

Single-Particle Data Analysis using cryoSPARC

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cryoSPARC

- A streamlined end-to-end single particle cryo-EM workflow
- Rapidly solve high-resolution structures
- SSH into one of the ports according to the instruction provided.
- A browser-based user interface and command line tools
- Work best on Google Chrome, may also work on Firefox and Safari.

Organization: Projects, Workspaces, Jobs

Project: a new sample on which you have collected data.

Workspace: created inside a project. Each project can contain multiple workspaces.

Job: One unit of processing work. Many jobs within each workspace.

Organization: Projects, Workspaces, Jobs

Card View

Project **Workspace** **Job**

The interface displays a grid of job cards. Each card represents a specific processing step in a cryo-EM workflow. The top navigation bar allows switching between projects and workspaces. The right sidebar provides detailed information about the selected job, including its title, tags, creation date, and status.

Job Details:

- Title:** tutorial
- Tags:** No tags applied.
- Created:** Jun 19, 2023, 2:03:44 PM
- Created By:** Dongyan Tan
- Last Accessed:** Jun 20, 2023, 10:56:23 PM
- Last Accessed By:** Dongyan Tan

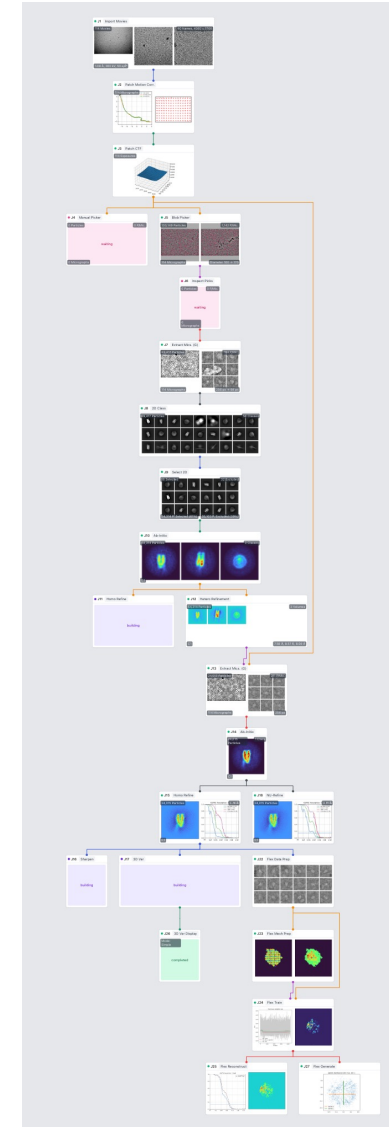
Description:

Statistics:

- Last Updated:** Jun 20, 2023, 10:05:30 PM
- Total Jobs:** 25
- Job Status:** 23 completed, 1 building, 1 failed

Actions: View Workspace →

Tree View



CryoSPARC Web Interface: Dashboard

Navigation bar

Navigation control

Side bar

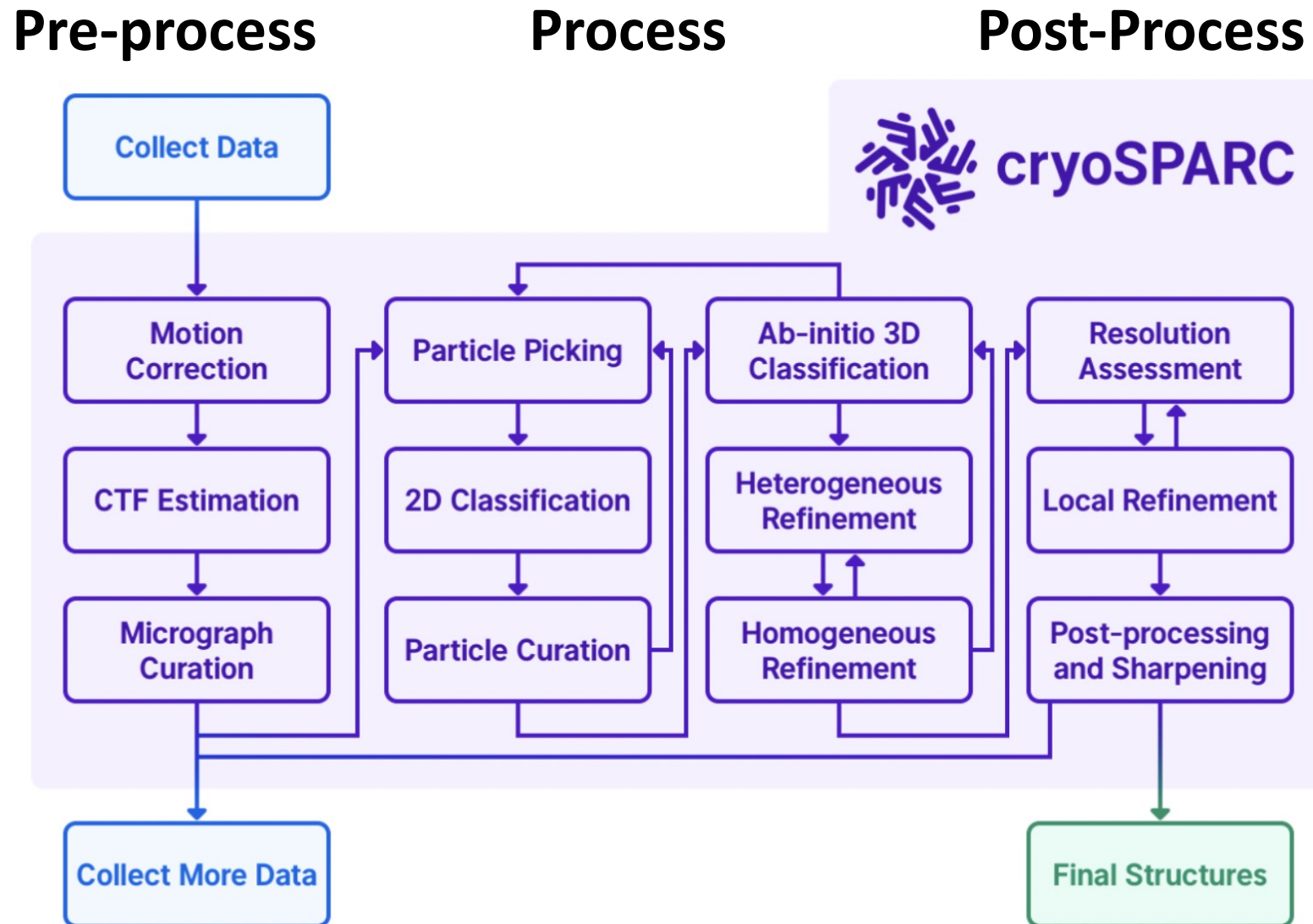
The dashboard displays a workflow with the following jobs:

- J1 Import Movies**: 46 Movies, 0.66 Å, 300 kV, 53 e/Å², 38 x 7676, 00m 22s, 6 settings.
- J2 Patch Motion Corr.**: 0 Micrographs, completed, 01m 02s, default, 2 settings.
- J3 Patch Motion Corr.**: 46 Micrographs, 03m 37s, default, 4 settings.
- J4 Patch CTF**: 46 Exposures, 01m 02s, default, 4 settings.
- J5 Blob Picker**: 51,410 Particles, 46 Micrographs, 1,118 P/Mic., 00m 33s, default, 1 setting.
- J6 Inspect Picks**: 20,108 Particles, 437 P/Mic., 25 Jobs, 19 Job Types, 3 Statuses.
- J7 Extract Mics. (G)**: 17,313 Particles, 376 P/Mic.

The right sidebar shows details for the selected job (P16 W1 tutorial):

- Details**: Title (tutorial), Tags (No tags applied), Created (Jun 19, 2023, 2:03:44 PM), Created By (Dongyan Tan), Last Accessed (Jun 20, 2023, 10:56:23 PM), Last Accessed By (Dongyan Tan).
- Description**: (Expandable section).
- Statistics**: Last Updated (Jun 20, 2023, 10:05:30 PM), Total Jobs (25), Job Status (23 completed, 1 building, 1 failed).
- Actions**: View Workspace →

Typical Workflow of Image Processing in cryoSPARC



Tutorial Data Set: nucleosome

- Subset of 26 movies in TIFF format
- Data collected at a 300kV microscope
- Pixel size: 1.08 Å
- Total Dosage : 50 e/ Å²
- Stable 200 KDa DNA-protein complex

Exploring Heterogeneity





Journal of Structural Biology

Volume 213, Issue 2, June 2021, 107702



3D variability analysis: Resolving continuous flexibility and discrete heterogeneity from single particle cryo-EM

Ali Punjani^{a b c}  , David J. Fleet^{a b}  

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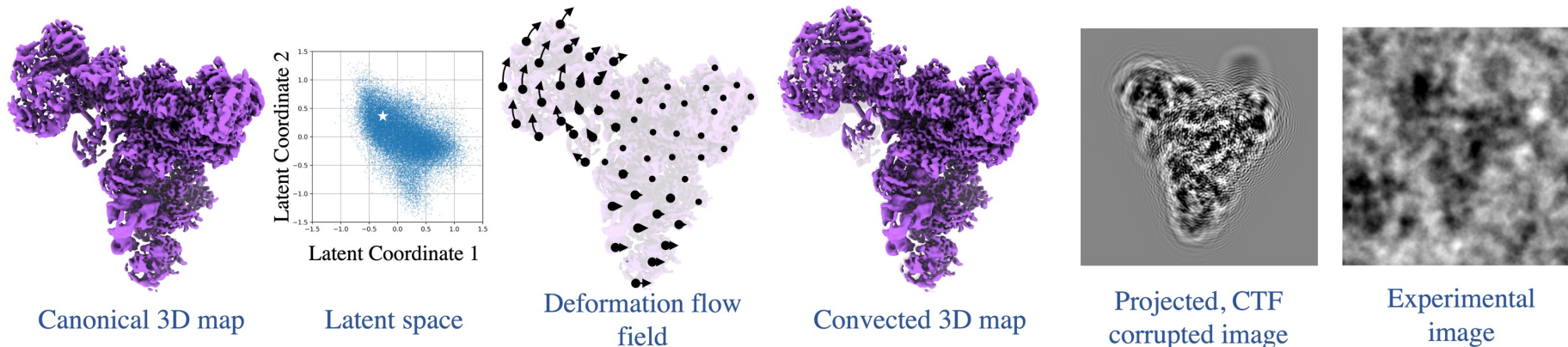
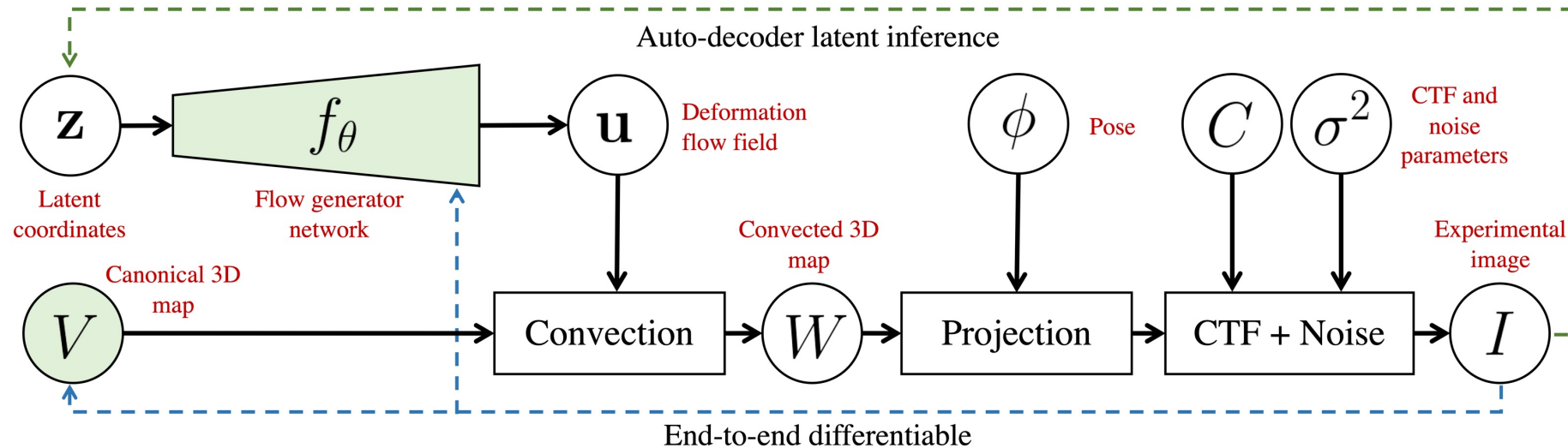
3DFlex: determining structure and motion of flexible proteins from cryo-EM

Ali Punjani  & David J. Fleet 

[Nature Methods](#) **20**, 860–870 (2023) | [Cite this article](#)

3DFlex Refinement

A advanced motion-based deep generative model for continuous heterogeneity



3DFlex Refinement

5 Steps

- 3D Flex Data Prep
- 3D Flex Mesh Prep – create a mesh
- 3D Flex Training – to model the movement of the particles
- 3D Flex Reconstruction

Limitation

- Compositional heterogeneity.
- Intricate motions such as side chain or loop motion
- Intermediate states with no data
- Interpretation of latent space, how it relates to a physically meaningful notion of energy