

# Contact us

- Applicants with systems:
- With custom parameters or molecules that are not included in the standard distribution of the supported force fields.
- Have dozens of restraints and/or restraints involving thousands of atoms.
- Shaped such that one dimension of the simulation cell is much larger than the others
- Please contact anton-support@psc.edu

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# Common Proposal Pitfalls

- Poor grantsmanship (probably #1 issue), including:
  - *lack of clear hypothesis ("fishing expeditions")*
  - *lack of explanation of why the proposed system is important or what contribution the results will have on the field* **(looking for breakthrough science)**
- Insufficient justification of:
  - the differences between 2 proposals submitted by a PI/Co-PI pair and demonstration that the work will happen in PI's lab.
  - the number of requested simulation units
  - the need for Anton over standard supercomputing cluster
  - unused prior Anton allocation
- Weak explanation of progress since last received allocation

# Submit the proposal

- Submit through the Portal as described in : https://www.psc.edu/resources/anton/
- RFP
- **Recall deadline Tuesday, October 21, 2025. Submit a few days prior to create account.**
- Proposals are first reviewed for feasibility, missing documents, etc. at the PSC. Then sent to a review panel convened by the National Academy of Sciences (NAS).
- Rigorous and transparent process: The review committee is made public and there is a community comment period prior to the review. The entire committee must agree on the recommendation report.
- If notified of acceptance, you will receive info about login in to Anton, the documentation and how to get started.

# After the Review

- Expect a notice of proposal acceptance by ~ end of January. The full NAS report is also published on their website.
- Allocation is for one year. Target starting day is April 1 2026.
- Access to files for an extra year.
- A “Getting Started Workshop” will be offered in the spring 2026:
  an intensive 1-day Anton training workshops for new users to help them prepare and start running their simulations.
- Acknowledge Anton in all publications resulting from this work.
- We collect publications and Ph.D. Theses resulting from Anton work,

so keep them coming!

# Trajectories

- Trajectories generated on Anton and all their associated data will be kept private until publication, or up to one year after the end of an Anton allocation, whichever comes first.

- After this  period, the trajectories and data will become part of a collection of hundreds of long-timescale trajectories that will be made widely available to the research and education communities.

Slides and RFP are at
https://www.psc.edu/resources/anton/

Please fill out Survey

https://forms.gle/5YqBYRVgJ52mRrDF7

Best of Luck
Questions?
Thank you!