

## Full information on catdcd options (on stampede)

```
catdcd -o catenated_file.dcd 1.dcd 2.dcd 3.dcd ...
```

```
catdcd -o shortfile.dcd -stride 10 longfile.dcd
```

Suppose I want to capture atoms 1-999.

Open the PSF/PDB in VMD and then type in the tkcon:

```
set sel [atomselect top "my selection"] (e.g. "chain G")
set out [open "prot-ind.dat" w]
puts $out [$sel get index]
close $out
```

prot-ind.dat is a line of indices you feed to catdcd, like this:

```
catdcd -o reduced.dcd -i prot-ind.dat 1.dcd 2.dcd ...
```

You can also add a "-stride" to cut down the frames.

```
login3.stampede(1)$ /opt/apps/vmd/1.9.2/bin/plugins/LINUXAMD64/bin/catdcd
5.1/catdcd
CatDCD 5.1
/opt/apps/vmd/1.9.2/bin/plugins/LINUXAMD64/bin/catdcd5.1/catdcd -o
outputfile [-otype <filetype>] [-i indexfile]
[-stype <filetype>] [-s structurefile]
[-first firstframe] [-last lastframe] [-stride stride]
[-<filetype>] inputfile1 [-<filetype>] inputfile2 ...
```

Allowed input file types:

```
ABINIT Alchemy AMBERPREP BallStick MSIBGF BiosymCAR Boogie Cacao CADPAC
CHARMm Chem3d-1 Chem3d-2 CSSR FDAT GSTAT Dock DockPDB Feature Fractional
GAMESSoutput GaussianZmatrix Gaussian92output Gaussian94output Gromos96A
Gromos96N HyperchemHIN IsisSDF M3D MacMolecule Macromodel MicroWorld
MM2Input MM2Output MM3 MMADS MDLMOL MOLIN MopacCartesian MopacInternal
MopacOutput PCModel PSGVBin PSGVBout QuantaMSF Schakal ShelX SMILES
Spartan SpartanSE SpartanMM SybylMol SybylMol2 Conjure UniChemXYZ XYZ XED
bgf binpos car cor cpmd crd crdbox cube dcd dlpolyhist dlpoly3hist gro
g96 trr trj xtc js lammstrj mol2 namdbin pdb pqr rst7 tinker OUTCAR
POSCAR VASP_XDATCAR5 XDATCAR xml xbgf xsf xyz dtr mae vcf vtf webpdb
```

Allowed output file types:

```
ABINIT bgf binpos crd crdbox dcd gro trr js lammstrj mol2 namdbin pdb
pqr rst7 POSCAR xbgf xyz dtr mae
login3.stampede(2)$
```