NERSC

Checkpointing and Restarting Jobs with DMTCP

User Training on Checkpoint/Restart (I)

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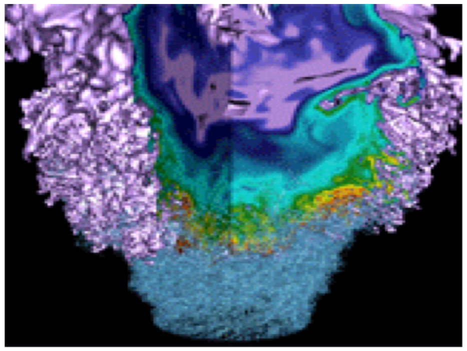
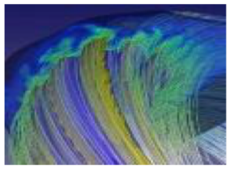
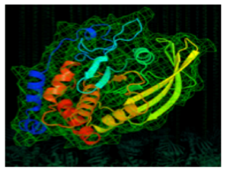
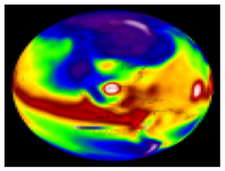
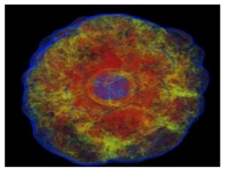
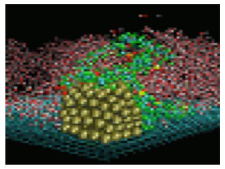
Outline

- Introduction
- DMTCP overview
- Checkpoint/restart serial and threaded applications on Cori
- Automatic job resubmission of checkpoint/restart jobs with DMTCP
- Summary

Introduction

What is Checkpointing/Restarting?

- *Checkpointing* is the action of saving the state of a running process to a checkpoint image file
    - Dump a running process’s memory, state, etc. into a file
- The process can be *restarted* later from the checkpoint file: continuing the execution from where it left off, on the same or different computer

Why Checkpoint/Restart?

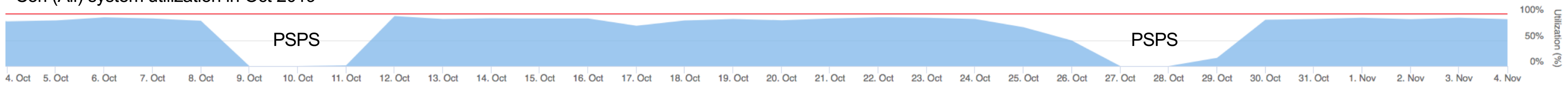
User Perspective

- Enable my jobs to run longer than walltime limit
- Improve my jobs' throughput by exploiting the holes in the Slurm schedule
- Extend interactive sessions by saving & restarting where I left off
- Debug long-running jobs by pausing just before the error & restarting from that point multiple times

NERSC Perspective

- Increased flexibility in scheduling jobs
- (Potentially) enables preempting of jobs for more important or time-sensitive jobs
- Better backfill when reserving nodes for large job, increasing utilization
- Run checkpointing jobs right up to system maintenance
- (Potentially) checkpoint all jobs before unexpected power outage

Cori (All) system utilization in Oct 2019



Checkpoint/Restart: A Great Idea, Hard to Implement

- Requires extensive effort to create transparent-to-users implementation
  - MPI support is especially challenging: combination of MPI implementations (e.g., MPICH, OpenMPI) & networks (e.g., ethernet, Cray Aries) means multiple versions required (MxN problem)
- Earlier checkpoint/restart project, BLCR, shifted development/ maintenance burdens to MPI developers, OS kernels, and batch system developers
  - Required cooperation from all these entities
  - No longer being developed

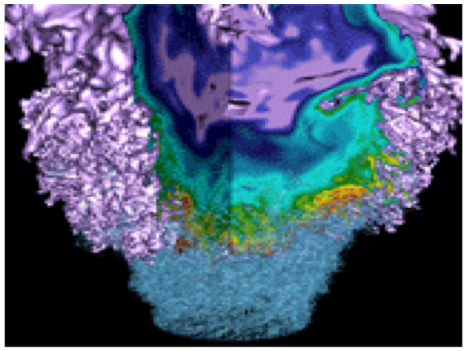
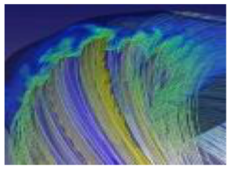
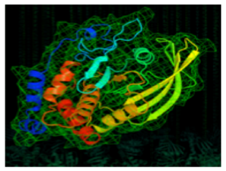
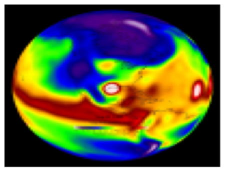
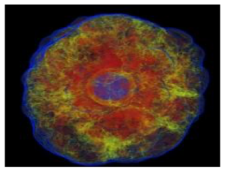
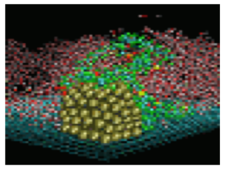
Checkpoint/Restart: A Great Idea, Hard to Implement

- DMTCP (topic of today’s training) takes a different approach & lives completely in user space
  - No kernel modifications or hooks into MPI or lower communication layers are required
- A new implementation of DMTCP, MANA, has addressed the MPI MxN maintainability issue, and proven to be scalable to large number of processes
  - Work in progress: need to experiment with production workloads at NERSC to further harden the code
  - Subject of future training

Schedule of NERSC User Trainings on Checkpoint/Restart

- A series of user training sessions on C/R are planned in November, January, and February
  - **November (today): focus on using DMTCP with serial/threaded applications**
  - January: focus on applications with internal C/R support - get good job throughput with variable-time jobs
  - February: Checkpoint/restart MPI applications with DMTCP (MANA)

DMTCP: Distributed MultiThreaded CheckPointing

DMTCP website, http://dmtcp.sourceforge.net/index.html

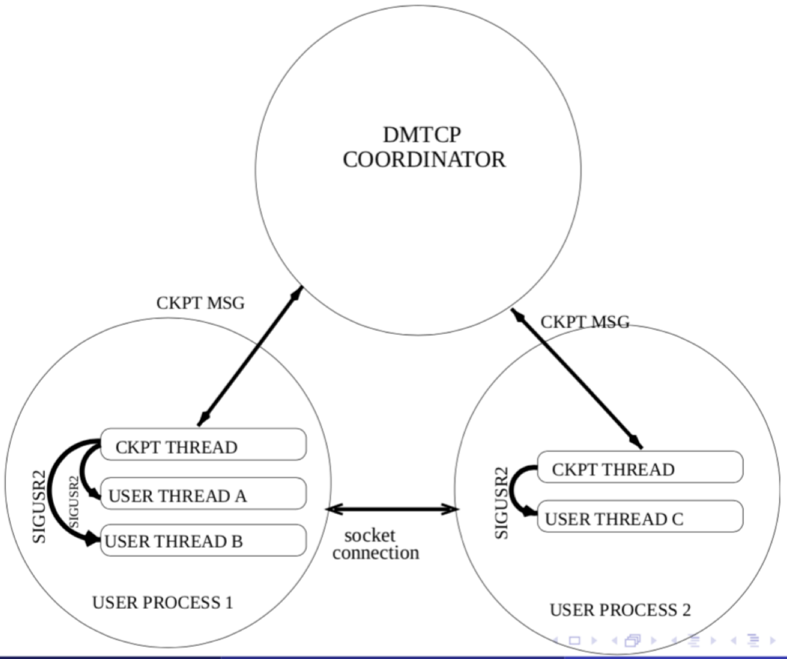
This work was partially supported by National Science Foundation Grants OAC-1740218 and ACI-1440788.

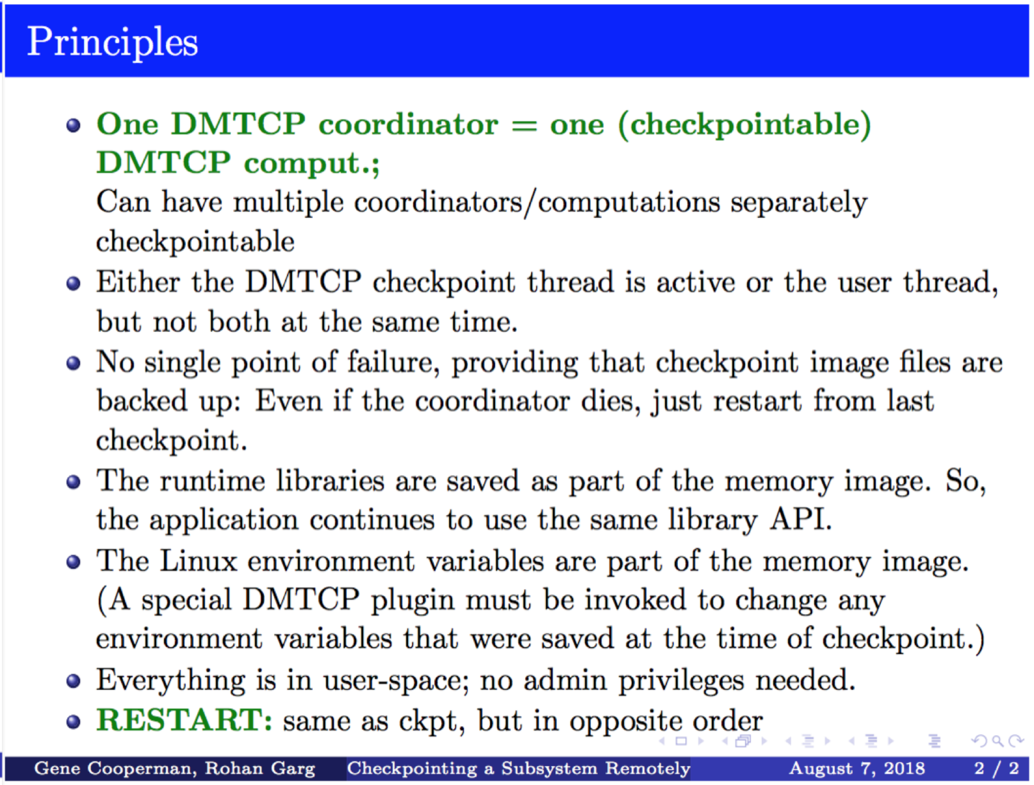
DMTCP: Distributed MultiThreaded CheckPointing

- DMTCP transparently checkpoints a single-host or distributed computation in user-space -- with no modifications to user code or to the O/S.
- DMTCP supports a variety of applications, including MPI (various implementations over TCP/IP or InfiniBand), OpenMP, MATLAB, Python, and many programming languages including C/C++/Fortran, shell scripting languages, and resource managers (e.g., Slurm)

How does DMTCP Work?

DMTCP Architecture: Coordinated Checkpointing





Principles

- **One DMTCP coordinator = one (checkpointable) DMTCP comput.;**
  Can have multiple coordinators/computations separately checkpointable
- Either the DMTCP checkpoint thread is active or the user thread, but not both at the same time.
- No single point of failure, providing that checkpoint image files are backed up: Even if the coordinator dies, just restart from last checkpoint.
- The runtime libraries are saved as part of the memory image. So, the application continues to use the same library API.
- The Linux environment variables are part of the memory image. (A special DMTCP plugin must be invoked to change any environment variables that were saved at the time of checkpoint.)
- Everything is in user-space; no admin privileges needed.
- **RESTART:** same as ckpt, but in opposite order

DMTCP Usage

Terminal 1

```
rm -f ckpt_a.out*.dmtcp

dmtcp_launch -j ./a.out arg1 …
^C
dmtcp_restart ckpt_a.out*.dmtcp
```

Terminal 2

```
dmtcp_coordinator  --interval 30
```

Or

```
dmtcp_launch --interval 30 ./a.out
^C
dmtcp_restart ckpt_a.out*.dmtcp
```

Or

```
dmtcp_launch ./a.out arg1 …

^C
dmtcp_restart ckpt_a.out*.dmtcp
```

```
dmtcp_command --checkpoint
```

DMTCP Commands

`dmtcp_coordinator` -- coordinates checkpoints between multiple processes.

Usage: `dmtcp_coordinator [OPTIONS] [port]`

Options:

`-p, --coord-port PORT_NUM` (`env DMTCP_COORD_PORT`), Port to listen on (default: 7779)

`--port-file` *`filename`*, File to write listener port number. (Useful with '`--port 0`', which is used to assign a random port)

`--exit-on-last`, Exit automatically when last client disconnects

`--exit-after-ckpt`, Kill peer processes of computation after first checkpoint is created

`--daemon`, Run silently in the background after detaching from the parent process.

`-i, --interval` (`env DMTCP_CHECKPOINT_INTERVAL`): Time in seconds between automatic checkpoints (default: 0, disabled)

COMMANDS:

type '`?<return>`' at runtime for list

DMTCP Commands (cont.)

`dmtcp_launch` -- Start a process under DMTCP control.

Usage: `dmtcp_launch [OPTIONS] <command> [args...]`

- `-h, --coord-host` *`HOSTNAME`* (`env DMTCP_COORD_HOST`), hostname where `dmtcp_coordinator` is run (default: `localhost`)
- `-p, --coord-port` *`PORT_NUM`* (`env DMTCP_COORD_PORT`), port where `dmtcp_coordinator` is run (default: 7779)
- `--port-file` *`FILENAME`*, file to write listener port number.
- `-j, --join-coordinator`, join an existing coordinator, raise error if one doesn't already exist
- `-i, --interval` *`SECONDS`* (`env DMTCP_CHECKPOINT_INTERVAL`), time in seconds between automatic checkpoints.
- `--ckpt-signal` *`signum`*, signal number used internally by DMTCP for checkpointing (default: `SIGUSR2` (signal 12)).

DMTCP Commands (cont.)

`dmtcp_restart` -- Restart processes from a checkpoint image.

Usage: `dmtcp_restart [OPTIONS] <ckpt1.dmtcp> [ckpt2.dmtcp...]`

`-h, --coord-host` *`HOSTNAME`* (`env DMTCP_COORD_HOST`), Hostname where `dmtcp_coordinator` is run (default: `localhost`)

`-p, --coord-port` *`PORT_NUM`* (`env DMTCP_COORD_PORT`), Port where `dmtcp_coordinator` is run (default: 7779)

`--port-file` *`FILENAME`*, File to write listener port number.

`-j, --join-coordinator`, Join an existing coordinator, raise error if one doesn't already exist

`-i, --interval` *`SECONDS`* (`env DMTCP_CHECKPOINT_INTERVAL`), Time in seconds between automatic checkpoints.

DMTCP Commands (cont.)

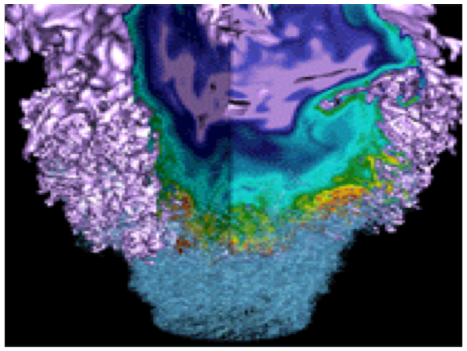
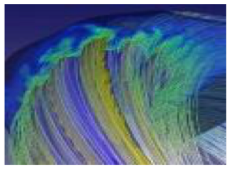
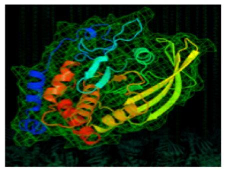
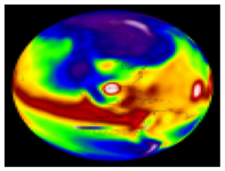
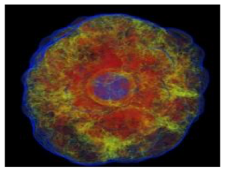
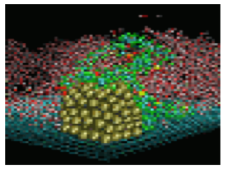
`dmtcp_command` -- Send a command to the `dmtcp_coordinator` remotely.

Usage: `dmtcp_command [OPTIONS] COMMAND [COMMAND...]`	
`-s, --status`	Print status message
`-l, --list`	List connected clients
`-c, --checkpoint`	Checkpoint all nodes
`-bc, --bcheckpoint`	Checkpoint all nodes, blocking until done
`-i, --interval <val>`	Update ckpt interval to `<val>` seconds (0=never)
`-k, --kill`	Kill all nodes
`-q, --quit`	Kill all nodes and quit

MPI Status of DMTCP on Cori

- We are working with the DMTCP developers to get "MANA for MPI: MPI-Agnostic Network-Agnostic Transparent Checkpointing", which works with Cray MPICH, to work on Cori.
    - The openmpi module (tcp/ip) may work with your MPI applications now
    - However, we recommend the to-be-released MANA version of DMTCP for MPI applications (target date Feb 2020)
- Confirmed that serial/threaded apps work with DMTCP on Cori
    - We invite users to experiment DMTCP with their production workloads, and report bugs
    - DMTCP development team will prioritize bugs reported by NERSC

Checkpoint/Restart Serial/Threaded Applications with DMTCP on Cori

Demo: C/R Jobs with DMTCP Interactively

Terminal 1 (batch session)

Step 1
```
module load dmtcp
#get a compute node
salloc -N1 -C knl -t 1:00:00 -q interactive
```

Step 4
```
#launch job under DMTCP control
dmtcp_launch -j ./a.out arg1 ...
```

Step 6
```
^c kill the running job
```

Step 7
```
#restart from checkpoint image file
dmtcp_restart ckpt-*.dmtcp
#or run dmtcp_restart_script.sh
```

Terminal 2

Step 2
```
#ssh to the compute node of your running job
ssh_job <jobid>
```

Step 3
```
#launch dmtcp_coordinator
module load dmtcp
dmtcp_coordinator
```

Step 5
```
#checkpoint
c


q
--------
#or use dmtcp_command to send checkpoint command
remotely
dmtcp_command -c
```

The application (`a.out`) must be linked dynamically!

Notes on DMTCP Usage

- **Must link applications dynamically**
- Use `--help` option with `dmtcp_*` commands to see available options
- Checkpoint options:
    - checkpoint periodically
    - checkpoint once and quit (detect allocated time)
    - checkpoint remotely as needed
    - for batch jobs, use `--port-file` number (`-p`), because host (`-h`) could be different between restarted jobs
- For restart jobs, can use `dmtcp_coordinator`-generated restart script `dmtcp_restart_script.sh` instead of `dmtcp_restart ckpt*`
    - This file is a link to the most recent restart script

Sample Job Script: C/R Using DMTCP on Cori Haswell

Original job script

```
#!/bin/bash
#SBATCH -J test
#SBATCH -q regular
#SBATCH -N 1
#SBATCH -C haswell
#SBATCH -t 48:00:00
#SBATCH -o test-%j.out
#SBATCH -e test-%j.err

#user settings
export OMP_PROC_BIND=true
export OMP_PLACES=threads
export OMP_NUM_THREADS=32

./a.out
```

run.slurm

```
#!/bin/bash
#SBATCH -J test_cr
#SBATCH -q regular
#SBATCH -N 1
#SBATCH -C haswell
#SBATCH -t 48:00:00
#SBATCH -o test_cr-%j.out
#SBATCH -e test_cr-%j.err
#SBATCH --time-min=6:00:00

#user settings
export OMP_PROC_BIND=true
export OMP_PLACES=threads
export OMP_NUM_THREADS=32

#for c/r with dmtcp
module load dmtcp nersc_cr

#checkpointing once every hour
start_coordinator -i 3600

#run job under dmtcp control
dmtcp_launch ./a.out
```

restart.slurm

```
#!/bin/bash
#SBATCH -J test_cr
#SBATCH -q regular
#SBATCH -N 1
#SBATCH -C haswell
#SBATCH -t 48:00:00
#SBATCH -o test_cr-%j.out
#SBATCH -e test_cr-%j.err
#SBATCH --time-min=6:00:00

#user settings
export OMP_PROC_BIND=true
export OMP_PLACES=threads
export OMP_NUM_THREADS=32

#for c/r with dmtcp
module load dmtcp nersc_cr

#checkpointing once every hour
start_coordinator -i 3600

#restart the job from dmtcp
checkpoint files
./dmtcp_restart_script.sh
```

To run: `sbatch run.slurm`; `sbatch restart.slurm`; `sbatch restart.slurm`; …
or submit dependency jobs

The “flex” QOS is Available for You (on Cori KNL Only)

- The flex QOS is for user jobs that can produce useful work with a relatively short amount of run time before terminating
  - For example, jobs that are capable of checkpointing and restarting from where they left off
- **Benefits to using the flex QOS include improved job throughput and a 75% discount in charging.**
- Access via “`#SBATCH -q flex`” and must use “`#SBATCH --time-min=2:00:00`” or less
- A flex QOS job can use up to 256 KNL nodes for 48 hours

Sample Job Script: C/R Using DMTCP with flex QOS on Cori KNL

original job script

```
#!/bin/bash
#SBATCH -J test
#SBATCH -q regular
#SBATCH -N 1
#SBATCH -C knl
#SBATCH -t 48:00:00
#SBATCH -o test-%j.out
#SBATCH -e test-%j.err

#user settings
export OMP_PROC_BIND=true
export OMP_PLACES=threads
export OMP_NUM_THREADS=64

./a.out
```

run.slurm

```
#!/bin/bash
#SBATCH -J test_cr
#SBATCH -q flex
#SBATCH -N 1
#SBATCH -C knl
#SBATCH -t 48:00:00
#SBATCH -o test_cr-%j.out
#SBATCH -e test_cr-%j.err
#SBATCH --time-min=2:00:00

#user settings
export OMP_PROC_BIND=true
export OMP_PLACES=threads
export OMP_NUM_THREADS=64

#for c/r with dmtcp
module load dmtcp nersc_cr

#checkpointing once every hour
start_coordinator -i 3600

#run job under dmtcp control
dmtcp_launch ./a.out
```

restart.slurm

```
#!/bin/bash
#SBATCH -J test
#SBATCH -q flex
#SBATCH -N 1
#SBATCH -C knl
#SBATCH -t 48:00:00
#SBATCH -o test_cr-%j.out
#SBATCH -e test_cr-%j.err
#SBATCH --time-min=2:00:00

#user settings
export OMP_PROC_BIND=true
export OMP_PLACES=threads
export OMP_NUM_THREADS=64

#for c/r with dmtcp
module load dmtcp nersc_cr

#checkpointing once every hour
start_coordinator -i 3600

#restart the job from dmtcp
checkpoint files
./dmtcp_restart_script.sh
```

To run: `sbatch run.slurm`; `sbatch restart.slurm`; `sbatch restart.slurm`; …
or submit depency jobs

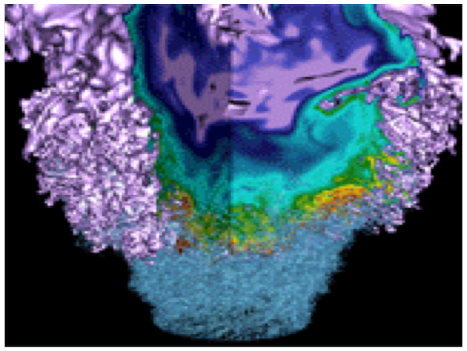
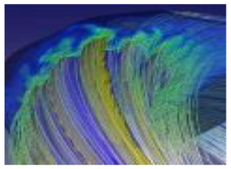
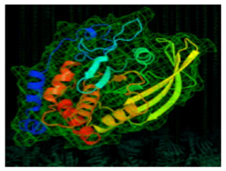
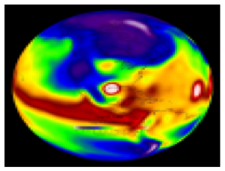
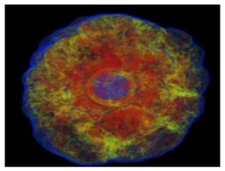
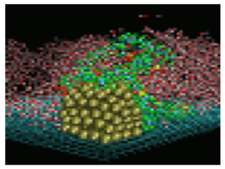
Notes on the DMTCP Job Script

- `nersc_cr` module provides a set of bash functions to manage C/R jobs
  - See `/global/common/sw/cray/cnl7/haswell/nersc_cr/19.10/etc/env_setup.sh`
- `start_coordinator` is a bash function (from `nersc_cr` module) that wraps the `dmtcp_coordinator` command and sets two envs to save coordinator host & port number, and generate `dmtcp_command.<jobid>` file in the run directory for communication with your running jobs as needed

```
dmtcp_coordinator --daemon --exit-on-last -p 0 --port-file $fname $@
1>/dev/null 2>&1
export DMTCP_COORD_HOST=$h
export DMTCP_COORD_PORT=$p
```

- User selects checkpoint interval (`-i` option for coordinator): periodic checkpoint vs checkpoint only once before the job terminates
  - The checkpoint overhead should be less than the time needed to dump the full memory on the node to the disk

Automatic Resubmission of Checkpoint/Restart Jobs with DMTCP

Automatic Resubmission of DMTCP Restart Jobs Using flex QOS (KNL Only)

Original Job script

```
#!/bin/bash
#SBATCH –J test
#SBATCH –q regular
#SBATCH –N 1
#SBATCH –C knl
#SBATCH –t 48:00:00
#SBATCH –o test-%j.out
#SBATCH –e test-%j.err

#user setting
export OMP_PROC_BIND=true
export OMP_PLACES=threads
export OMP_NUM_THREADS=64

./a.out
```

```
#!/bin/bash
#SBATCH –J test_cr
#SBATCH –q flex
#SBATCH –N 1
#SBATCH –C knl
#SBATCH –t 48:00:00
#SBATCH –o test_cr-%j.out
#SBATCH –e test_cr-%j.err
#SBATCH –time-min=2:00:00

#user setting
export OMP_PROC_BIND=true
export OMP_PLACES=threads
export OMP_NUM_THREADS=64

module load dmtcp nersc_cr
#checkpointing once every hour
start_coordinator -i 3600

#run job under dmtcp control
dmtcp_launch ./a.out
```

C/R jobs with DMTCP
Manual resubmission

```
#!/bin/bash
#SBATCH –J test
#SBATCH –q flex
#SBATCH –N 1
#SBATCH –C knl
#SBATCH –t 48:00:00
#SBATCH –o test_cr-%j.out
#SBATCH –e test_cr-%j.err
#SBATCH –time-min=2:00:00

#for c/r with dmtcp
module load dmtcp nersc_cr

#checkpointing once every hour
start_coordinator -i 3600

#restart the job from dmtcp checkpoint files
bash ./dmtcp_restart_script.sh
```

C/R jobs with DMTCP
Automatic resubmission

```
#!/bin/bash
#SBATCH -J test
#SBATCH -q flex
#SBATCH -N 1
#SBATCH -C KNL
#SBATCH --time=48:00:00
#SBATCH --error=test%j.err
#SBATCH --output=test%j.out
#SBATCH --time-min=02:00:00
#SBATCH --comment=48:00:00
#SBATCH --signal=B:USR1@300
#SBATCH --requeue
#SBATCH --open-mode=append

module load dmtcp nersc_cr
start_coordinator -i 3600

#checkpoint/restart job
if [[ $(restart_count) == 0 ]]; then
    #user setting
    export OMP_NUM_THREADS=64
    export OMP_PROC_BIND=spread
    export OMP_PLACES=threads
    dmtcp_launch -j ./a.out &
elif [[ $(restart_count) > 0 ]] && [[ -e dmtcp_restart_script.sh ]]; then
    bash ./dmtcp_restart_script.sh &
else
    echo "Failed to restart the job, exit”; exit
fi
# requeueing the job if remaining time >0
ckpt_command=
requeue_job func_trap USR1

wait
```

Automatic Resubmissions of DMTCP Jobs (cont.)

```
#SBATCH --time-min=02:00:00
```

Specify the minimum time for your job. Flex QOS requires time-min to be no more than 2 hours.

```
#SBATCH --comment=48:00:00
```

A flag to add comments about the job, used by the script to specify the desired walltime and to track the remaining walltime for the requeued jobs (after pre-termination). **You can specify any length of time, e.g., a week or even longer**

```
#SBATCH --signal=B:USR1@<sig_time>
```

Request the batch system to send user-defined signal USR1 to the batch shell (where the job is running) `sig_time` seconds (e.g., 300) before the job hits the wall clock limit

```
#SBATCH --requeue
```

Specify the job is eligible to requeue

```
#SBATCH --open-mode=append
```

Append the standard output/error of the requeued job to the same standard out/error files from the previously terminated job.

```
#SBATCH --comment=48:00:00
#SBATCH --signal=B:USR1@300
#SBATCH --requeue
#SBATCH --open-mode=append
```

Automatic Resubmission of DMTCP Jobs (cont.)

Bash functions used to automate job resubmission: `requeue_job`, `func_trap`, `start_coordinator`, ...

`requeue_job`

This function traps the user defined signal (e.g., `USR1`). Upon receiving the signal, it executes a function (e.g., `func_trap` below) provided on the command line.

```
requeue_job() {
    parse_job    # to calculate the remaining walltime
    if [ -n $remainingTimeSec ] && [ $remainingTimeSec -gt 0 ];
then
       commands=$1
       signal=$2
       trap $commands $signal
    fi
}
```

`func_trap`

This function contains the list of commands to be executed to initiate checkpointing, prepare inputs for the next job, requeue the job, and update the remaining walltime.

```
func_trap() {
    $ckpt_command
    scontrol requeue ${SLURM_JOB_ID}
    scontrol update JobId=${SLURM_JOB_ID} TimeLimit=${requestTime}
}
```

```
# requeueing the job if remaining
time >0
ckpt_command=
requeue_job func_trap USR1

wait
```

How Does Automatic Resubmission of DMTCP Jobs Work?

1. User submits job script.
2. The batch system looks for a backfill opportunity for the job. If it can allocate the requested number of nodes for this job for any duration (e.g., 6 hours) between the specified minimum time (2 hours) and the time limit (48 hours) before those nodes are used for other higher priority jobs, the job starts execution.
3. The job runs until it receives signal `USR1` (`--signal=B:USR1@300`) 300 seconds before it hits the allocated time limit (6 hours).
4. Upon receiving the signal, the `func_trap` function gets executed, which in turn executes
   a. `ckpt_command` if specified
   b. Requeues the job and then updates remaining walltime for requeued job.
5. Steps 2-4 repeat until job runs for the desired amount of time (48 hours) or job completes.
6. User checks results.

```
func_trap() {
    $ckpt_command
    scontrol requeue ${SLURM_JOB_ID}
    scontrol update JobId=${SLURM_JOB_ID} TimeLimit=${requestTime}
}
```

Summary

- DMTCP works with serial and threaded applications on Cori
    - You are encouraged to experiment with your workloads, and report bugs at help.nersc.gov
    - Benefits of checkpoint/restart jobs with DMTCP using the flex QOS on Cori KNL include increased job throughput, a large charging discount, and capability of running jobs of any length
    - For Haswell you can use DMTCP with regular QOS, just no charging discount
- For MPI applications, we recommend the to-be-released MANA implementation of DMTCP, which will work with Cray MPICH. We will host user training on MANA DMTCP in Feb 2020

Resources

- DMTCP website, http://dmtcp.sourceforge.net/index.html
- DMTCP github site https://github.com/dmtcp/dmtcp/blob/master/QUICK-START.md
- NERSC website, https://docs.nersc.gov/development/checkpoint-restart/
  - will be available on Nov 7, 2019
- Presentation slides will be posted in our training site after the training
- Our dmtcp module used Twinkle Jain's DMTCP fork, https://github.com/JainTwinkle/dmtcp.git (branch: spades-v2)

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- Rebecca Hartman-Baker for her vision on C/R, leading the C/R effort at NERSC
  - worked with a summer student (Tiffany Connors, now NERSC staff) developed the variable-time job script, automated the job resubmissions
  - Initiated the collaboration with DMTCP team
- Steve Leak - for working on improving/rewriting the variable-time job scripts (work in progress)
- Gene Cooperman, Twinkle Jain, and Rohan Garg for collaborations on getting DMTCP into production at NERSC (technical support, quick bug fixes, etc.)
- JGI SPADES team to adopt DMTCP in their workflow, resulting in multiple bug fixes
- NERSC team members, Chris Samuel, Eric Roman for helping system side debugging, batch system incorporation, etc.
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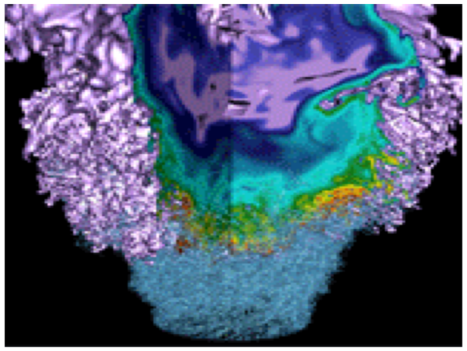
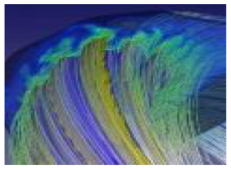
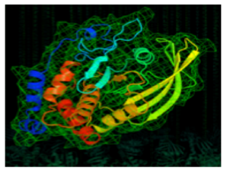
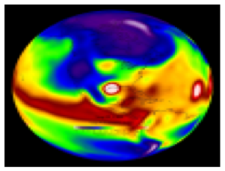
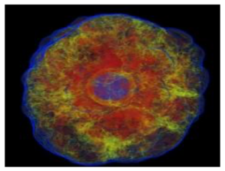
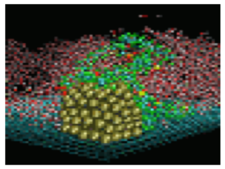
- DMTCP work (Gene Cooperman's research group at Northeastern Univ.) was partially supported by National Science Foundation Grants OAC-1740218 and ACI-1440788.

Thank You!

Backup slides

Running dmtcp_command from Cori Login Nodes

- From a Cori login node

```
mom_local.py dmtcp_command.<jobid> --checkpoint
```

  - `mom_local.py` script transfers current user environment, wd, and command line arguments precisely to the remote nodes and execs the command there

```
zz217@cori04:~> mom_local.py ./dmtcp_command.25583470 -s
Coordinator:
  Host: nid02471
  Port: 35241
Status...
  NUM_PEERS=0
  RUNNING=no
  CKPT_INTERVAL=3600
```

- Otherwise get on to the compute node first

```
ssh_job <jobid>
dmtcp_command.<jobid> --checkpoint
```

For a Quick Hands-on on Cori

- Using the binaries available at the test directory of the dmtcp modules, e.g., dmtcp1

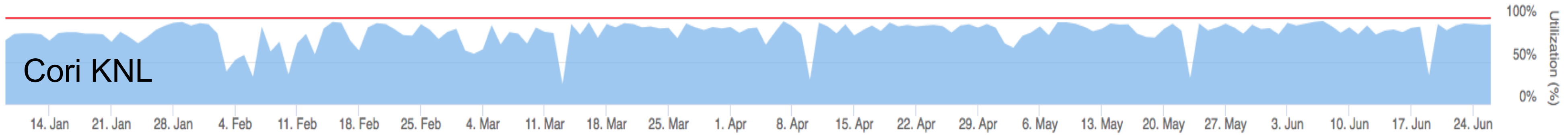
```
module load dmtcp
append_testpath  #so the DMTCP test directory in your path
cd $SCRATCH      #run on your scratch directory, because the image file
could be large
```

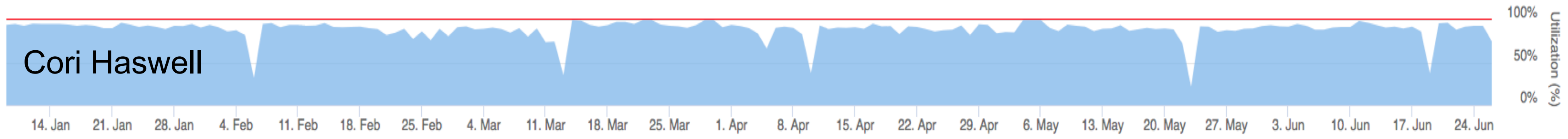
- Or use the jacobi.f90 available at /global/csratch1/sd/zz217/dmtcp_demo

```
cp -pr /global/csratch1/sd/zz217/dmtcp_demo $SCRATCH
cd $SCRATCH/dmtcp_demo
./compile.sh
```

  then run the jac.x under DMTCP control

System Utilizations





- Can we make use of the idle nodes when the system drains for larger jobs? Yes, we can! We just need many shorter jobs to backfill.
- The jobs submitted with a short ---time-min (on both Haswell and KNL nodes) will get higher job throughput, provided your jobs can do checkpoint/restart.

Automatic Resubmissions of VASP flex Jobs

```
# put any commands that need to run to continue the next
job here
ckpt_vasp() {
    set -x
    restarts=`squeue -h -O restartcnt -j $SLURM_JOB_ID`
    echo checkpointing the ${restarts}-th job

    # to terminate VASP at the next ionic step
    echo LSTOP = .TRUE. > STOPCAR
    # wait until VASP to complete the current ionic step,
write WAVECAR file and quit
    srun_pid=`ps -fle|grep srun|head -1|awk '{print $4}'`
    wait $srun_pid

    # copy CONTCAR to POSCAR
    cp -p CONTCAR POSCAR
    set +x
}

ckpt_command=ckpt_vasp
max_timelimit=48:00:00
ckpt_overhead=300

# requeueing the job if remaining time >0
. /global/common/cori/software/variable-time-job/setup.sh
requeue_job func_trap USR1
```

https://docs.nersc.gov/jobs/examples/#vasp-example

For automatic resubmissions of pre-terminated jobs

```
#!/bin/bash
#SBATCH -q flex
#SBATCH -N 2
#SBATCH -C knl
#SBATCH -t 48:00:00
#SBATCH --time-min=2:00:00

#SBATCH --comment=48:00:00
#SBATCH --signal=B:USR1@300
#SBATCH --requeue
#SBATCH --open-mode=append

module load vasp/20181030-knl
export OMP_NUM_THREADS=4

# srun must execute in background and catch signal
on wait command
# launching 1 task every 4 cores (16 CPUs)
srun -n32 -c16 --cpu-bind=cores vasp_std  &



 wait
```