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Compute Resources

Have questions or need help with compute, including activation or issues? Follow this link.

User Agreement

Docker Usage

The information on this page assumes that you have a knowledge base of using Docker to create images and push them to a repository for use. If you need to review that information, please see the links below.

https://washu.atlassian.net/wiki/spaces/RUD/pages/1705115761/Docker+and+the+RIS+Compute1+Platform?atlOrigin=eyJpIjoiNzc4YTZjNjIxYmQwNGI3OTk4M2Q0MW

https://washu.atlassian.net/wiki/spaces/RUD/pages/1864892726/Docker+Basics+Building+Tagging+Pushing+A+Custom+Docker+Image?atlOrigin=eyJpIjoiMTVjMjNlM

storageN

The use of `storageN` within these documents indicates that any storage platform can be used.

Current available storage platforms:

- storage1
- storage2

Software Included

AlphaFold v2.2.0 (https://github.com/deepmind/alphafold)

Getting Started

Connect to compute client.

Prepare the computing environment before submitting an AlphaFold job.

AlphaFold can run by default on both V100 and A100 GPU architectures. Modify the `-gpu` argument to specify the GPU architecture.

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A list of GPU models can be found here.

Jobs can be managed using job groups. Job groups are a way to submit a large number of jobs at once.

Additional Information

Please refer to official AlphaFold documentation for direction on setting up run options, expected output, example runs, etc.