**Caspers cheatsheet**

***Cluster***

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| Request GPU on izar | Sinteract -p gpu -q gpu -g gpu:1 -t 48:0:0 -m 32gb |
| Execute dMaSIF environment | source load\_env/load\_dMaSIF\_env.sh |
| dMaSIF search  (training) | python -W ignore -u main\_training.py --experiment\_name dMaSIF\_search\_3layer\_12A --batch\_size 64 --embedding\_layer dMaSIF --search True --device cuda:0 --random\_rotation True --radius 12.0 --n\_layers 3 |
| dMaSIF  search w more points (training) | python -W ignore -u main\_training.py --experiment\_name max\_more\_points --batch\_size 64 --embedding\_layer dMaSIF --search True --device cuda:0 --random\_rotation True --resolution 0.5 --sup\_sampling 100 --radius 12.0 --n\_layers 3 |
| dMaSIF search  (inference) | python -W ignore -u main\_inference.py --experiment\_name dMaSIF\_search\_3layer\_12A\_epoch37 --batch\_size 64 --embedding\_layer dMaSIF --search True --device cuda:0 --random\_rotation True --radius 12.0 --n\_layers 3 |
| dMaSIF site  (training) | python -W ignore -u main\_training.py --experiment\_name dMaSIF\_site\_3layer\_15A --batch\_size 64 --embedding\_layer dMaSIF --site True --single\_protein True --random\_rotation True --radius 15.0 --n\_layers 3 |
| Start jupyter notebook server | jupyter notebook --no-browser --port 8080  ssh -NL 8080:localhost:8080 jansen@izar.epfl.ch |
| Start jupyter notebook server from node | jupyter notebook --no-browser --port=1234 --ip=$(hostname -i)  ssh -NL 1234:10.91.27.35:1234 goverde@izar.epfl.ch |
| Start tensorboard from cluster | tensorboard --logdir=runs --port=1234  ssh -NL 1234:localhost:1234 goverde@izar.epfl.ch |
| Copy files | scp -r goverde@izar.epfl.ch:/home/goverde/dMaSIF/preds/dMaSIF\_search\_3layer\_12A\_epoch37 /Users/goverde/Documents/MaSIF\_search\_output |
| Mount | sshfs -o reconnect jansen@fidis.epfl.ch:/work/upcorreia/users/jansen/masif\_site\_selected/data/masif\_site/ mnt |
| Unmount | umount -f ~/mnt |

***Tmux***

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| New session | tmux new -s mysession |
| Close session | tmux kill-session -t mysession |
| Attach to session | tmux a -t mysession |
| Create new window | Ctrl + b, c |

***Conda***

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| **New environment** | conda create --name py35 python=3.5 |
| **List environments** | conda env list |
| **Install package**  **for env** | conda install PACKAGENAME |

***Pymol***

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| **Load MaSIF pointcloud into PyMol** | ﻿loadpred /Users/goverde/Documents/MaSIF\_search\_output, 2VE6\_A |
| **Pymol align proteins** | ﻿pair\_fit GD\_original\_prot///1-89/N+CA+C, GD\_designed\_prot///1-89/N+CA+C |
| **Load dMaSIF pointcloud into PyMol** | loadvtk 1A2K\_C\_pred.vtk |
| **Load specific patch** | ﻿loadpred .,ALA91 (leave out ‘\_pred’ part) |
| **Color whole pdb** | ﻿color white, 1A2K\_AB |
| **Color specific residue** | ﻿color gold, Chain B and resi 91 |
| **Label specific residue** | label n. CA **and** i. 44, "(**%s**, **%s**, **%s**)" % (resn, resi, b) |
| **Set transparency** | set cartoon\_transparency, 0.5, <sele> |
| **Color chain, b factor (confidence score for AF2)** | spectrum b, blue\_white\_red, minimum=50, maximum=100 |

***GPU checks and queues in general***

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| Check jobs | Squeue |
| Check user jobs (no caps) | squeue -u |
| Check GPU | nvidia-smi |
| Check GPU | gpustat (must be installed first, use pip in venv). |
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