



Hewlett Packard
Enterprise

OLAF
CRYOSPARC TUTORIAL



HPE Cray
April, 2020

WHAT IS CRYOSPARC?

- CryoSPARC (**Cryo**-EM **S**ingle **P**article **A**b-Initio **R**econstruction and **C**lassification) is a state of the art HPC software solution for complete processing of single-particle cryo-electron microscopy (cryo-EM) data.
- <https://cryosparc.com/>



INSTALL AND SETUP

- Export your License ID as an environment variable
 - `export LICENSE_ID="<license_id>"`
- Download the two files into tarball archives
 - `curl -L https://get.cryosparc.com/download/master-latest/$LICENSE_ID -o cryosparc_master.tar.gz`
 - `curl -L https://get.cryosparc.com/download/worker-latest/$LICENSE_ID -o cryosparc_worker.tar.gz`
- Extract the downloaded files
 - `tar -xf cryosparc_master.tar.gz cryosparc_master`
 - `tar -xf cryosparc_worker.tar.gz cryosparc_worker`



INSTALL CRYSPARC MASTER PACKAGE

- Install the cryosparc_master package
 - `cd cryosparc_master`
 - `./install.sh --license $LICENSE_ID --hostname <master_hostname> --dbpath <db_path> --port <port_number> [-insecure] [--allowroot] [--yes]`
 - Example
 - `./install.sh --license $LICENSE_ID --hostname olaf1 --port 39200 --dbpath /opt/cryoem/cryosparc-center/3.0.1/cryosparc2_database`
- Start cryoSPARC
 - `./bin/cryosparcm start`
- Create the first user
 - `cryosparcm createuser --email “<user email>” --password “<user password>” --name “<login username>” --firstname “<given name>” --lastname “<surname>”`
 - Example
 - `cryosparcm createuser --email crayadmin@olaf --password crayadm --username crayadm --firstname edu --lastname edu`



INSTALL CRYOPARC WORKER PACKAGE

- GPU Worker node cryoSPARC installation
 - `cd cryosparc_worker`
 - `./install.sh --license $LICENSE_ID --cudapath <cuda_path> [--yes]`
 - Example
 - `./install.sh --license $LICENSE_ID --cudapath /opt/compiler/nvidia/cuda-10.2`



CONNECTION OF CLUSTER WORKLOAD MANAGER

- Connecting a Cluster to cryoSPARC
 - To register the cluster, cluster_info.json and clusters_script.sh need to be provided.
 - cluster_info.json

```
name : "cluster1"
# A unique name for the cluster to be connected (multiple clusters can be connected)
worker_bin_path : "/path/to/cryosparc_worker/bin/cryosparcw"
# Path on cluster nodes to the cryosparcw entry point for worker process
cache_path : "/path/to/local/SSD/on/cluster/nodes"
# Path on cluster nodes that is a writable location on local SSD on each cluster node. This might be /scratch or similar. This path MUST be the same
on all cluster nodes. Note that the installer does not check that this path exists, so make sure it does and is writable. If you plan to use the cluster
nodes without SSD, you can leave this blank.
send_cmd_tpl : "ssh loginnode {{ command }}"
# Used to send a command to be executed by a cluster node (in case the cryosparc master is not able to directly use cluster commands). If your
cryosparc master node is able to directly use cluster commands (like qsub etc) then this string can be just "{{ command }}"
qsub_cmd_tpl : "qsub {{ script_path_abs }}"
# The exact command used to submit a job to the cluster, where the job is defined in the cluster script located at {{ script_path_abs }}. This string
can also use any of the variables defined below that are available inside the cluster script (num_gpus, num_cpus, etc)
qstat_cmd_tpl : "qstat -as {{ cluster_job_id }}"
# Cluster command that will report back the status of cluster job with id {{ cluster_job_id }}.
qdel_cmd_tpl : "qdel {{ cluster_job_id }}"
# Cluster command that will kill and remove {{ cluster_job_id }} from the queue.
qinfo_cmd_tpl : "qstat -q"
# General cluster information command
transfer_cmd_tpl : "scp {{ src_path }} loginnode:{{ dest_path }}"
# Command that can be used to transfer a file {{ src_path }} on the cryosparc master node to {{ dest_path }} on the cluster nodes. This is used when
the master node is remotely updating a cluster worker installation. This is optional - if it is incorrect or omitted, you can manually update the cluster
worker installation.
```

CONNECTION OF CLUSTER WORKLOAD MANAGER

- cluster_script.sh

```
{{ script_path_abs }} # the absolute path to the generated submission script
{{ run_cmd }} # the complete command-line string to run the job
{{ num_cpu }} # the number of CPUs needed
{{ num_gpu }} # the number of GPUs needed.
{{ ram_gb }} # the amount of RAM needed in GB
{{ job_dir_abs }} # absolute path to the job directory
{{ project_dir_abs }} # absolute path to the project dir
{{ job_log_path_abs }} # absolute path to the log file for the job
{{ worker_bin_path }} # absolute path to the cryosparc worker command
{{ run_args }} # arguments to be passed to cryosparcw run
{{ project_uid }} # uid of the project
{{ job_uid }} # uid of the job
{{ job_creator }} # name of the user that created the job (may contain spaces)
{{ cryosparc_username }} # cryosparc username of the user that created the job (usually an email)
```

- To actually create or set a configuration for a cluster in cryoSPARC
 - cryosparcm cluster connect # connects new or updates existing cluster configuration, reading cluster_info.json and cluster_script.sh from the current directory, using the name from cluster_info.json
 - Other commands
 - cryosparcm cluster example <cluster_type> # dumps out config and script template files to current working directory. Examples are available for pbs and slurm schedulers but others should be very similar
 - cryosparcm cluster dump <name> # dumps out existing config and script to current working directory
 - cryosparcm cluster remove <name> # removes a cluster configuration from the scheduler

CONNECTION OF CLUSTER WORKLOAD MANAGER

- Example

- cluster_info.json

```
{
  "qdel_cmd_tpl": "scancel {{ cluster_job_id }}",
  "worker_bin_path": "/opt/cryoem/cryosparc-center/3.0.1/cryosparc2_worker/bin/cryosparcw",
  "title": "cryo_all",
  "qinfo_cmd_tpl": "sinfo --format=%8N %6D %10P %6T %14C %5c %6z %7m %7G %9d %20E",
  "qsub_cmd_tpl": "sbatch {{ script_path_abs }}",
  "qstat_cmd_tpl": "squeue -j {{ cluster_job_id }}",
  "cache_quota_mb": null,
  "cache_reserve_mb": null,
  "send_cmd_tpl": "{{ command }}",
  "name": "cryo_all"
}
```

- Cluster_script.sh

```
#!/bin/bash
#SBATCH --job-name=cryosparc_center_{{ project_uid }}_{{ job_uid }}
#SBATCH --partition=cryoem
#SBATCH --output={{ job_log_path_abs }}
#SBATCH --error={{ job_log_path_abs }}
#SBATCH --gpus={{ num_gpu }}
#SBATCH --gres=gpu:{{ num_gpu }}
#SBATCH --ntasks={{ num_cpu }}
#SBATCH --cpus-per-task=1

source $MODULESHOME/init/bash
module load cuda/10.2
module load cryosparc-center/3.0.1-worker

{{ run_cmd }}
```

UPDATES

- Run cryosparcm update command to check for cryoSPARC updates

- cryosparcm update --check

- Example

```
$ cryosparcm update --check  
CryoSPARC current version v2.15.0  
update starting on Wed Mar 18 12:09:52 EDT 2020  
current version v2.15.0  
new version v3.0.0  
Update available!
```

- cryosparcm update --list

- Example

```
$ cryosparcm update --list  
CryoSPARC current version v2.14.0  
update starting on Wed Mar 18 12:11:42 EDT 2020  
Available versions:  
v2.0.18  
v2.0.20  
v2.0.23  
...  
v2.14.2  
v2.15.0  
v3.0.0  
To install a specific version, use  
$ cryosparcm update --version=vXX.YY.ZZ[-branchname]
```



UPDATES

- Master update
 - cryosparcm update or cryosparcm update --version=vXX.YY.ZZ
- Worker update
 - Copy cryosparc2_worker.tar.gz that it is downloaded when updating master into worker installation directory.
 - bin/cryosparcm update



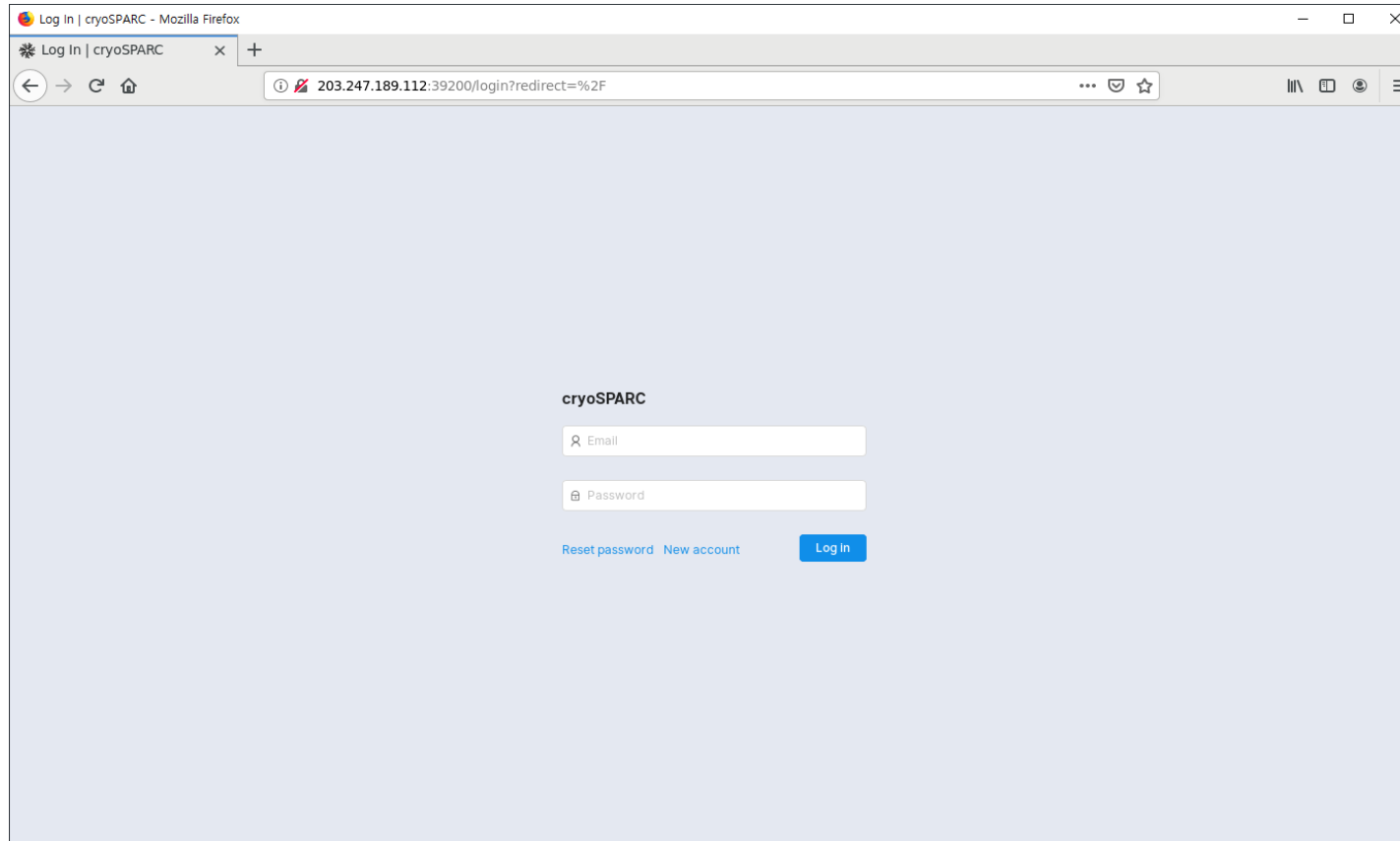
CRYO-EM DATA PROCESSING IN CRYOSPARC: INTRODUCTORY TUTORIAL

- <https://guide.cryosparc.com/processing-data/cryo-em-data-processing-in-cryosparc-introductory-tutorial>
- A subset of 20 movies from the EMPIAR-10025 T20S Proteasome dataset
- Launch firefox or web browser on your laptop
 - module load cryosparc-center/3.0.1-master
 - firefox



CONNECT TO MASTER

- **http://203.247.189.112:39200**



INTRODUCTION: DASHBOARD, PROJECTS, WORKSPACES AND JOBS

- Dashboard
 - At-a-glance information on your Projects, Workspaces and status of jobs
- Workflow is organized by Project, e.g. P1, P2, etc
- Projects contain one or more Workspaces, which in turn house jobs.

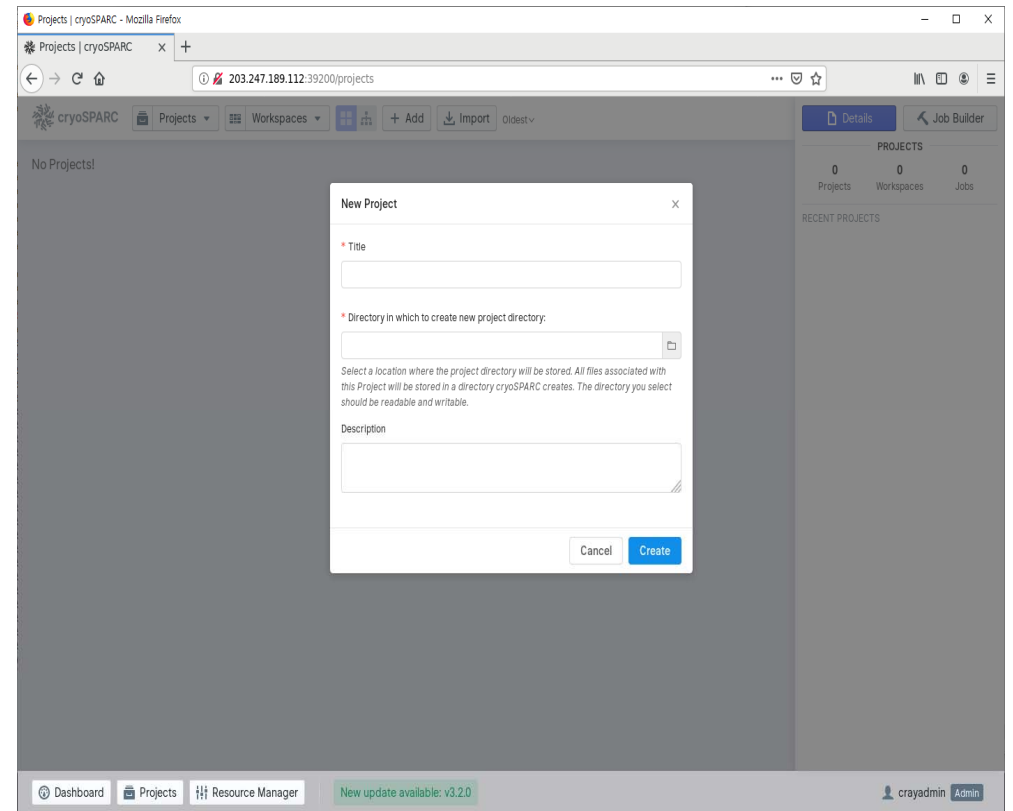
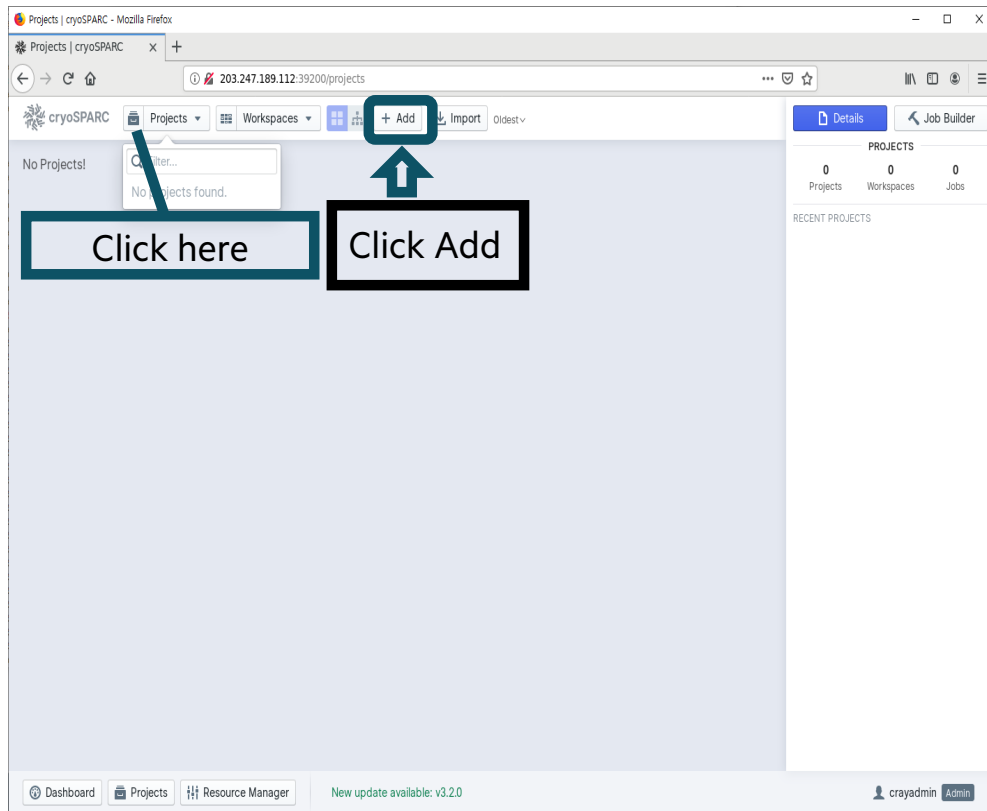
The screenshot displays the cryoSPARC dashboard in a Mozilla Firefox browser window. The dashboard is organized into several sections:

- Statistics:** A table showing counts for Projects, Workspaces, and Jobs across three time periods: This week, This month, and Total. All counts are currently zero.
- Change Log:** A list of updates for version v3.2.0, dated Mar 29, 2021. Updates include options for sorting jobs, performance improvements, and new features like Deep Particle Picking Jobs and Metadata tab enhancements.
- My Recent Jobs:** A section showing zero recent jobs.
- Links:** A sidebar with various resources including the CryoSPARC Guide, Tutorials and Case Studies, and Job Reference.
- Details Panel:** A right-hand panel showing counts for Projects, Workspaces, and Jobs (all zero) and a list of recent projects.

The bottom of the dashboard features navigation buttons for Dashboard, Projects, and Resource Manager, along with a notification for a new update available (v3.2.0) and a user profile for 'crayadmin'.

STEP 1

- Create a Project



STEP 1

The screenshot shows the cryoSPARC web interface in a Mozilla Firefox browser. The browser address bar shows the URL `203.247.189.112:39200/projects`. The main content area displays a "New Project" dialog box with the following fields:

- Title:** `cryoSPARC tutorial - crayadmin`
- Directory in which to create new project directory:** `/mnt/lustre/ibs/center/EDU/crayadmin`
- Description:** (empty text area)

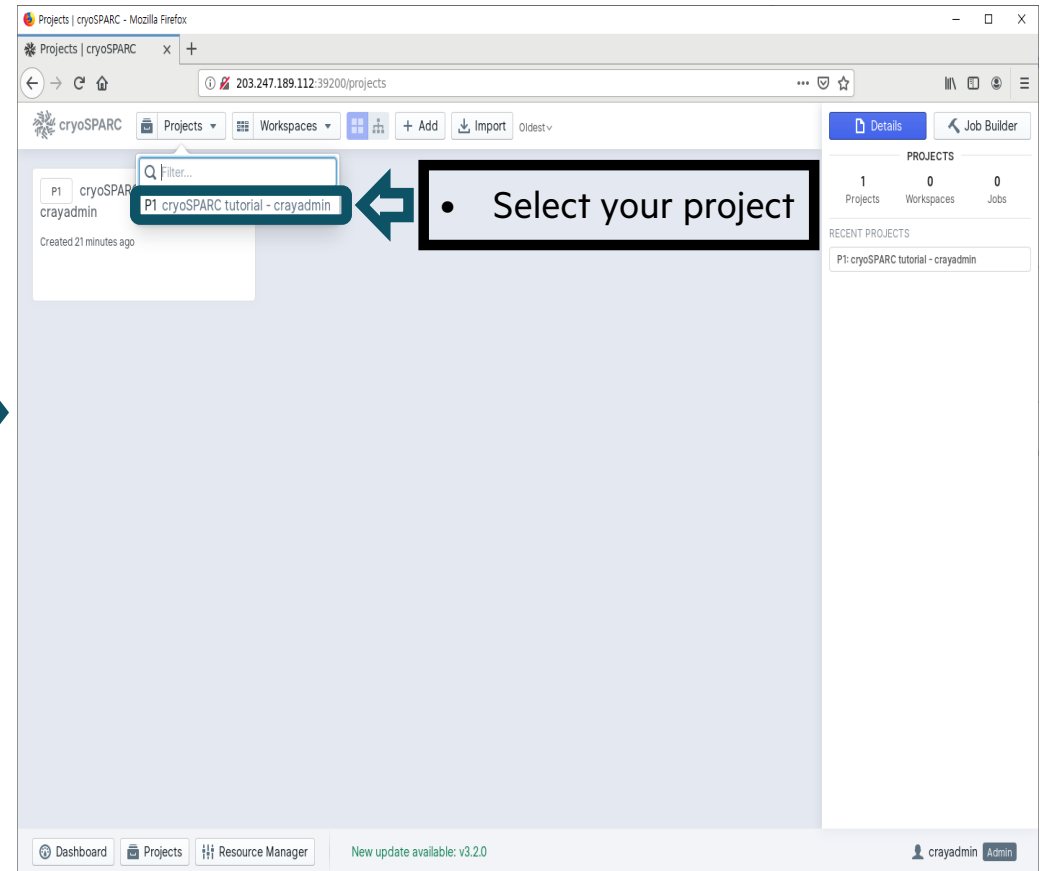
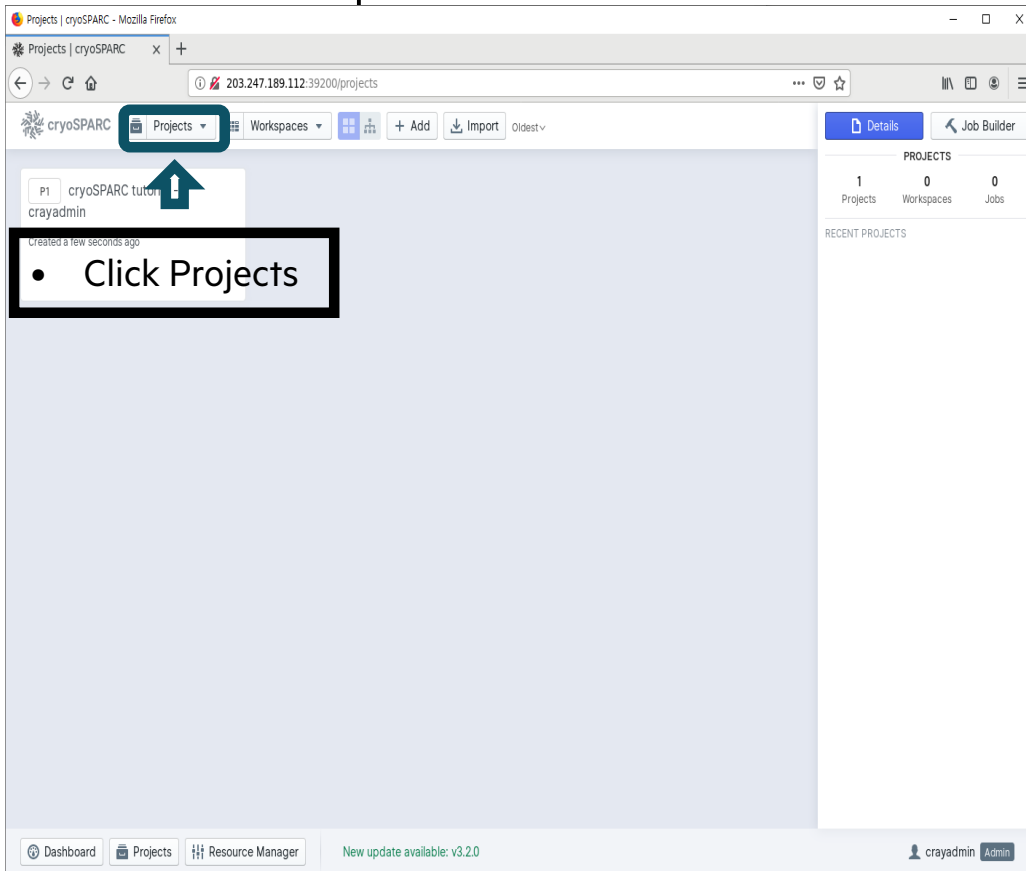
At the bottom of the dialog are "Cancel" and "Create" buttons. The "Create" button is highlighted with a blue border. To the right of the dialog, three callout boxes with arrows point to the input fields and the "Create" button:

- cryoSPARC tutorial – edu[01-40]
- /mnt/lustre/ibs/center/EDU/edu[01-40]
- Click here



STEP 2

- Create a Workspace



STEP 2

The screenshot shows the cryoSPARC web interface in a Mozilla Firefox browser. The address bar displays the URL `203.247.189.112:39200/projects/P1`. The main content area shows "No workspaces!". A red box highlights the "+ Add" button in the top navigation bar. A red arrow points from the callout box to the button. The callout box contains the text "Click Add".



The screenshot shows the cryoSPARC web interface with a "New Workspace in P1" dialog box open. The dialog box has a "Title" field, a "Description" field, and "Cancel" and "Create" buttons. The background interface is dimmed.



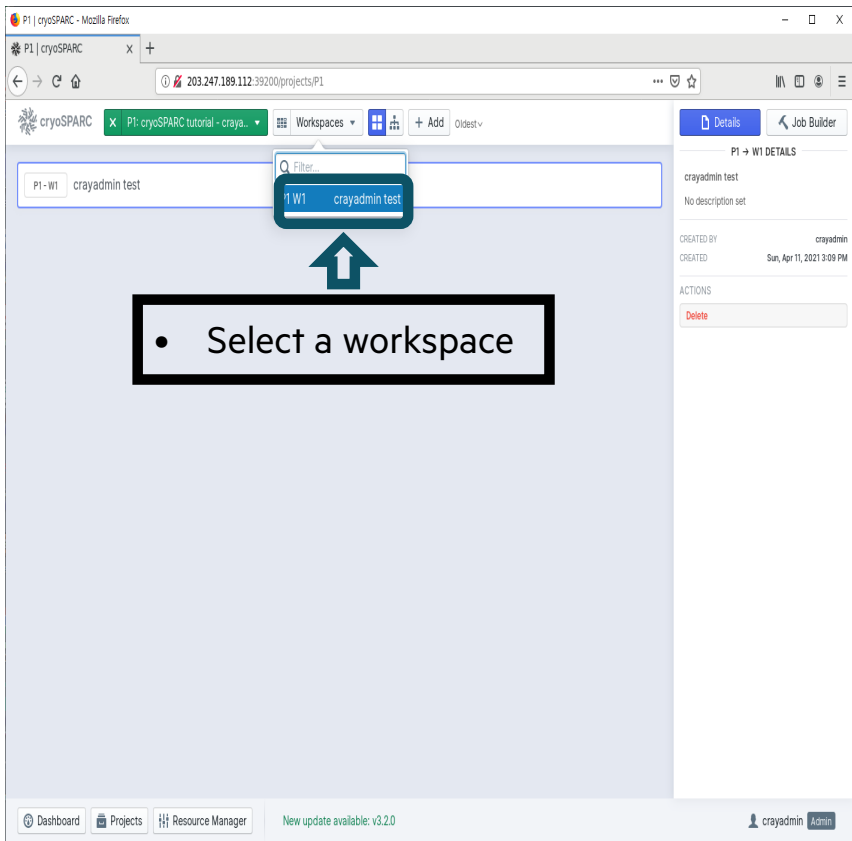
STEP 2

The screenshot displays the cryoSPARC web interface. A modal dialog titled "New Workspace in P1" is open, featuring a "Title" field with the text "crayadmin test" and a "Description" field. A blue arrow points to the "Create" button at the bottom right of the dialog. A callout box with the text "Set a title" points to the "Title" field. Another callout box with the text "Click Create" points to the "Create" button. The background shows the "P1 DETAILS" panel with various project information and actions.

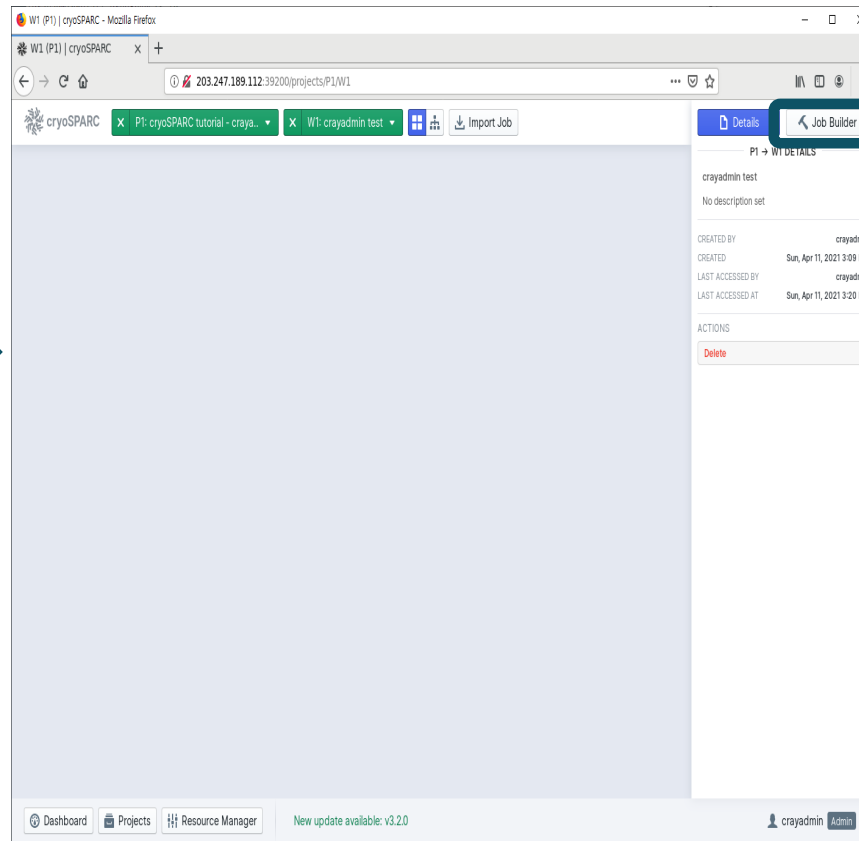


STEP 3

- Import Movies



• Select a workspace



• Select Job Builder



STEP 3

W1 (P1) | cryoSPARC - Mozilla Firefox

W1 (P1) | cryoSPARC

203.247.189.112:39200/projects/P1/W1

cryoSPARC

PI: cryoSPARC tutorial - craya... | W1: crayadmin test | Import Job

Details | Job Builder

JOB BUILDER

Search...

Workflows (1)

Extensive Workflow for T20s (BENCH) (BETA)

Imports (6)

- Import Movies
- Import Micrographs
- Import Particle Stack
- Import 3D Volumes
- Import Templates
- Import Result Group

Motion Correction (5)

- Full-frame motion correction (multi)
- Patch motion correction (multi)
- Local motion correction
- Local motion correction (multi)
- MotionCor2

CTF Estimation (4)

- Patch CTF estimation (multi)
- Patch CTF Extraction
- CTF Estimation (CTFFIND4)
- CTF Estimation (Gctf) (BETA)

Exposure Curation (1)

Dashboard | Projects | Resource Manager | New update available: v3.2.0 | crayadmin Admin

- Click Import Movies

W1 (P1) | cryoSPARC - Mozilla Firefox

W1 (P1) | cryoSPARC

203.247.189.112:39200/projects/P1/W1

cryoSPARC

PI: cryoSPARC tutorial - craya... | W1: crayadmin test | Import Job

Details | Job Builder

JOB BUILDER

J1 (Import Movies) BUILDING

New Job J1

PARAMETERS

Movies

- Movies data path:
- Gain reference path:
- Defect file path:
- Flip gain ref & defect file in X?:
- Flip gain ref & defect file in Y?:
- Rotate gain ref?:
- Raw pixel size (Å):
- Accelerating Voltage (kV):
- Spherical Aberration (mm):
- Total exposure dose (e/Å²):

Cancel | Queue

Dashboard | Projects | Resource Manager | New update available: v3.2.0 | crayadmin Admin



STEP 3

- Movies data path:
- /mnt/lustre/ibs/center/EDU/crayadmin/empiar_10025_subset/*.tif

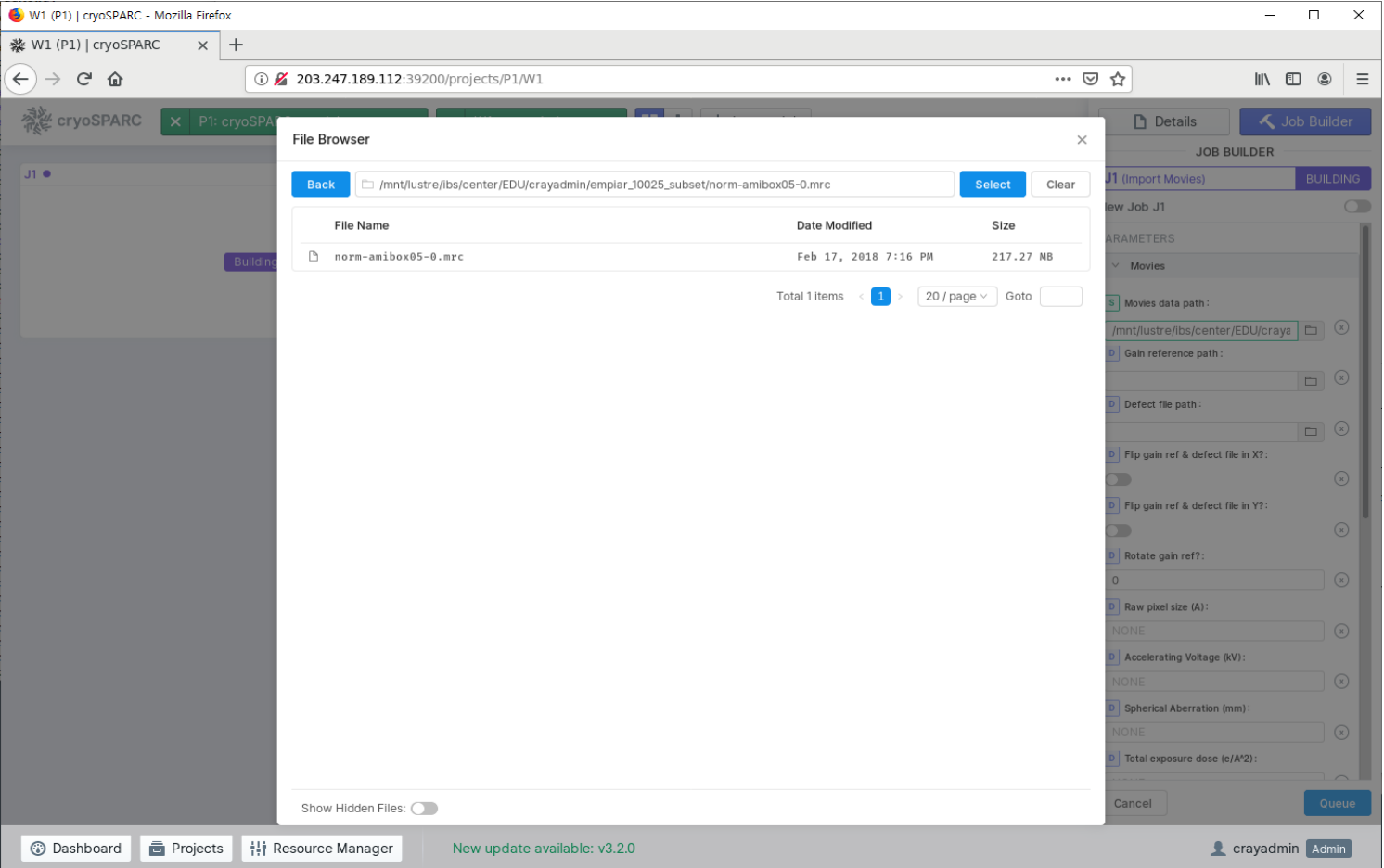
The screenshot shows the cryoSPARC web interface in a Mozilla Firefox browser. A 'File Browser' dialog is open, displaying a list of files in the directory /mnt/lustre/ibs/center/EDU/crayadmin/empiar_10025_subset/*.tif. The files are listed with their names, modification dates, and sizes. The background interface shows the 'JOB BUILDER' section with various parameters for job J1.

File Name	Date Modified	Size
14sep05c_00024sq_00003hl_00002es.frames.tif	Feb 16, 2018 8:51 PM	403.15 MB
14sep05c_00024sq_00003hl_00005es.frames.tif	Feb 16, 2018 8:52 PM	400.69 MB
14sep05c_00024sq_00004hl_00002es.frames.tif	Feb 16, 2018 8:54 PM	402.37 MB
14sep05c_00024sq_00006hl_00003es.frames.tif	Feb 16, 2018 8:55 PM	401.85 MB
14sep05c_c_00003gr_00014sq_00002hl_00005es.frames.tif	Feb 16, 2018 8:56 PM	403.74 MB
14sep05c_c_00003gr_00014sq_00004hl_00004es.frames.tif	Feb 16, 2018 8:57 PM	402.03 MB
14sep05c_c_00003gr_00014sq_00005hl_00002es.frames.tif	Feb 16, 2018 8:58 PM	403.39 MB
14sep05c_c_00003gr_00014sq_00005hl_00003es.frames.tif	Feb 16, 2018 8:59 PM	403.45 MB
14sep05c_c_00003gr_00014sq_00005hl_00005es.frames.tif	Feb 16, 2018 9:00 PM	403.86 MB
14sep05c_c_00003gr_00014sq_00006hl_00002es.frames.tif	Feb 16, 2018 9:02 PM	403.39 MB
14sep05c_c_00003gr_00014sq_00006hl_00003es.frames.tif	Feb 16, 2018 9:03 PM	402.79 MB
14sep05c_c_00003gr_00014sq_00006hl_00005es.frames.tif	Feb 16, 2018 9:04 PM	403.86 MB
14sep05c_c_00003gr_00014sq_00007hl_00004es.frames.tif	Feb 16, 2018 9:05 PM	402.33 MB
14sep05c_c_00003gr_00014sq_00007hl_00005es.frames.tif	Feb 16, 2018 9:06 PM	404.22 MB
14sep05c_c_00003gr_00014sq_00008hl_00005es.frames.tif	Feb 16, 2018 9:08 PM	403.07 MB
14sep05c_c_00003gr_00014sq_00009hl_00004es.frames.tif	Feb 16, 2018 9:09 PM	404.44 MB
14sep05c_c_00003gr_00014sq_00010hl_00002es.frames.tif	Feb 16, 2018 9:10 PM	403.81 MB
14sep05c_c_00003gr_00014sq_00011hl_00002es.frames.tif	Feb 16, 2018 9:11 PM	404.37 MB
14sep05c_c_00003gr_00014sq_00011hl_00003es.frames.tif	Feb 16, 2018 9:13 PM	403.88 MB
14sep05c_c_00003gr_00014sq_00011hl_00004es.frames.tif	Feb 16, 2018 9:14 PM	404.40 MB



STEP 3

- Gain reference path:
- /mnt/lustre/ibs/center/EDU/crayadmin/empiar_10025_subset/norm-amibox05-0.mrc

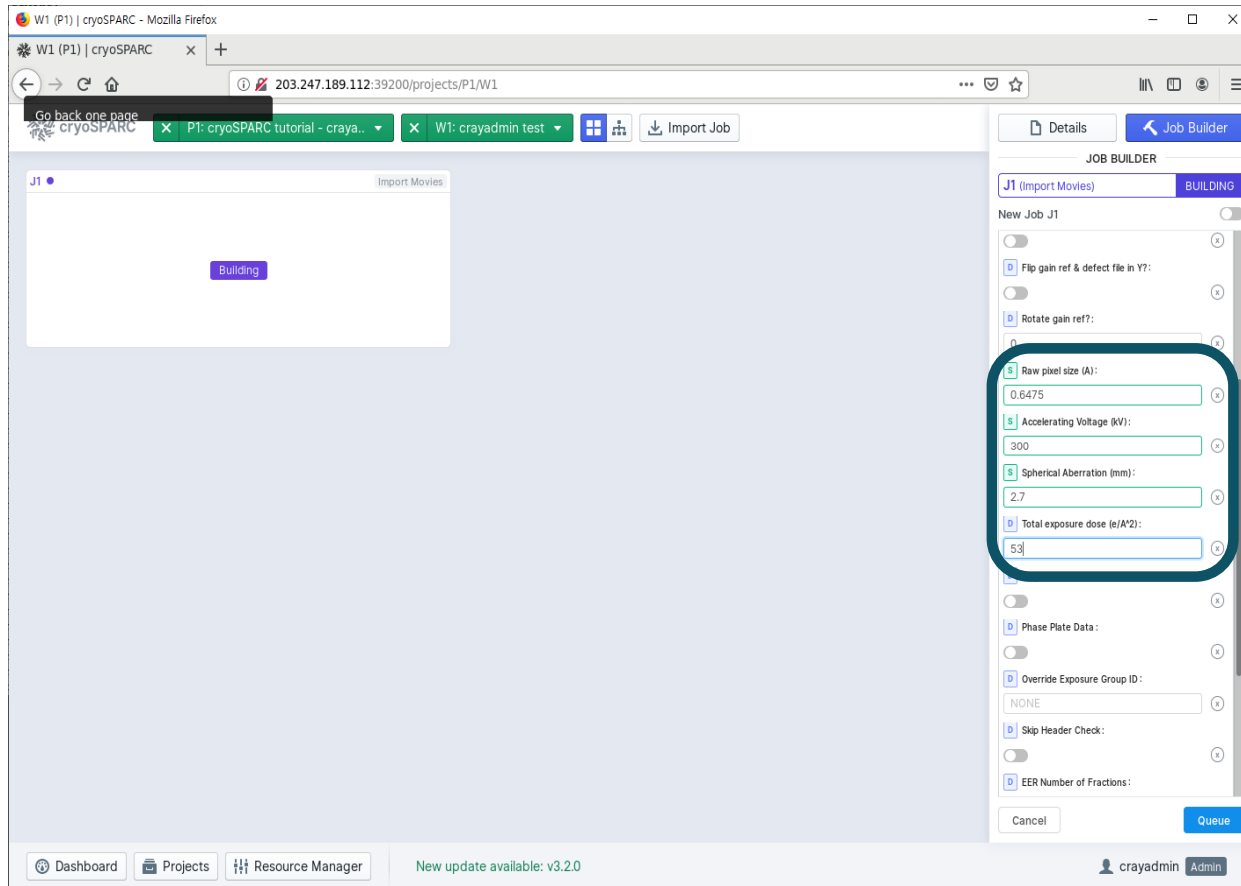


The screenshot shows the cryoSPARC web interface in Mozilla Firefox. A 'File Browser' dialog is open, displaying a file named 'norm-amibox05-0.mrc' with a date modified of 'Feb 17, 2018 7:16 PM' and a size of '217.27 MB'. The dialog also shows a 'Back' button, a 'Select' button, and a 'Clear' button. The background interface shows the 'JOB BUILDER' section with various parameters and a 'Queue' button.

File Name	Date Modified	Size
norm-amibox05-0.mrc	Feb 17, 2018 7:16 PM	217.27 MB



STEP 3



- Raw pixel size (A): 0.6475
- Accelerating Voltage (kV): 300
- Spherical Aberration (mm): 2.7
- Total exposure dose (e/A²): 53



STEP 3

W1 (P1) | cryoSPARC - Mozilla Firefox

W1 (P1) | cryoSPARC

203.247.189.112:39200/projects/P1/W1

cryoSPARC

P1: cryoSPARC tutorial - craya... W1: crayadmin test Import Job

J1 Import Movies

Building

Details Job Builder

J1 (Import Movies) BUILDING

New Job J1

300

Spherical Aberration (mm): 2.7

Total exposure dose (e/Å²): 53

Negative Stain Data:

Phase Plate Data:

Override Exposure Group ID: NONE

Skip Header Check:

EER Number of Fractions: 40

EER Upsampling Factor: 2

Compute settings

Number of CPUs to parallelize: 1

Cancel Queue

Dashboard Projects Resource Manager New update available: v3.2.0

crayadmin Admin

- Number of CPUs to parallelize: 1

- Click Queue

STEP 3

- Select cryo_all lane

W1 (P1) | cryoSPARC - Mozilla Firefox

W1 (P1) | cryoSPARC

203.247.189.112:39200/projects/P1/W1

Queue P1 → J1 (import_movies)

* Lane

- Lane cryo_all (cluster) (cluster)
cryo_all
- Lane jepyc (cluster) (cluster)
jepyc
- Lane jepyc-rtx (cluster) (cluster)
jepyc-rtx

Description

Enter a description.

* Run Job In

- Current Workspace (W1)
- New Workspace

Cancel Create

• Click Create



STEP 3

- Import Movies - Done

Overview Inputs and Parameters Outputs Metadata

Show from top Select checkpoint Follow latest Filter Types Filter Flags

```
> [CPU: 161.3 MB] -----
> [CPU: 161.3 MB] Loaded 20 movies.
> [CPU: 161.3 MB] Common fields:
> [CPU: 161.5 MB] mscope_params/accel_kv : {300.0}
> [CPU: 161.5 MB] mscope_params/cs_mm : {2.7}
> [CPU: 161.5 MB] mscope_params/total_dose_e_per_A2 : {53.0}
> [CPU: 161.5 MB] mscope_params/exp_group_id : {0}
> [CPU: 161.5 MB] mscope_params/phase_plate : {0}
> [CPU: 161.5 MB] mscope_params/neg_stain : {0}
> [CPU: 161.5 MB] movie_blob/psize_A : {0.6475}
> [CPU: 161.5 MB] movie_blob/shape : [ 38 7676 7420]
> [CPU: 161.5 MB] movie_blob/is_gain_corrected : {0}
> [CPU: 161.5 MB] -----
> [CPU: 161.5 MB] Making example plots. Exposures will be displayed without defect correction.
> [CPU: 161.5 MB] Reading file ...
```

Raw data J1/imported/14sep05c_00024sq_00003hl_00002es.frames.tif [png]

Outputs

- imported_movies
exposure Count: 20
- failed_movies
exposure Count: 0

JOB DETAILS

J1 (Import Movies) COMPLETED

New Job J1
Enter a description.

CREATED BY: crayadmin
LAST ACCESSED BY: crayadmin
LAST ACCESSED AT: Sun, Apr 11, 2021 3:55 PM
INTERACTIVE: No
CREATED: Sun, Apr 11 2021 3:26:35 PM
QUEUED: Sun, Apr 11 2021 3:55:11 PM
LAUNCHED: Sun, Apr 11 2021 3:55:15 PM
STARTED: Sun, Apr 11 2021 3:55:43 PM
COMPLETED: Sun, Apr 11 2021 3:57:56 PM

SIZE: 19.57 KB

ACTIONS

- Queue Job on cryo_all
- Queue Job on jepyc
- Queue Job on jepyc-rtx
- Kill Job
- Clear Job
- Clear Intermediate Results
- Export Job
- Clone Job

Job Builder

• Click Job Builder to go to next step



STEP 4

- Motion Correction

The screenshot shows the cryoSPARC web interface. The main content area displays a terminal window with the following output:

```
> [CPU: 161.3 MB] -----
> [CPU: 161.3 MB] Loaded 20 movies.
> [CPU: 161.3 MB] Common fields:
> [CPU: 161.3 MB]     mscope_params/accel_kv : {300.0}
> [CPU: 161.5 MB]     mscope_params/cs_mm : {2.7}
> [CPU: 161.5 MB]     mscope_params/total_dose_e_per_A2 : {53.0}
> [CPU: 161.5 MB]     mscope_params/exp_group_id : {0}
> [CPU: 161.5 MB]     mscope_params/phase_plate : {0}
> [CPU: 161.5 MB]     mscope_params/neg_stain : {0}
> [CPU: 161.5 MB]     movie_blob/psize_A : {0.6475}
> [CPU: 161.5 MB]     movie_blob/shape : [ 38 7676 7420]
> [CPU: 161.5 MB]     movie_blob/is_gain_corrected : {0}
> [CPU: 161.5 MB] -----
> [CPU: 161.5 MB] Making example plots. Exposures will be displayed without defect correction.
> [CPU: 161.5 MB] Reading file ...
```

Below the terminal output is a preview of the raw data: `J1/imported/14sep05c_00024sq_00003hl_00002es.frames.tif [png]`. The right sidebar shows the 'JOB BUILDER' workflow with the following sections:

- Workflows (1)
- Imports (6)
- Motion Correction (5)
 - Full-frame motion correction (multi)
 - Patch motion correction (multi)** (highlighted)
 - Local motion correction
 - Local motion correction (multi)
 - MotionCor2
- CTF Estimation (4)
- Exposure Curation (1)

• Select Patch motion correction(multi)



STEP 4

The screenshot displays the cryoSPARC web interface in a Mozilla Firefox browser. The main content area shows the 'Overview' tab for a job, with a terminal window displaying the following output:

```
> [CPU: 161.3 MB] =====
> [CPU: 161.3 MB] Loaded 20 movies.
> [CPU: 161.3 MB] Common fields:
> [CPU: 161.5 MB] mscope_params/accel_kv : {300.0}
> [CPU: 161.5 MB] mscope_params/cs_mm : {2.7}
> [CPU: 161.5 MB] mscope_params/total_dose_e_per_A2 : {53.0}
> [CPU: 161.5 MB] mscope_params/exp_group_id : {0}
> [CPU: 161.5 MB] mscope_params/phase_plate : {0}
> [CPU: 161.5 MB] mscope_params/neg_stain : {0}
> [CPU: 161.5 MB] movie_blob/psize_A : {0.6475}
> [CPU: 161.5 MB] movie_blob/shape : [ 38 7676 7420]
> [CPU: 161.5 MB] movie_blob/is_gain_corrected : {0}
> [CPU: 161.5 MB] =====
> [CPU: 161.5 MB] Making example plots. Exposures will be displayed without defect correction.
> [CPU: 161.6 MB] Reading file ...
```

Below the terminal output, a raw data image is shown: `Raw data J1/imported/14sep05c_00024sq_00003h1_00002es.frames.tif [png]`. The image is a grayscale micrograph showing a textured surface.

On the right side, the 'JOB BUILDER' panel is visible, showing a job named 'J2 (Patch motion correction (multi))' in a 'BUILDING' state. The 'INPUTS' section includes a field for 'movies (exposure)' with a value of '0' and a red dashed box around it containing the text 'Min: 1, Max: Infinity, Repeats: no'. The 'PARAMETERS' section is expanded to show 'General settings' and 'Motion correction' options.

A callout box with the text 'Drag and Drop' and an arrow points to the 'movies (exposure)' input field, indicating that users can drag and drop files into this field.

STEP 4

The screenshot shows the cryoSPARC web interface. The main panel displays the 'JOB BUILDER' for 'J2 (Patch motion correction (multi))'. The 'INPUTS' section is highlighted with a red box, showing 'movies (exposure)' with a count of 1 and 'Group 1 -> J1Imported_movies'. The 'PARAMETERS' section is also visible, with 'Number of GPUs to parallelize' set to 1. The 'Outputs' section shows 'Imported_movies' and 'failed_movies'.

The screenshot shows the cryoSPARC web interface. The main panel displays the 'JOB BUILDER' for 'J2 (Patch motion correction (multi))'. The 'PARAMETERS' section is highlighted with a red box, showing 'Number of GPUs to parallelize' set to 1. A red box also highlights the 'Queue' button, with an arrow pointing to it and the text 'Click Queue'.

- Number of GPUs to parallelize: 1



STEP 4

• Select cryo_all lane



• Click Create



STEP 4

• Motion correction - Done

Overview Inputs and Parameters Outputs Metadata

Show from top Select checkpoint Follow latest Filter Types Filter Flag

```
> license is valid.
> Launching job on lane cryo_all target cryo_all ...
> Launching job on cluster cryo_all
>
> ***** Cluster submission script: *****
>
> #!/bin/bash
> #SBATCH --job-name=cryosparc_center_P1_J2
> #SBATCH --partition=cryoem
> #SBATCH --output=/mnt/lustre/ibs/center/EDU/crayadmin/P1/J2/job.log
> #SBATCH --error=/mnt/lustre/ibs/center/EDU/crayadmin/P1/J2/job.log
> #SBATCH --gpus=1
> #SBATCH --gres-gpu:1
> #SBATCH --ntasks=6
> #SBATCH --cpus-per-task=1
>
> source $MODULESHOME/init/bash
> module load cuda/10.2
> module load cryosparc-center/3.0.1-worker
>
> /opt/cryoem/cryosparc-center/3.0.1/cryosparc2_worker/bin/cryosparcw run --project P1 --job J2 --master_hostname olaf1
> --master_command_core_port 39202 > /mnt/lustre/ibs/center/EDU/crayadmin/P1/J2/job.log 2>&1
>
> *****
> ----- Submission command:
> sbatch /mnt/lustre/ibs/center/EDU/crayadmin/P1/J2/queue_sub_script.sh
> ----- Cluster Job ID:
> 105116
> ----- Queued on cluster at 2021-04-11 16:29:46.867616
> ----- Job status at 2021-04-11 16:29:46.987934
>
> JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
> 105116 cryoem cryospar center PD 0:00 1 (None)
```

Outputs

- micrographs exposure Count: 0
- micrographs_incomplete exposure Count: 0

JOB DETAILS

J2 [Patch motion correction (multi)] LAUNCHED

New Job J2
Enter a description.

CREATED BY: crayadmin
INTERACTIVE: No
CREATED: Sun, Apr 11 2021 4:14:10 PM
QUEUED: Sun, Apr 11 2021 4:29:42 PM
LAUNCHED: Sun, Apr 11 2021 4:29:46 PM
PARENTS: J1
SIZE: 0 Bytes

ACTIONS

- Queue Job on cryo_all
- Queue Job on jupyter
- Queue Job on jupyter-rtx
- Kill Job
- Clear Job
- Clear Intermediate Results
- Export Job
- Clone Job
- Mark Job as Complete
- Delete Job

Overview Inputs and Parameters Outputs Metadata

```
Done in 0.25s
Writing 120x120 micrograph thumbnail to J2/thumbnails
/10574882217909946971_14sep05c_c_00003gr_00014sq_00011h1_00004es.frames_thumb_01x.png ...
Done in 0.00s
Writing 240x240 micrograph thumbnail to J2/thumbnails
/10574882217909946971_14sep05c_c_00003gr_00014sq_00011h1_00004es.frames_thumb_02x.png ...
Done in 0.00s
Writing dose-weighted result to J2/motioncorrected
/10574882217909946971_14sep05c_c_00003gr_00014sq_00011h1_00004es.frames_patch_aligned_doseweighted.mrc ...
Done in 0.25s
Writing background estimate to J2/motioncorrected
/10574882217909946971_14sep05c_c_00003gr_00014sq_00011h1_00004es.frames_background.mrc ...
Done in 0.01s
Writing motion estimates ...
Done in 0.00s
> [CPU: 365.7 MB] Outputting partial results now ...
> [CPU: 341.7 MB] -----
> [CPU: 341.7 MB] Compiling job outputs ...
> [CPU: 341.7 MB] Passing through outputs for output group micrographs from input group movies
> [CPU: 342.0 MB] This job outputted results ['micrograph_blob_non_dw', 'micrograph_thumbnail_blob_1x',
'micrograph_thumbnail_blob_2x', 'micrograph_blob', 'background_blob', 'rigid_motion', 'spline_motion']
> [CPU: 342.0 MB] Loaded output dset with 20 items
> [CPU: 342.0 MB] Passthrough results ['movie_blob', 'gain_ref_blob', 'mscope_params']
> [CPU: 342.0 MB] Loaded passthrough dset with 20 items
> [CPU: 342.1 MB] Intersection of output and passthrough has 20 items
> [CPU: 342.1 MB] Passing through outputs for output group micrographs_incomplete from input group movies
> [CPU: 342.1 MB] This job outputted results ['micrograph_blob']
> [CPU: 342.1 MB] Loaded output dset with 0 items
> [CPU: 342.1 MB] Passthrough results ['movie_blob', 'gain_ref_blob', 'mscope_params']
> [CPU: 342.1 MB] Loaded passthrough dset with 20 items
> [CPU: 342.1 MB] Intersection of output and passthrough has 0 items
> [CPU: 342.1 MB] Checking outputs for output group micrographs
> [CPU: 342.2 MB] Checking outputs for output group micrographs_incomplete
> [CPU: 342.2 MB] Updating job size ...
> [CPU: 342.2 MB] Exporting job and creating csg files ...
> [CPU: 342.2 MB] *****
> [CPU: 342.2 MB] Job complete. Total time 353.91s
```

JOB DETAILS

J2 [Patch motion correction (multi)] COMPLETED

New Job J2
Enter a description.

CREATED BY: crayadmin
INTERACTIVE: No
CREATED: Sun, Apr 11 2021 4:14:10 PM
QUEUED: Sun, Apr 11 2021 4:29:42 PM
LAUNCHED: Sun, Apr 11 2021 4:29:46 PM
STARTED: Sun, Apr 11 2021 4:30:16 PM
COMPLETED: Sun, Apr 11 2021 4:36:32 PM
PARENTS: J1
SIZE: 8.57 GB

ACTIONS

- Queue Job on cryo_all
- Queue Job on jupyter
- Queue Job on jupyter-rtx
- Kill Job
- Clear Job
- Clear Intermediate Results
- Export Job
- Clone Job
- Mark Job as Complete
- Delete Job

STEP 5

- CTF estimation

The screenshot shows the cryoSPARC web interface. At the top, there are tabs for 'P1: cryoSPARC tutorial - craya..' and 'W1: crayadmin test'. The main content area is divided into 'Overview', 'Inputs and Parameters', 'Outputs', and 'Metadata'. The 'Overview' tab is active, displaying a terminal window with logs and a 'Rigid motion' plot. On the right side, there is a 'JOB BUILDER' sidebar with a search bar and a list of workflows. The 'Job Builder' button is highlighted with a blue arrow pointing to it from a callout box. Below it, the 'CTF Estimation (4)' section is expanded, and the 'Patch CTF estimation (multi)' option is highlighted with a blue arrow pointing to it from another callout box. The bottom of the interface shows a navigation bar with 'Dashboard', 'Projects', and 'Resource Manager' buttons, along with a 'New update available: v3.2.0' notification and a user profile for 'crayadmin Admin'.

• Select Job Builder

• Select Patch CTF estimation (multi)



STEP 5

The screenshot displays the cryoSPARC web interface in a Firefox browser window. The address bar shows the URL `203.247.189.112:39200/projects/P1/W1/J2`. The interface includes a navigation bar with tabs for 'P1: cryoSPARC tutorial - craya..' and 'W1: crayadmin test', and a 'Job Builder' button. The main content area is divided into 'Overview', 'Inputs and Parameters', 'Outputs', and 'Metadata' tabs. The 'Overview' tab is active, showing a terminal log of a job's progress. The log includes the following text:

```
> [CPU: 250.3 MB] -----
> [CPU: 250.3 MB] Processed 0 of 20 movies in 41.86s
> [CPU: 3.13 GB] -- 0.0: processing 2 of 20: J1/imported/14sep05c_00024sq_00004hl_00002es.frames.tif
loading /mnt/lustre/ibs/center/EDU/crayadmin/P1/J1/imported/14sep05c_00024sq_00004hl_00002es.frames.tif
Loading raw movie data from J1/imported/14sep05c_00024sq_00004hl_00002es.frames.tif ...
Done in 5.70s
Loading gain data from J1/imported/norm-amibox05-0.mrc ...
Done in 0.00s
Processing ...
Done in 10.25s
Completed rigid and patch motion with (Z:5,Y:8,X:8) knots
Writing non-dose-weighted result to J2/motioncorrected
/14677808006177856559_14sep05c_00024sq_00004hl_00002es.frames_patch_aligned.mrc ...
Done in 0.29s
Writing 120x120 micrograph thumbnail to J2/thumbnails
/14677808006177856559_14sep05c_00024sq_00004hl_00002es.frames_thumb_@1x.png ...
Done in 0.00s
Writing 240x240 micrograph thumbnail to J2/thumbnails
/14677808006177856559_14sep05c_00024sq_00004hl_00002es.frames_thumb_@2x.png ...
Done in 0.00s
Writing dose-weighted result to J2/motioncorrected
/14677808006177856559_14sep05c_00024sq_00004hl_00002es.frames_patch_aligned_doseweighted.mrc ...
Done in 0.30s
Writing background estimate to J2/motioncorrected
/14677808006177856559_14sep05c_00024sq_00004hl_00002es.frames_background.mrc ...
Done in 0.01s
Writing motion estimates ...
Done in 0.01s
```

Below the log, there are two plots: 'Rigid motion for 14sep05c_00024sq_00003hl_00005es.frames [png] [pdf]' showing 'x-motion' and 'y-motion' plots. The 'x-motion' plot has a legend with 'raw coarse' (blue), 'smooth coarse' (orange), and 'smooth fine' (green). The 'y-motion' plot has a legend with 'raw coarse' (blue), 'smooth coarse' (orange), and 'smooth fine' (green).

The 'Outputs' section on the right shows a grid of micrographs with a 'Count: 20' and a 'micrographs_incomplete' section with a 'Count: 0'. A callout box with the text 'Drag and Drop' has arrows pointing to the 'micrographs' output folder and the 'exposure' input field in the job configuration panel. The job configuration panel on the right shows the 'exposure' input field with a value of '0' and a 'PARAMETERS' section with various settings.



STEP 5

The screenshot shows the cryoSPARC Job Builder interface for job J3. The 'Overview' tab is active, displaying a log of the job's progress. The 'Parameters' section is expanded, showing the following settings:

- General settings: Make motion diagnostic plots: ; Number of moves to plot: 10; Only process this many moves: NONE; Classic mode:
- CTF estimation: Amplitude Contrast: 0.1
- Compute settings: Number of GPUs to parallelize: 1

The 'Outputs' section shows a grid of micrographs. The 'Queue' button is highlighted with a blue box.

This screenshot is similar to the previous one but includes several annotations:

- A blue box highlights the 'exposures (exposure)' field in the 'Inputs' section, with a value of 1.
- A blue box highlights the 'Number of GPUs to parallelize' field in the 'Compute settings' section, with a value of 1.
- A blue box highlights the 'Queue' button.
- A callout box with an arrow pointing to the 'Queue' button contains the text 'Click Queue'.
- A larger callout box with an arrow pointing to the 'Number of GPUs to parallelize' field contains the text 'Number of GPUs to parallelize: 1'.

Click Queue

Number of GPUs to parallelize: 1

STEP 5

- Select cryo_all lane

The screenshot displays the cryoSPARC web interface. A modal dialog box titled "Queue P1 -> J3 (patch_ctf_estimation_multi)" is open. In the "Lane" section, the "Lane cryo_all (cluster) (cluster)" option is selected, and its input field contains the text "cryo_all". Below the "Lane" section is a "Description" field with the placeholder text "Enter a description.". In the "Run Job In" section, the "Current Workspace (W1)" option is selected. At the bottom right of the dialog, there are "Cancel" and "Create" buttons. The "Create" button is highlighted with a red box and a red arrow. The background interface shows a "JOB BUILDER" section with a job "J3 (Patch CTF estimation (multi))" in a "BUILDING" state. There are also tabs for "Overview", "Inputs and Parameters", "Outputs", and "Metadata". A log window on the left shows system messages and progress indicators.

- Click Create

STEP 5

• CTF estimation - Done

Job J3 (Patch CTF estimation (multi)) is in the **STARTED** state. The interface shows the job's execution details, including the submission script and job parameters. A notification at the bottom indicates a new notification system is active.

Job J3 (Patch CTF estimation (multi)) is in the **COMPLETED** state. The interface displays the final output logs, confirming the successful completion of the patch CTF estimation process. The job size is 47.62 MB.



THANK YOU

