#### **Contents**

Gummary	1
Outline of the CAP process:	1
General features of the CAP system:	2
Reporting requirements:	4
Beamtime allocation:	
Beamtime usage:	
Access to CAP data:	
xpert User Training:	5
Fravel budget and reimbursement	6

# **Summary**

The Australian Synchrotron <u>Collaborative Access Program</u> (or CAP) is designed to:

- reduce workload for PIs, beam line staff, the MX Program Advisory Committee (PAC) and its reviewers and the AS
- create a system where PIs submit one proposal for beamtime per year
- increase flexibility for users as to when they access beam time
- allow the users to know the amount of beam time they have allocated well in advance
- improve the efficiency with which beamtime is used
- maximise science productivity on the MX beamlines.

The implementation of CAP time recognises that this system better reflects the needs of the MX community where labs require regular access to beamtime in order to advance a series of different projects to the point of publication. Combining beamtime from different PIs allows the CAP to have the flexibility to chose which samples and staff to send for a given allocation period and provides all members with more regular access to beamtime.

# **Outline of the CAP process:**

- 1. In May each year the AS User Office issues a call for CAP proposals. (To be submitted in late May / early June each year)
- 2. New CAP proposals are assessed by the MX Proposal Assessment Committee (or PAC). The CAP proposal is scored and the individual projects within the CAP proposal have time allocations adjusted for the two MX beamlines.
- 3. In August CAP members are informed as to the success of their proposals and the amount of beamtime allocated.

- 4. During the 12 month period that the CAP is in operation no additional beamtime requests are required).
- 5. The User office informs the CAP spokesperson of the dates of the CAPs experiments for the next 4 month cycle.
- 6. The CAP spokesperson submits Experimental Authorisation (EA) forms as usual prior to each experiment.
- 7. The CAP spokesperson is informed of the dates of the next cycles of experiments before the end of the current cycle.
- 8. At the end of the CAPs allocation the CAP will need to submit a new CAP proposal in order to continue getting beamtime. This will include a summary of the outcomes from the beamtime that was used during the time of the CAP.

### **General features of the CAP system:**

Pls group together to form Collaborative Access Programs (CAPs). A PI can belong to only one CAP. The intent of this is to group all of the beamtime requirements for a lab or group of labs into a single block.

There are only two modes of access for beamtime on the MX beamlines; CAP and rapid access.

Rapid access time is intended for emergency access, overseas applications from non-CAP labs or new labs that have formed during the CAP cycle.

All MX labs are expected to belong to a CAP as it is the standard mode of access.

A CAP can be any group of PIs (and must include their associated staff, post-docs and students), not necessarily from the same institution and not necessarily involved in the same projects.

The minimum size expected for a CAP is two or more PIs where the combined samples and staff of the CAP are able to efficiently use six shifts (2 days) of beamtime on each MX beamline per cycle. This is a total of 6 days on MX1 and 6 days on MX2 per 12 month period.

Where CAP applications are made for CAPs that fall below the minimum size expected they will be considered on a case-by-case basis. There must be valid reasons why the PIs cannot form a larger CAP.

Once a PI joins a CAP all of their staff, post-docs and students are also classed as members of the same CAP. It is not permitted for lab members to belong to different CAPs as all of a lab's projects should be bundled together into the PIs single CAP application.

Each CAP drafts a scientific proposal once a year wherein their science and proposed type of experiments CAP's different PIs are outlined as well as the total number of days of beam time required for the year. This proposal is submitted to the AS and then to the MX PAC for review. The MX PAC then recommends to the AS a time allocation for that CAP for the year.

In advance of the start of each year, each CAP is allocated a set number of days for that year. It is up to the CAP to decide which PI or group of PIs within the CAP will use which of their allocated days (subject to the usual experiment authorisation processes).

Only a fixed percentage of the total MX beam time will be available for CAP allocation and CAP time will be allocated in a block like fashion. If the number of days requested by all CAPs exceeds that available for CAP allocation, the allocation of CAP time will be at the discretion of the AS on advice from the PAC.

CAP members, their post-docs and their students may make use of rapid access time or other forms of fill-in time that may be made available; however priority for rapid access time will be given firstly to non-CAP researchers.

The amount of time allocated between CAP and rapid access would be set by the AS in an attempt to optimize efficiency whilst maintaining fairness to the whole MX community.

New members can be enrolled within a CAP at any stage, but the CAP will not be allocated any additional time under the existing proposal as a consequence.

All researchers working at the AS under the auspices of a CAP would be expected to comply with the usual user obligations. This would include appropriate lead times for submission of travel applications, experimental authorization etc. As with all experimental visits, failure to submit crucial documentation in a timely fashion could result in a visit cancellation and potentially (in the absence of a suitable replacement group organized by the CAP) loss of CAP beamtime.

The maximum travel funding made available to a CAP would be based on the total amount of time available to the CAP in a cycle, the apportionment of beamtime among the member groups, and where those member groups are based. It will have to be acquitted in a similar fashion to any other AS user travel funding.

The AS would reserve the right to dissolve a CAP. This could be as a result of demonstratively poor organization or an inability to agree internally on beamtime scheduling. In this case the re-allocation of the remaining CAP beamtime would be at the discretion of the AS.

A condition of renewal of a CAP will include an assessment of how effectively the member groups had utilized previous CAP beamtime.

CAPs will report to the AS on CAP activities as required.

CAPs may dissolve themselves on the basis of a simple majority of PIs voting to do so (or one in the case of a two PI CAP). If this occurs the beamtime is treated as if the AS had dissolved the CAP.

If a PI chooses to leave a functioning CAP that CAP loses the shifts of beamtime that were allocated to that CAP to carry out the leaving PIs research. This "lost" beamtime reverts to the AS not the PI. It will be at the discretion of the AS as to whether the departing PI will be able to apply for other merit time during the remaining life of the CAP.

Each CAP will appoint a CAP-coordinator who will be the single point of contact between the CAP and the user office for user administration. For administrative purposes it may be necessary for this person to be the named in the Web Portal as the principal investigator for the CAP proposal.

It is the responsibility of the CAP-coordinator to ensure that the CAP beamtime is used effectively and that the CAP is able to provide sufficient staff and samples to use the allocated time effectively.

# **Reporting requirements:**

At the completion of each experiment the user group attending the beamline must complete:

- 1. The end-of-experiment feedback survey.
- 2. MX User survey

At the end of the CAP period the CAP PIs submit a new CAP proposal. This will include:

- 1. The number of structures solved.
- 2. The number of structures deposited to the PDB.
- 3. The number of papers published with a citation for each paper.
- 4. Number of and details for undergraduate and graduate theses submitted that contain research outputs produced using CAP beamtime.
- 5. Advances in the project that have not lead to items 1-3 above such as improvement in resolution of crystals, native data without experimental phases, partial models under refinement and so forth.

#### **Beamtime allocation:**

The CAP proposal allows the PIs in the CAP to request beamtime on each MX beamline on a project-by-project basis. The total beamtime assigned to the CAP will be pooled and it is assumed that the CAP provides beamtime to the projects in a similar manner to that laid down in the CAP proposal. It is up to the PIs in the CAP to decide how to allocate their time so as to maximise scientific productivity from their beamtime and to ensure efficient usage of the beamtime allocated.

The CAP renewal also enables the CAP to discuss the usage of beamtime from the previous year. The CAP may request more time for some projects due to experimental needs or based on track record. The allocated beamtime for each project in the CAP proposal will be derived from the requested beamtime but will be weighted by the MX PAC based on usage, productivity and the scientific merit of that project.

The CAP system is a merit-based system and all proposals are scored on their scientific merit and the track record on the projects included in the proposal. There is an expectation that beamtime will result in publication. Not all experiments will result in publication and some difficult projects such as membrane proteins or large complexes may take many experiments (or even years) to reach the point where they can be published. This is taken into account during the assessment of proposals and it is expected that if no publication has been produced for a project the proposal is able to show the strategy to overcome the experimental issues and some progress such as improved crystal quality, resolution etc.

# Beamtime usage:

It is expected that allocated beamtime is used effectively. One of the strengths of the CAP system is that the CAP members are able to coordinate their samples so as to be able to effectively use the beamtime allocated. This should provide frequent access to beamtime for those projects that have crystals. It is also inevitable that there is some idle beamtime during experiments. However, repeated long periods of idle beamtime will be taken as inefficient usage and result in a decrease in allocated beamtime for subsequent proposals.

If a CAP is unable to provide sufficient samples or staff for an upcoming experiment the CAP coordinator should contact the AS User Office and ask for the experiment to either be reduced in time or cancelled. Should this be done more than 8 working ways from the date of the experiment this will not be counted as inefficient usage (unless this happens repeatedly).

At the completion of each CAP experiment all PIs in the CAP will receive an activity report listing the number of screening images, datasets, scans and idle hours. This is intended to allow the CAP to track usage and to allow the CAP members to react with any issues of usage as they occur rather than this coming as a surprise during the CAP renewal process. Should there be errors in the activity report the CAP spokesperson should contact beamline staff within a week of the experiment. The data from the activity reports is collated and forms part of the CAP renewal process. The MX PAC will amend the amount of beamtime allocated to a CAP partly based on these usage statistics.

#### Access to CAP data:

All CAP members will have access to all data generated by the members of their own CAP. PIs may add access for individuals via the usual experimental access management tools on the Virtual Beamline. CAP members will be collecting data on each other's samples and so all CAP members will be provided access to all experiments.

# **Expert User Training:**

As part of the CAP process it is expected that each CAP nominate a pool of their staff to become "Expert Users" (EU). These staff members will undergo separate training at the MX beamlines on safety and user training, how the beamline operates and how to fix common failure modes. After training has taken place it is expected that the CAP arrange for at least one EU to be present at each experiment. During an experiment the EU will also act as the User Group Spokesperson.

Until the EU training program is finalised and is in place, and sufficient training cycles have been run to allow each CAP to train several staff, the requirement for EUs to be present during all experiments will be waived. It is anticipated that this requirement will come into force in January 2017.

### Travel budget and reimbursement.

When a CAP is offered beamtime the CAP coordinator is given the total travel budget for the CAP for the 12 month period of the CAP's beamtime allocation. This is calculated as if the allocated CAP beamtime was made up of three shift experiments and based on the allocation to the PIs. The current funding template used by the User Office lists the maximum travel reimbursement per experiment based on the location of the PIs lab. The total amount of travel funding allocated to the CAP is based on the approved shifts per PI and each PIs location. For example a CAP with three PIs, based in Perth, Queensland and Sydney, would have the total budget for CAP travel based on the rates for each location and the proportion of time allocated to each of the PIs. If the travel budget is spent before the end of the CAP time the CAP will be required to pay for the remaining travel. The AS will not pay for CAP travel costs above the approved budget. Only one invoice may be submitted per institution per CAP.

### **Experimental Authorisation (EA):**

An EA must be submitted by the CAP spokesperson via the user portal no later than 5 working days from the start of the experiment. Sample information may be amended to add new samples up to the morning of the experiment. Should an EA form not contain sufficient information the CAP spokesperson will be asked to submit.

#### For protein samples:

At a minimum the following is required in the "Details of experiment" section:

- 1. A statement that all samples are: non-toxic, non-hazardous, non-infectious protein samples.
- 2. Should #1 above not be correct the exact nature of the hazard, toxicity or infectivity risks posed by the samples must be detailed. Risk control measures must be detailed including a risk-assessment.
- 3. The full name of the sample and its abbreviation such as "crystals of beta-2 adrenergic receptor, B2A-(GPCR).
- 4. A statement that the protein samples are recombinant and purified from laboratory organisms. The name of the lab organism shall be given e.g. "Expressed recombinately in *E. coli.*"
- 5. Should #3 not be correct the name of the source organism should be given e.g. "Purified from wombat blood."
- 6. The level of purity shall be given e.g. "Crystals of pure protein."
- 7. Should #1 or #3 above not be correct and risks relating to the purity of the sample should be discussed e.g. "While this protein is purified from live virus these crystals are non-infectious and non-hazardous" or "While this sample is purified from snake venom the pure protein present in the crystals has limited toxicity and the amount present is below that needed to pose a risk to human health".

- 8. That all samples will be removed from the beamline at the end of the experiment and returned to the user's lab.
- 9. Should #7 above not be correct the planned process of disposal of samples is needed.
- 10. For each sample the name of the protein and its abbreviation is required e.g. "Human cytidine deaminase (CDA)".

Forms simply stating "protein crystals" will not be accepted.

#### For non-protein samples:

At a minimum the information required is:

- 1. Name of compound.
- 2. Abbreviation.
- 3. Expected structure. This should be an image of the structure as output from packages such as Chemdraw.
- 4. The cell dimensions (if known).
- 5. The spacegroup symbol and number, including unique axis (if known).
- 6. Empirical formula.
- 7. Chemical formula mass (Da).
- 8. Safety information if available.

Some samples have no available safety information and if this is the case a statement on the handling and safety precautions used in the researchers lab must be included.

The information on the EA form is confidential.