**Codes**

**Marvin:**

>screen

>cp -R /home/databases/SCALE-META-reads /home/tiffany

>scp -r SCALE-META-reads tiffdp@wonko.bi.up.ac.za:/home/tiffdp

**Wonko:**

>screen

>cp -R /home/tiffdp/SCALE-META-reads /nlustre/users/tiffdp/

>cd /nlustre/users/tiffdp/SCALE-META-reads

>nano atlas.sh

#!/bin/bash

#PBS -l nodes=1:ppn=8

#PBS -l walltime=120:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/stdout.log

#PBS -e /nlustre/users/tiffdp/stderr.log

#PBS -k oe

#PBS -m ae

#PBS -M 17duplti@gmail.com

module load metagenome-atlas

source /apps/miniconda3/etc/profile.d/cond/sh

conda activate atlasenv

atlas init –db-dir databases /nlustre/users/tiffdp/SCALE-META-reads

atlas run qc –-keep-going

>qsub atlas.sh

>cd /home/tiffdp/

>ls -al 20082D\*/sequence\_quality\_control

>cd /nlustre/users/tiffdp/SCALE-META-reads/

>module load fastqc-0.11.7

>fastqc 20082D-04-01\_S1\_L003\_R1\_001\_fastqc.gz

>fastqc 20082D-04-18\_S11\_L003\_R1\_001\_fastqc.gz

>fastqc 20082D-04-39\_S21\_L003\_R1\_001\_fastqc.gz

>fastqc 20082D-04-41\_S23\_L003\_R1\_001\_fastqc.gz

>cd /home/tiffdp/20082D-04-01-S1-L003-001/sequence\_quality\_control

>fastqc 20082D-04-01-S1-L003-001\_QC\_R1.fastqc.gz

>cd /home/tiffdp/20082D-04-18-S11-L003-001/sequence\_quality\_control

>fastqc 20082D-04-18-S11-L003-001\_QC\_R1.fastqc.gz

>cd /home/tiffdp/20082D-04-39-S21-L003-001/sequence\_quality\_control

>fastqc 20082D-04-39-S21-L003-001\_QC\_R1.fastqc.gz

>cd /home/tiffdp/20082D-04-41-S23-L003-001/sequence\_quality\_control

>fastqc 20082D-04-41-S23-L003-001\_QC\_R1.fastqc.gz

**Marvin:**

>cd /home/tiffany/SCALE-META-reads

>nano trimmomatic.sh

#!/bin/bash

for f in $(ls \*fastq.gz | sed -e 's/\_R1\_001.fastq.gz//' -e 's/\_R2\_001.fastq.gz//' | sort -u)

do java -jar /usr/local/src/Trimmomatic-0.36/trimmomatic-0.36.jar PE -phred33 -threads 8 ${f}\_R1\_001.fastq.gz ${f}\_R2\_001.fastq.gz ${f}\_R1\_001\_paired.fastq.gz ${f}\_R1\_001\_unpaired.fastq.gz ${f}\_R2\_001\_paired.fastq.gz ${f}\_R2\_001\_unpaired.fastq.gz ILLUMINACLIP:/usr/local/src/Trimmomatic-0.36/adapters/NexteraPE-PE.fa:2:30:10 LEADING:3 TRAILING:3 SLIDINGWINDOW:4:15 MINLEN:36

done

>chmod +x trimmomatic.sh

>./trimmomatic.sh

>scp 20082D-04-18\_S11\_L003\_R1\_001\_paired.fastq.gz 20082D-04-18\_S11\_L003\_R2\_001\_paired.fastq.gz 20082D-04-23\_S15\_L003\_R1\_001\_paired.fastq.gz 20082D-04-23\_S15\_L003\_R2\_001\_paired.fastq.gz 20082D-04-38\_S20\_L003\_R1\_001\_paired.fastq.gz 20082D-04-38\_S20\_L003\_R2\_001\_paired.fastq.gz 20082D-04-42\_S24\_L003\_R1\_001\_paired.fastq.gz 20082D-04-42\_S24\_L003\_R2\_001\_paired.fastq.gz 20082D-04-45\_S27\_L003\_R1\_001\_paired.fastq.gz 20082D-04-45\_S27\_L003\_R2\_001\_paired.fastq.gz 20082D-04-49\_S30\_L003\_R1\_001\_paired.fastq.gz 20082D-04-49\_S30\_L003\_R2\_001\_paired.fastq.gz 20082D-04-64\_S38\_L003\_R1\_001\_paired.fastq.gz 20082D-04-64\_S38\_L003\_R2\_001\_paired.fastq.gz tiffdp@wonko.bi.up.ac.za:/nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/

**Wonko:**

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples

>nano spades\_1500.sh

#!/bin/bash

#PBS -l nodes=1:ppn=24

#PBS -l walltime=300:00:00

#PBS -q bigmem

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/stdout.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples /stderr.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load SPAdes-3.13.0

for f in $(ls \*fastq.gz | sed -e 's/\_R1\_001\_paired.fastq.gz//' -e 's/\_R2\_001\_paired.fastq.gz//' | sort -u)

do spades.py --pe1-1 ${f}\_R1\_001\_paired.fastq.gz --pe1-2 ${f}\_R2\_001\_paired.fastq.gz --meta -t 24 -o ${f}\_metaspades\_results -m 500

done

>qsub spades\_1500.sh

**Marvin:**

>scp 20082D-04-01\_S1\_L003\_R1\_001\_paired.fastq.gz 20082D-04-01\_S1\_L003\_R2\_001\_paired.fastq.gz 20082D-04-03\_S43\_L003\_R1\_001\_paired.fastq.gz 20082D-04-03\_S43\_L003\_R2\_001\_paired.fastq.gz 20082D-04-05\_S4\_L003\_R1\_001\_paired.fastq.gz 20082D-04-05\_S4\_L003\_R2\_001\_paired.fastq.gz 20082D-04-11\_S6\_L003\_R1\_001\_paired.fastq.gz 20082D-04-11\_S6\_L003\_R2\_001\_paired.fastq.gz 20082D-04-15\_S9\_L003\_R1\_001\_paired.fastq.gz 20082D-04-15\_S9\_L003\_R2\_001\_paired.fastq.gz 20082D-04-26\_S17\_L003\_R1\_001\_paired.fastq.gz 20082D-04-26\_S17\_L003\_R2\_001\_paired.fastq.gz 20082D-04-21\_S13\_L003\_R1\_001\_paired.fastq.gz 20082D-04-21\_S13\_L003\_R2\_001\_paired.fastq.gz 20082D-04-31\_S18\_L003\_R1\_001\_paired.fastq.gz 20082D-04-31\_S18\_L003\_R2\_001\_paired.fastq.gz 20082D-04-40\_S22\_L003\_R1\_001\_paired.fastq.gz 20082D-04-40\_S22\_L003\_R2\_001\_paired.fastq.gz 20082D-04-43\_S25\_L003\_R1\_001\_paired.fastq.gz 20082D-04-43\_S25\_L003\_R2\_001\_paired.fastq.gz 20082D-04-47\_S28\_L003\_R1\_001\_paired.fastq.gz 20082D-04-47\_S28\_L003\_R2\_001\_paired.fastq.gz 20082D-04-53\_S31\_L003\_R1\_001\_paired.fastq.gz 20082D-04-53\_S31\_L003\_R2\_001\_paired.fastq.gz 20082D-04-56\_S34\_L003\_R1\_001\_paired.fastq.gz 20082D-04-56\_S34\_L003\_R2\_001\_paired.fastq.gz 20082D-04-58\_S36\_L003\_R1\_001\_paired.fastq.gz 20082D-04-58\_S36\_L003\_R2\_001\_paired.fastq.gz 20082D-04-65\_S39\_L003\_R1\_001\_paired.fastq.gz 20082D-04-65\_S39\_L003\_R2\_001\_paired.fastq.gz 20082D-04-68\_S41\_L003\_R1\_001\_paired.fastq.gz 20082D-04-68\_S41\_L003\_R2\_001\_paired.fastq.gz tiffdp@wonko.bi.up.ac.za:/nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/

>scp 20082D-04-02\_S2\_L003\_R1\_001\_paired.fastq.gz 20082D-04-02\_S2\_L003\_R2\_001\_paired.fastq.gz 20082D-04-04\_S3\_L003\_R1\_001\_paired.fastq.gz 20082D-04-04\_S3\_L003\_R2\_001\_paired.fastq.gz 20082D-04-06\_S5\_L003\_R1\_001\_paired.fastq.gz 20082D-04-06\_S5\_L003\_R2\_001\_paired.fastq.gz 20082D-04-12\_S7\_L003\_R1\_001\_paired.fastq.gz 20082D-04-12\_S7\_L003\_R2\_001\_paired.fastq.gz 20082D-04-16\_S10\_L003\_R1\_001\_paired.fastq.gz 20082D-04-16\_S10\_L003\_R2\_001\_paired.fastq.gz 20082D-04-22\_S14\_L003\_R1\_001\_paired.fastq.gz 20082D-04-22\_S14\_L003\_R2\_001\_paired.fastq.gz 20082D-04-32\_S19\_L003\_R1\_001\_paired.fastq.gz 20082D-04-32\_S19\_L003\_R2\_001\_paired.fastq.gz 20082D-04-41\_S23\_L003\_R1\_001\_paired.fastq.gz 20082D-04-41\_S23\_L003\_R2\_001\_paired.fastq.gz 20082D-04-44\_S26\_L003\_R1\_001\_paired.fastq.gz 20082D-04-44\_S26\_L003\_R2\_001\_paired.fastq.gz 20082D-04-48\_S29\_L003\_R1\_001\_paired.fastq.gz 20082D-04-48\_S29\_L003\_R2\_001\_paired.fastq.gz 20082D-04-54\_S32\_L003\_R1\_001\_paired.fastq.gz 20082D-04-54\_S32\_L003\_R2\_001\_paired.fastq.gz 20082D-04-55\_S33\_L003\_R1\_001\_paired.fastq.gz 20082D-04-55\_S33\_L003\_R2\_001\_paired.fastq.gz 20082D-04-57\_S35\_L003\_R1\_001\_paired.fastq.gz 20082D-04-57\_S35\_L003\_R2\_001\_paired.fastq.gz 20082D-04-66\_S40\_L003\_R1\_001\_paired.fastq.gz 20082D-04-66\_S40\_L003\_R2\_001\_paired.fastq.gz 20082D-04-69\_S42\_L003\_R1\_001\_paired.fastq.gz 20082D-04-69\_S42\_L003\_R2\_001\_paired.fastq.gz tiffdp@wonko.bi.up.ac.za:/nlustre/users/tiffdp/SCALE-META-reads/500\_samples/

>scp 20082D-04-14\_S8\_L003\_R1\_001\_paired.fastq.gz 20082D-04-14\_S8\_L003\_R2\_001\_paired.fastq.gz 20082D-04-20\_S12\_L003\_R1\_001\_paired.fastq.gz 20082D-04-20\_S12\_L003\_R2\_001\_paired.fastq.gz 20082D-04-24\_S16\_L003\_R1\_001\_paired.fastq.gz 20082D-04-24\_S16\_L003\_R2\_001\_paired.fastq.gz 20082D-04-37\_S44\_L003\_R1\_001\_paired.fastq.gz 20082D-04-37\_S44\_L003\_R2\_001\_paired.fastq.gz 20082D-04-39\_S21\_L003\_R1\_001\_paired.fastq.gz 20082D-04-39\_S21\_L003\_R2\_001\_paired.fastq.gz 20082D-04-63\_S37\_L003\_R1\_001\_paired.fastq.gz 20082D-04-63\_S37\_L003\_R2\_001\_paired.fastq.gz tiffdp@wonko.bi.up.ac.za:/nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/

**Wonko:**

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples

>module load fastqc-0.11.7

>fastqc 20082D-04-18\_S11\_L003\_R1\_001\_paired.fastq.gz

>cd /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples

>module load fastqc-0.11.7

>fastqc 20082D-04-01\_S1\_L003\_R1\_001\_paired.fastq.gz

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples

>module load fastqc-0.11.7

>fastqc 20082D-04-41\_S23\_L003\_R1\_001\_paired.fastq.gz

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples

>module load fastqc-0.11.7

>fastqc 20082D-04-39\_S21\_L003\_R1\_001\_paired.fastq.gz

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples

>nano spades\_500.sh

#!/bin/bash

#PBS -l nodes=1:ppn=24

#PBS -l walltime=300:00:00

#PBS -q bigmem

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/stdout.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/stderr.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load SPAdes-3.13.0

for f in $(ls \*fastq.gz | sed -e 's/\_R1\_001\_paired.fastq.gz//' -e 's/\_R2\_001\_paired.fastq.gz//' | sort -u)

do spades.py --pe1-1 ${f}\_R1\_001\_paired.fastq.gz --pe1-2 ${f}\_R2\_001\_paired.fastq.gz --meta -t 24 -o ${f}\_metaspades\_results -m 500

done

>qsub spades\_500.sh

>qsub -I -q interactive -N quast -l nodes=1:ppn=2 -l walltime=02:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples

> module load quast-5.0.2

> quast.py \*.fasta -o quast\_results -t 2

[in each metaspades\_results directory]

>qsub -I -q interactive -N bbmap -l nodes=1:ppn=2 -l walltime=02:00:00

>module load bbmap

>module load samtools-1.7

>cp /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_R1\_001\_paired.fastq.gz /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results

>cp /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_R2\_001\_paired.fastq.gz /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results

>bbmap.sh ref=contigs.fasta in=20082D-04-18\_S11\_L003\_R1\_001\_paired.fastq.gz in2=20082D-04-18\_S11\_L003\_R2\_001\_paired.fastq.gz out=metaspades.sam bamscript=sam2bam.sh

>./sam2bam.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N quast -l nodes=1:ppn=2 -l walltime=02:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples

>module load quast-5.0.2

>quast.py \*.fasta -o quast\_results -t 2

[in each metaspades\_results directory]

>qsub -I -q interactive -N bbmap -l nodes=1:ppn=2 -l walltime=02:00:00

>module load bbmap

>module load samtools-1.7

>cp /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_R1\_001\_paired.fastq.gz /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results

>cp /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_R2\_001\_paired.fastq.gz /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results

>bbmap.sh ref=contigs.fasta in=20082D-04-02\_S2\_L003\_R1\_001\_paired.fastq.gz in2=20082D-04-02\_S2\_L003\_R2\_001\_paired.fastq.gz out=metaspades.sam bamscript=sam2bam.sh

>./sam2bam.sh

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads

>mkdir atlas

**Marvin:**

>screen

>cd /home/tiffany

>scp -r SCALE-META-reads tiffdp@wonko.bi.up.ac.za:/nlustre/users/tiffdp/SCALE-META-reads/atlas

**Wonko:**

>cd /nlustre/users/tiffdp/SCALE-META-reads/atlas

>nano atlas.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=720:00:00

#PBS -q bigmem

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/atlas/stdout.log

#PBS -e /nlustre/users/tiffdp/ SCALE-META-reads/atlas/stderr.log

#PBS -k oe

#PBS -m ae

#PBS -M 17duplti@gmail.com

Cd $PBS\_O\_WORKDIR

module load metagenome-atlas

source /apps/miniconda3/etc/profile.d/cond/sh

conda activate atlasenv

atlas init –db-dir databases /nlustre/users/tiffdp/SCALE-META-reads/atlas/ --working-dir /nlustre/users/tiffdp/SCALE-META-reads/atlas/SCALE-META-reads

atlas run qc assembly binning --resources mem=250 --jobs 20 –-keep-going

>qsub atlas.sh

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results

>nano metabat\_11.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=20:00:00

#PBS -q normal

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/stdout.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/stderr.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load metabat

module load bamtools

jgi\_summarize\_bam\_contig\_depths --outputDepth depth.txt \*.bam

metabat -i contigs.fasta -a depth.txt –verysensitive -o metabat\_verysensitive -v > log.txt

metabat -i contigs.fasta -a depth.txt –sensitive -o metabat\_sensitive -v > log.txt

>qsub metabat\_11.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=02:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/

>module load checkm

>checkm lineage\_wf -t 2 -x .fa /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results 20082D-04-18\_S11\_L003\_metaspades\_results > checkm.txt

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results

>nano metabat\_2.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=20:00:00

#PBS -q normal

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/stdout.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/stderr.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load metabat

module load bamtools

jgi\_summarize\_bam\_contig\_depths --outputDepth depth.txt \*.bam

metabat -i contigs.fasta -a depth.txt –verysensitive -o metabat\_verysensitive -v > log.txt

metabat -i contigs.fasta -a depth.txt –sensitive -o metabat\_sensitive -v > log.txt

>qsub metabat\_2.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/

>module load checkm

>checkm lineage\_wf -t 2 -x .fa /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results 20082D-04-02\_S2\_L003\_metaspades\_results > checkm.txt

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results

>nano maxbin\_11.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=05:00:00

#PBS -q normal

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/x\_stdout.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/x\_stderr.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load maxbin-2.2.6

module load bbmap

module load samtools-1.10

pileup.sh in=metaspades.sam out=cov.txt

awk '{print $1"\t"$5}' cov.txt | grep -v '^#' > abundance.txt

run\_MaxBin.pl -thread 20 -contig contigs.fasta -out maxbin -abund abundance.txt

>qsub maxbin\_11.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/

>module load checkm

>checkm lineage\_wf -t 2 -x fasta /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/maxbin\_bins 20082D-04-18\_S11\_L003\_metaspades\_results > checkm\_x.txt

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results

>nano maxbin\_2.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=05:00:00

#PBS -q normal

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/x\_stdout.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/x\_stderr.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load maxbin-2.2.6

module load bbmap

module load samtools-1.10

pileup.sh in=metaspades.sam out=cov.txt

awk '{print $1"\t"$5}' cov.txt | grep -v '^#' > abundance.txt

run\_MaxBin.pl -thread 20 -contig contigs.fasta -out maxbin -abund abundance.txt

>qsub maxbin\_2.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/

>module load checkm

>checkm lineage\_wf -t 2 -x fasta /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/maxbin\_bins 20082D-04-02\_S2\_L003\_metaspades\_results > checkm\_x.txt

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results

>nano concoct\_11.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=120:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/stdout\_c.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/stderr\_c.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load concoct

source /apps/miniconda3/etc/profile.d/conda.sh

conda activate concoct

module load bedtools-2.28.0

module load bamtools

cut\_up\_fasta.py contigs.fasta -c 10000 -o 0 --merge\_last -b contigs\_10K.bed > contigs\_10K.fa

concoct\_coverage\_table.py contigs\_10K.bed metaspades\_sorted.bam > coverage\_table.tsv

concoct --composition\_file contigs\_10K.fa --coverage\_file coverage\_table.tsv -b concoct\_output/

merge\_cutup\_clustering.py concoct\_output/clustering\_gt1000.csv > concoct\_output/clustering\_merged.csv

mkdir concoct\_output/fasta\_bins

extract\_fasta\_bins.py contigs.fasta concoct\_output/clustering\_merged.csv --output\_path concoct\_output/fasta\_bins

>qsub concoct\_11.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/concoct\_output

>module load checkm

>checkm lineage\_wf -t 2 -x fa /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/concoct\_output/fasta\_bins/ checkm\_concoct > checkm\_o.txt

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results

>nano concoct\_2.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=120:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/stdout\_c.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/stderr\_c.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load concoct

source /apps/miniconda3/etc/profile.d/conda.sh

conda activate concoct

module load bedtools-2.28.0

module load bamtools

cut\_up\_fasta.py contigs.fasta -c 10000 -o 0 --merge\_last -b contigs\_10K.bed > contigs\_10K.fa

concoct\_coverage\_table.py contigs\_10K.bed metaspades\_sorted.bam > coverage\_table.tsv

concoct --composition\_file contigs\_10K.fa --coverage\_file coverage\_table.tsv -b concoct\_output/

merge\_cutup\_clustering.py concoct\_output/clustering\_gt1000.csv > concoct\_output/clustering\_merged.csv

mkdir concoct\_output/fasta\_bins

extract\_fasta\_bins.py contigs.fasta concoct\_output/clustering\_merged.csv --output\_path concoct\_output/fasta\_bins

>qsub concoct\_2.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/concoct\_output

>module load checkm

>checkm lineage\_wf -t 2 -x .fa /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/concoct\_output/fasta\_bins checkm\_concoct > checkm\_o.txt

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/concoct\_output

>module load das\_tool-1.1

>module load perl-5.26.1

>perl -pe "s/,/\tconcoct./g;" /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/concoct\_output/clustering\_merged.csv > concoct.scaffolds2bin.tsv

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/

>nano dast\_11.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=120:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/stdout\_d.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/stderr\_d.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load das\_tool-1.1

module load R-3.6.3

module load ruby-2.7.1

module load perl-5.26.1

module load prodigal-2.6.3

module load diamond-2.0.7

DAS\_Tool -i /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/metabat\_bins/metabat.scaffolds2bin.tsv,/nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/maxbin\_bins/maxbin.scaffolds2bin.tsv,/nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/concoct\_output/concoct.scaffolds2bin.tsv -l metabat,maxbin,concoct -c contigs.fasta -o DAST\_1500 --write\_bins 1 --db\_directory /nlustre/users/tiffdp/SCALE-META-reads/db -t 20

>qsub dast\_11.sh

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/dast\_bins

>module load checkm

>checkm lineage\_wf -t 2 -x .fa /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/dast\_bins/DAST\_1500\_DASTool\_bins checkm\_dast > checkm\_d.txt

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/

>nano dast\_2.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=120:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/stdout\_d.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/stderr\_d.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load das\_tool-1.1

module load R-3.6.3

module load ruby-2.7.1

module load perl-5.26.1

module load prodigal-2.6.3

module load diamond-2.0.7

DAS\_Tool -i /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/metabat\_bins/metabat.scaffolds2bin.tsv,/nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/maxbin\_bins/maxbin.scaffolds2bin.tsv,/nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/concoct\_output/concoct.scaffolds2bin.tsv -l metabat,maxbin,concoct -c contigs.fasta -o DAST\_1500 --write\_bins 1 --db\_directory /nlustre/users/tiffdp/SCALE-META-reads/db -t 20

>qsub dast\_2.sh

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/dast\_bins

>module load checkm

>checkm lineage\_wf -t 2 -x .fa /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/dast\_bins/DAST\_1500\_DASTool\_bins checkm\_dast > checkm\_d.txt

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/

>nano gtdbtk\_11.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=120:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/stdout\_g.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/stderr\_g.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load gtdbtk

gtdbtk identify --genome\_dir /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/dast\_bins/DAST\_1500\_DASTool\_bins --out\_dir gtdbtk\_identify -x fa --cpus 2

gtdbtk align --identify\_dir /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/gtdbtk\_identify --out\_dir gtdbtk\_align --cpus 2

gtdbtk classify --genome\_dir /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/dast\_bins/DAST\_1500\_DASTool\_bins --align\_dir /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/gtdbtk\_align --out\_dir gtdbtk\_classify -x fa --cpus 2

>qsub gtdbtk\_11.sh

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/

>nano gtdbtk\_2.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=120:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/stdout\_g.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/stderr\_g.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load gtdbtk

gtdbtk identify --genome\_dir /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/dast\_bins/DAST\_1500\_DASTool\_bins --out\_dir gtdbtk\_identify -x fa --cpus 2

gtdbtk align --identify\_dir /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/gtdbtk\_identify --out\_dir gtdbtk\_align --cpus 2

gtdbtk classify --genome\_dir /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/dast\_bins/DAST\_1500\_DASTool\_bins --align\_dir /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/gtdbtk\_align --out\_dir gtdbtk\_classify -x fa --cpus 2

>qsub gtdbtk\_2.sh

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples

>nano spades\_deep.sh

#!/bin/bash

#PBS -l nodes=1:ppn=24

#PBS -l walltime=300:00:00

#PBS -q bigmem

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/stdout.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/stderr.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load python-3.8.2

module load SPAdes-3.13.0

for f in $(ls \*fastq.gz | sed -e 's/\_R1\_001\_paired.fastq.gz//' -e 's/\_R2\_001\_paired.fastq.gz//' | sort -u)

do spades.py --pe1-1 ${f}\_R1\_001\_paired.fastq.gz --pe1-2 ${f}\_R2\_001\_paired.fastq.gz --meta -t 24 -o ${f}\_metaspades\_results -m 500

done

>qsub spades\_deep.sh

>qsub -I -q interactive -N quast -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples

>module load quast-5.0.2

>quast.py \*.fasta -o quast\_results -t 2

[in each metaspades\_results directory]

>qsub -I -q interactive -N bbmap -l nodes=1:ppn=2 -l walltime=04:00:00

>module load bbmap

>module load samtools-1.7

>cp /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_R1\_001\_paired.fastq.gz /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results

>cp /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_R2\_001\_paired.fastq.gz /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results

>bbmap.sh ref=contigs.fasta in=20082D-04-14\_S8\_L003\_R1\_001\_paired.fastq.gz in2=20082D-04-14\_S8\_L003\_R2\_001\_paired.fastq.gz out=metaspades.sam bamscript=sam2bam.sh

>./sam2bam.sh

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results

>nano metabat\_8.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=20:00:00

#PBS -q normal

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/stdout.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/stderr.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load metabat

module load bamtools

jgi\_summarize\_bam\_contig\_depths --outputDepth depth.txt \*.bam

metabat -i contigs.fasta -a depth.txt –verysensitive -o metabat\_verysensitive -v > log.txt

metabat -i contigs.fasta -a depth.txt –sensitive -o metabat\_sensitive -v > log.txt

>qsub metabat\_8.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=02:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/metabat\_bins

>module load checkm

>checkm lineage\_wf -t 2 -x .fa /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/metabat\_bins 20082D-04-14\_S8\_L003\_metaspades\_results > checkm.txt

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results

>nano maxbin\_8.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=05:00:00

#PBS -q normal

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/x\_stdout.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/x\_stderr.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load maxbin-2.2.6

module load bbmap

module load samtools-1.10

pileup.sh in=metaspades.sam out=cov.txt

awk '{print $1"\t"$5}' cov.txt | grep -v '^#' > abundance.txt

run\_MaxBin.pl -thread 20 -contig contigs.fasta -out maxbin -abund abundance.txt

>qsub maxbin\_8.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/maxbin\_bins

>module load checkm

>checkm lineage\_wf -t 2 -x fasta /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/maxbin\_bins 20082D-04-14\_S8\_L003\_metaspades\_results > checkm\_x.txt

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results

>nano concoct\_8.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=120:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/stdout\_c.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/stderr\_c.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load concoct

source /apps/miniconda3/etc/profile.d/conda.sh

conda activate concoct

module load bedtools-2.28.0

module load bamtools

cut\_up\_fasta.py contigs.fasta -c 10000 -o 0 --merge\_last -b contigs\_10K.bed > contigs\_10K.fa

concoct\_coverage\_table.py contigs\_10K.bed metaspades\_sorted.bam > coverage\_table.tsv

concoct --composition\_file contigs\_10K.fa --coverage\_file coverage\_table.tsv -b concoct\_output/

merge\_cutup\_clustering.py concoct\_output/clustering\_gt1000.csv > concoct\_output/clustering\_merged.csv

mkdir concoct\_output/fasta\_bins

extract\_fasta\_bins.py contigs.fasta concoct\_output/clustering\_merged.csv --output\_path concoct\_output/fasta\_bins

>qsub concoct\_8.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/concoct\_output/fasta\_bins

>module load checkm

>checkm lineage\_wf -t 2 -x fa /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/concoct\_output/fasta\_bins/ checkm\_concoct > checkm\_o.txt

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/concoct\_output

>module load das\_tool-1.1

>module load perl-5.26.1

>perl -pe "s/,/\tconcoct./g;" /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/concoct\_output/clustering\_merged.csv > concoct.scaffolds2bin.tsv

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results

>nano dast\_8.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=120:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/stdout\_d.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/stderr\_d.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load das\_tool-1.1

module load R-3.6.3

module load ruby-2.7.1

module load perl-5.26.1

module load prodigal-2.6.3

module load diamond-2.0.7

DAS\_Tool -i /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/metabat\_bins/metabat.scaffolds2bin.tsv,/nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/maxbin\_bins/maxbin.scaffolds2bin.tsv,/nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/concoct\_output/concoct.scaffolds2bin.tsv -l metabat,maxbin,concoct -c contigs.fasta -o DAST\_1500 --write\_bins 1 --db\_directory /nlustre/users/tiffdp/SCALE-META-reads/db -t 20

>qsub dast\_8.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/dast\_bins

>module load checkm

>checkm lineage\_wf -t 2 -x .fa /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/dast\_bins/DAST\_1500\_DASTool\_bins checkm\_dast > checkm\_d.txt

[in each metaspades\_results directory]

>nano gtdbtk\_8.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=120:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/stdout\_g.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/stderr\_g.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

module load gtdbtk

gtdbtk identify --genome\_dir /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/dast\_bins/DAST\_1500\_DASTool\_bins --out\_dir gtdbtk\_identify -x fa --cpus 2

gtdbtk align --identify\_dir /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/gtdbtk\_identify --out\_dir gtdbtk\_align --cpus 2

gtdbtk classify --genome\_dir /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/dast\_bins/DAST\_1500\_DASTool\_bins --align\_dir /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/gtdbtk\_align --out\_dir gtdbtk\_classify -x fa --cpus 2

>qsub gtdbtk\_8.sh

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples

>nano spades\_200.sh

#!/bin/bash

#PBS -l nodes=1:ppn=24

#PBS -l walltime=300:00:00

#PBS -q bigmem

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/stdout.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/stderr.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load python-3.8.2

module load SPAdes-3.13.0

for f in $(ls \*fastq.gz | sed -e 's/\_R1\_001\_paired.fastq.gz//' -e 's/\_R2\_001\_paired.fastq.gz//' | sort -u)

do spades.py --pe1-1 ${f}\_R1\_001\_paired.fastq.gz --pe1-2 ${f}\_R2\_001\_paired.fastq.gz --meta -t 24 -o ${f}\_metaspades\_results -m 700

done

>qsub spades\_200.sh

>qsub -I -q interactive -N quast -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples

>module load quast-5.0.2

>quast.py \*.fasta -o quast\_results -t 2

[in each metaspades\_results directory]

>qsub -I -q interactive -N bbmap -l nodes=1:ppn=2 -l walltime=04:00:00

>module load bbmap

>module load samtools-1.7

>cp /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_R1\_001\_paired.fastq.gz /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results

>cp /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_R2\_001\_paired.fastq.gz /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results

>cd /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results

>bbmap.sh ref=contigs.fasta in=20082D-04-01\_S1\_L003\_R1\_001\_paired.fastq.gz in2=20082D-04-01\_S1\_L003\_R2\_001\_paired.fastq.gz out=metaspades.sam bamscript=sam2bam.sh

>./sam2bam.sh

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results

>nano metabat\_1.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=20:00:00

#PBS -q normal

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/stdout\_m.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/stderr\_m.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load metabat

module load bamtools

jgi\_summarize\_bam\_contig\_depths --outputDepth depth.txt \*.bam

metabat -i contigs.fasta -a depth.txt –verysensitive -o metabat\_verysensitive -v > log.txt

metabat -i contigs.fasta -a depth.txt –sensitive -o metabat\_sensitive -v > log.txt

>qsub metabat\_1.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=02:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/

>module load checkm

>checkm lineage\_wf -t 2 -x .fa /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results 20082D-04-01\_S1\_L003\_metaspades\_results > checkm.txt

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results

>nano maxbin\_1.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=05:00:00

#PBS -q normal

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/stdout\_x.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/stderr\_x.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load maxbin-2.2.6

module load bbmap

module load samtools-1.10

pileup.sh in=metaspades.sam out=cov.txt

awk '{print $1"\t"$5}' cov.txt | grep -v '^#' > abundance.txt

run\_MaxBin.pl -thread 20 -contig contigs.fasta -out maxbin -abund abundance.txt

>qsub maxbin\_1.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/

>module load checkm

>checkm lineage\_wf -t 2 -x fasta /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/maxbin\_bins 20082D-04-01\_S1\_L003\_metaspades\_results > checkm\_x.txt

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results

>nano concoct\_1.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=120:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/stdout\_c.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/stderr\_c.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load concoct

source /apps/miniconda3/etc/profile.d/conda.sh

conda activate concoct

module load bedtools-2.28.0

module load bamtools

cut\_up\_fasta.py contigs.fasta -c 10000 -o 0 --merge\_last -b contigs\_10K.bed > contigs\_10K.fa

concoct\_coverage\_table.py contigs\_10K.bed metaspades\_sorted.bam > coverage\_table.tsv

concoct --composition\_file contigs\_10K.fa --coverage\_file coverage\_table.tsv -b concoct\_output/

merge\_cutup\_clustering.py concoct\_output/clustering\_gt1000.csv > concoct\_output/clustering\_merged.csv

mkdir concoct\_output/fasta\_bins

extract\_fasta\_bins.py contigs.fasta concoct\_output/clustering\_merged.csv --output\_path concoct\_output/fasta\_bins

>qsub concoct\_1.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/concoct\_output/

>module load checkm

>checkm lineage\_wf -t 2 -x fa /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/concoct\_output/fasta\_bins/ checkm\_concoct > checkm\_o.txt

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/concoct\_output

>module load das\_tool-1.1

>module load perl-5.26.1

>perl -pe "s/,/\tconcoct./g;" /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/concoct\_output/clustering\_merged.csv > concoct.scaffolds2bin.tsv

>cd /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results

>nano dast\_1.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=120:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/stdout\_d.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/stderr\_d.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load das\_tool-1.1

module load R-3.6.3

module load ruby-2.7.1

module load perl-5.26.1

module load prodigal-2.6.3

module load diamond-2.0.7

DAS\_Tool -i /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/metabat\_bins/metabat.scaffolds2bin.tsv,/nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/maxbin\_bins/maxbin.scaffolds2bin.tsv,/nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/concoct\_output/concoct.scaffolds2bin.tsv -l metabat,maxbin,concoct -c contigs.fasta -o DAST\_200 --write\_bins 1 --db\_directory /nlustre/users/tiffdp/SCALE-META-reads/db -t 20

>qsub dast\_1.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N checkm -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/dast\_bins

>module load checkm

>checkm lineage\_wf -t 2 -x .fa /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/dast\_bins/DAST\_200\_DASTool\_bins checkm\_dast > checkm\_d.txt

[in each metaspades\_results directory]

>nano gtdbtk\_1.sh

#!/bin/bash

#PBS -l nodes=1:ppn=20

#PBS -l walltime=120:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/stdout\_g.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/stderr\_g.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

module load gtdbtk

gtdbtk identify --genome\_dir /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/dast\_bins/DAST\_200\_DASTool\_bins --out\_dir gtdbtk\_identify -x fa --cpus 2

gtdbtk align --identify\_dir /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/gtdbtk\_identify --out\_dir gtdbtk\_align --cpus 2

gtdbtk classify --genome\_dir /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/dast\_bins/DAST\_200\_DASTool\_bins --align\_dir /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/gtdbtk\_align --out\_dir gtdbtk\_classify -x fa --cpus 2

>qsub gtdbtk\_1.sh

[in each metaspades\_results directory]

>qsub -I -q interactive -N prodigal -l nodes=1:ppn=2 -l walltime=02:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/dast\_bins

>mkdir proteins

>cd DAST\_1500\_DASTool\_bins

>module load prodigal-2.6.3

>for items in \*fa; do prodigal -i $items -a $items\.proteins.faa -p meta; done

>mv \*proteins.faa nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/dast\_bins/proteins

[in each metaspades\_results directory]

>qsub -I -q interactive -N prodigal -l nodes=1:ppn=2 -l walltime=02:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/dast\_bins

>mkdir proteins

>cd DAST\_1500\_DASTool\_bins

>module load prodigal-2.6.3

>for items in \*fa; do prodigal -i $items -a $items\.proteins.faa -p meta; done

>mv \*proteins.faa nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/dast\_bins/proteins

[in each metaspades\_results directory]

>qsub -I -q interactive -N prodigal -l nodes=1:ppn=2 -l walltime=02:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/dast\_bins

>mkdir proteins

>cd DAST\_1500\_DASTool\_bins

>module load prodigal-2.6.3

>for items in \*fa; do prodigal -i $items -a $items\.proteins.faa -p meta; done

>mv \*proteins.faa nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/dast\_bins/proteins

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/dast\_bins/proteins

>nano microbean\_11.sh

#!/bin/bash

#PBS -l nodes=1:ppn=24

#PBS -l walltime=120:00:00

#PBS -q bigmem

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/stdout\_a.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/stderr\_a.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load anaconda3-2021.05

source activate microbeannotator

microbeannotator -i $(ls \*.faa) -d /nlustre/data/MicrobeAnnotator\_DB -o microbean -m blast -p 2 -t 12

>qsub microbean\_11.sh

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/dast\_bins/proteins

>nano microbean\_2.sh

#!/bin/bash

#PBS -l nodes=1:ppn=24

#PBS -l walltime=120:00:00

#PBS -q bigmem

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/stdout\_a.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/stderr\_a.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load anaconda3-2021.05

source activate microbeannotator

microbeannotator -i $(ls \*.faa) -d /nlustre/data/MicrobeAnnotator\_DB -o microbean -m blast -p 2 -t 12

>qsub microbean\_2.sh

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/dast\_bins/proteins

>nano microbean\_8.sh

#!/bin/bash

#PBS -l nodes=1:ppn=24

#PBS -l walltime=120:00:00

#PBS -q bigmem

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/stdout\_a.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/stderr\_a.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load anaconda3-2021.05

source activate microbeannotator

microbeannotator -i $(ls \*.faa) -d /nlustre/data/MicrobeAnnotator\_DB -o microbean -m blast -p 2 -t 12

>qsub microbean\_8.sh

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples

>nano DRAM\_11.sh

#!/bin/bash

#PBS -l nodes=1:ppn=24

#PBS -l walltime=120:00:00

#PBS -q bigmem

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/stdout\_dr.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/stderr\_dr.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load DRAM

source /apps/anaconda3-2020.02/etc/profile.d/conda.sh

conda activate DRAM

DRAM.py annotate -i '\*.fa' -o annotation

DRAM.py distill -i annotation/annotations.tsv -o genome\_summaries --trna\_path annotation/trnas.tsv --rrna\_path annotation/rrnas.tsv

>qsub DRAM\_11.sh

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples

>nano DRAM\_2.sh

#!/bin/bash

#PBS -l nodes=1:ppn=24

#PBS -l walltime=120:00:00

#PBS -q bigmem

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/stdout\_dr.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/stderr\_dr.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load DRAM

source /apps/anaconda3-2020.02/etc/profile.d/conda.sh

conda activate DRAM

DRAM.py annotate -i '\*.fa' -o annotation

DRAM.py distill -i annotation/annotations.tsv -o genome\_summaries --trna\_path annotation/trnas.tsv --rrna\_path annotation/rrnas.tsv

>qsub DRAM\_2.sh

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples

>nano DRAM\_8.sh

#!/bin/bash

#PBS -l nodes=1:ppn=24

#PBS -l walltime=120:00:00

#PBS -q bigmem

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/stdout\_dr.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/stderr\_dr.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load DRAM

source /apps/anaconda3-2020.02/etc/profile.d/conda.sh

conda activate DRAM

DRAM.py annotate -i '\*.fa' -o annotation

DRAM.py distill -i annotation/annotations.tsv -o genome\_summaries --trna\_path annotation/trnas.tsv --rrna\_path annotation/rrnas.tsv

>qsub DRAM\_8.sh

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples

>nano DRAM\_1.sh

#!/bin/bash

#PBS -l nodes=1:ppn=24

#PBS -l walltime=120:00:00

#PBS -q bigmem

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/stdout\_dr.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/stderr\_dr.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load DRAM

source /apps/anaconda3-2020.02/etc/profile.d/conda.sh

conda activate DRAM

DRAM.py annotate -i '\*.fa' -o annotation

DRAM.py distill -i annotation/annotations.tsv -o genome\_summaries --trna\_path annotation/trnas.tsv --rrna\_path annotation/rrnas.tsv

>qsub DRAM\_1.sh

[in each metaspades\_results directory]

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples

>nano virsorter\_8.sh

#!/bin/bash

#PBS -l nodes=1:ppn=28

#PBS -l walltime=270:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/stdout\_v.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/20082D-04-14\_S8\_L003\_metaspades\_results/stderr\_v.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load virsorter2

source /apps/anaconda3-2020.02/etc/profile.d/conda.sh

conda activate vs2

for i in \*fa; do virsorter run -w $i\\_virs2\_output -d /nlustre/data/virsorter2 -i $i --include-groups dsDNAphage,ssDNA -j 28 --min-score 0.5 --min-length 1000 --keep-original-seq all; done

>qsub virsorter\_8.sh

[in each DASTools\_bins directory]

>qsub -I -q interactive -N checkv -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/deep\_samples/

>module load checkv

>for i in \*\_virs2\_output/final-viral-combined.fa; do checkv end\_to\_end $i $i\\_checkv\_output -t 2; done

[in each DASTools\_bins directory]

>for files in \*\_virs2\_output; do cat $files/final-viral-combined.fa\_checkv\_output/\*fna > $files/final-viral-combined.fa\_checkv\_output/combined.fna; done

>virsorter run --seqname-suffix-off --viral-gene-enrich-off --provirus-off --prep-for-dramv -i checkv/combined.fna -w virs2 --include-groups dsDNAphage,ssDNA --min-length 5000 --min-score 0.5 -j 28 all

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples

>nano virsorter\_11.sh

#!/bin/bash

#PBS -l nodes=1:ppn=28

#PBS -l walltime=270:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/stdout\_v.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/20082D-04-18\_S11\_L003\_metaspades\_results/stderr\_v.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load virsorter2

source /apps/anaconda3-2020.02/etc/profile.d/conda.sh

conda activate vs2

for i in \*fa; do virsorter run -w $i\\_virs2\_output -d /nlustre/data/virsorter2 -i $i --include-groups dsDNAphage,ssDNA -j 28 --min-score 0.5 --min-length 1000 --keep-original-seq all; done

>qsub virsorter\_11.sh

[in each DASTools\_bins directory]

>qsub -I -q interactive -N checkv -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/deeper\_samples/

>module load checkv

>for i in \*\_virs2\_output/final-viral-combined.fa; do checkv end\_to\_end $i $i\\_checkv\_output -t 2; done

[in each DASTools\_bins directory]

>for files in \*\_virs2\_output; do cat $files/final-viral-combined.fa\_checkv\_output/\*fna > $files/final-viral-combined.fa\_checkv\_output/combined.fna; done

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples

>nano virsorter\_2.sh

#!/bin/bash

#PBS -l nodes=1:ppn=28

#PBS -l walltime=270:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/stdout\_v.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/20082D-04-02\_S2\_L003\_metaspades\_results/stderr\_v.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load virsorter2

source /apps/anaconda3-2020.02/etc/profile.d/conda.sh

conda activate vs2

for i in \*fa; do virsorter run -w $i\\_virs2\_output -d /nlustre/data/virsorter2 -i $i --include-groups dsDNAphage,ssDNA -j 28 --min-score 0.5 --min-length 1000 --keep-original-seq all; done

>qsub virsorter\_2.sh

[in each DASTools\_bins directory]

>qsub -I -q interactive -N checkv -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/500\_samples/

>module load checkv

>for i in \*\_virs2\_output/final-viral-combined.fa; do checkv end\_to\_end $i $i\\_checkv\_output -t 2; done

[in each DASTools\_bins directory]

>for files in \*\_virs2\_output; do cat $files/final-viral-combined.fa\_checkv\_output/\*fna > $files/final-viral-combined.fa\_checkv\_output/combined.fna; done

>cd /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples

>nano virsorter\_1.sh

#!/bin/bash

#PBS -l nodes=1:ppn=28

#PBS -l walltime=270:00:00

#PBS -q long

#PBS -o /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/stdout\_v.log

#PBS -e /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/20082D-04-01\_S1\_L003\_metaspades\_results/stderr\_v.log

#PBS -m ae

#PBS -M 17duplti@gmail.com

cd $PBS\_O\_WORKDIR

module load virsorter2

source /apps/anaconda3-2020.02/etc/profile.d/conda.sh

conda activate vs2

for i in \*fa; do virsorter run -w $i\\_virs2\_output -d /nlustre/data/virsorter2 -i $i --include-groups dsDNAphage,ssDNA -j 28 --min-score 0.5 --min-length 1000 --keep-original-seq all; done

>qsub virsorter\_1.sh

[in each DASTools\_bins directory]

>qsub -I -q interactive -N checkv -l nodes=1:ppn=2 -l walltime=04:00:00

>cd /nlustre/users/tiffdp/SCALE-META-reads/surface\_samples/

>module load checkv

>for i in \*\_virs2\_output/final-viral-combined.fa; do checkv end\_to\_end $i $i\\_checkv\_output -t 2; done

[in each DASTools\_bins directory]

>for files in \*\_virs2\_output; do cat $files/final-viral-combined.fa\_checkv\_output/\*fna > $files/final-viral-