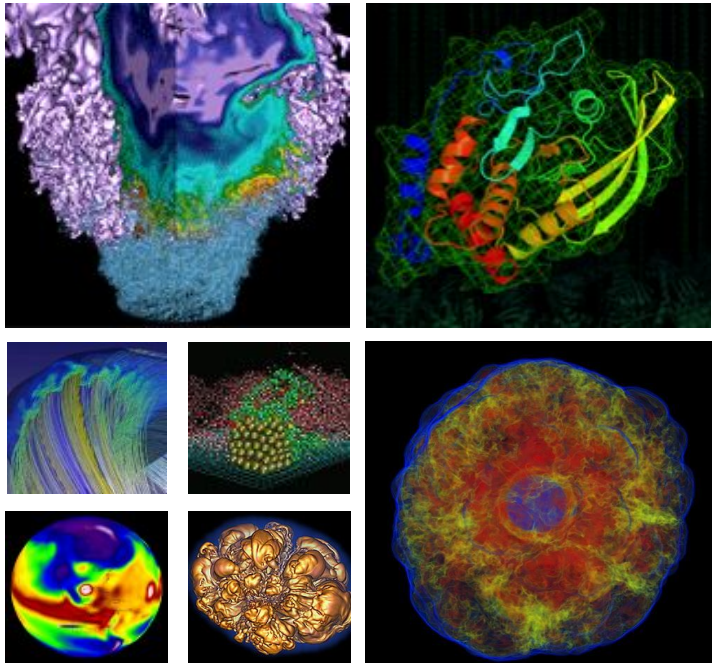
Optimizing Checkpoint-Restart Mechanism for HPC with DMTCP in Containers at NERSC



CUG Conference
May 5-9 2024
Perth, Australia

Madan Timalsina
NERSC/NESAP Postdoc
Data & AI Services

Coauthors (NERSC): W. Arndt, J. P. Blaschke, L. Gerhardt, and N. Tyler

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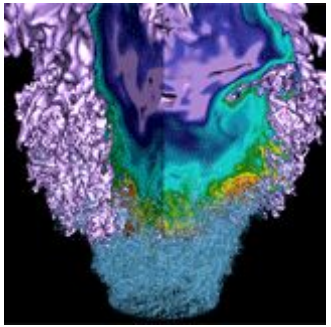
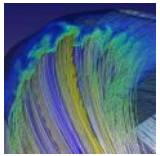
Outline

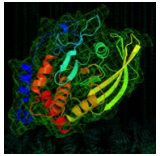
- National Energy Research Scientific Computing Center (NERSC)
- Checkpoint-Restart Mechanism
- DMTCP (Distributed MultiThreaded CheckPointing) Overview
- Checkpointing and Restarting Jobs using DMTCP
  - At NERSC Perlmutter
  - At NRSC Perlmutter inside the Containers
- Results
- Conclusion

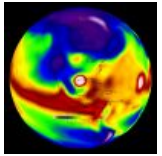
NERSC:

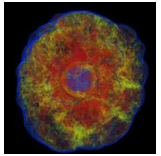
National Energy Research Scientific Computing Center

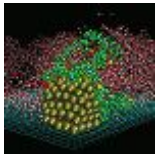












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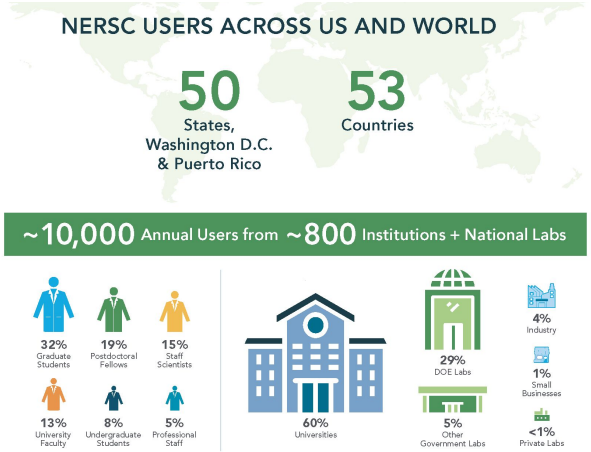
NERSC

- NERSC (at LBNL), a state-of-the-art supercomputer, is the mission High Performance Computing and Data facility for the DOE Office of Science
- Our mission involves deploying supercomputer systems designed for pioneering simulations and large-scale data analytics
- NERSC Science Acceleration Program (NESAP) fosters collaboration with partners to optimize scientific research for next-generation computational architectures and systems



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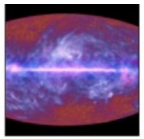
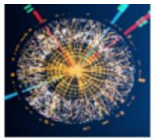
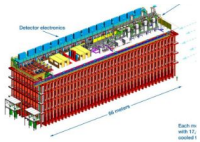
Palomar Transient Factory Supernova


Planck Satellite Cosmic Microwave Background Radiation

Star Particle Physics


Atlas Large Hadron Collider


APS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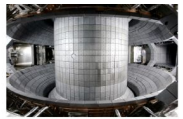
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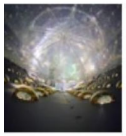
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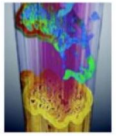

ALS Light Source

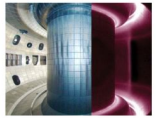

LCLS Light Source


Joint Genome Institute Bioinformatics


NSLS-II


HSX


Majorana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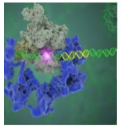
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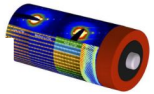
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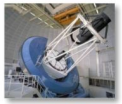
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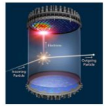

LZ


IceCube


EXO

JBEI Joint BioEnergy Institute

NERSC Center Architecture

TOP 500 The List. #12, 113PF Peak

>5 TB/s

35 PB All-Flash Scratch

HPE Slingshot 11 ethernet-compatible interconnect
4 NICs/GPU node,
1 NIC/CPU node

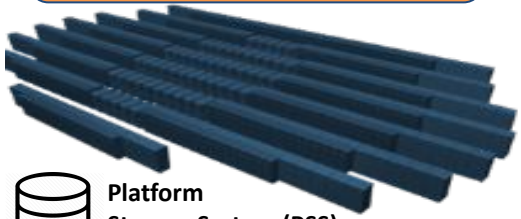
1,792 GPU-accelerated nodes
4 NVIDIA A100 GPUs+1 AMD "Milan" CPU
448 TB (CPU) + 320 TB (GPU) memory

3,072 CPU-only nodes
2 AMD "Milan" CPUs
1,536 TB CPU memory

1.6 TB/s

(2026)

NERSC-10



Platform Storage System (PSS)

Quality of Service Storage System (QSS)

Workflow Environment
Management Environment

Spin container services

Off Platform Storage

- HPSS Tape Archive >1 EB — 200 GB/s
- Community File System 240 PB — > 800 GB/s
- /home 450 TB — > 10 GB/s
- DTNs, Gateways

Ethernet

Science Friendly Security
Production Monitoring
Power Efficiency
LAN

3.25 TB/s (26 Tbps)

ESnet ENERGY SCIENCES NETWORK
2 x 400 Gb/s
2 x 100 Gb/s

Experimental Facility | ASCR Facility | Home Institution | Cloud | Edge

Containers at NERSC

Containers are valuable to our scientific computing users

- Encapsulation, isolation, reproducibility, portability, and even scalability

NERSC supports user container workloads via Shifter

- Developed at NERSC to address security concerns of docker
- Enables scalability on HPC systems
- Users can build their images with docker, then easily convert to shifter with a simple pull command

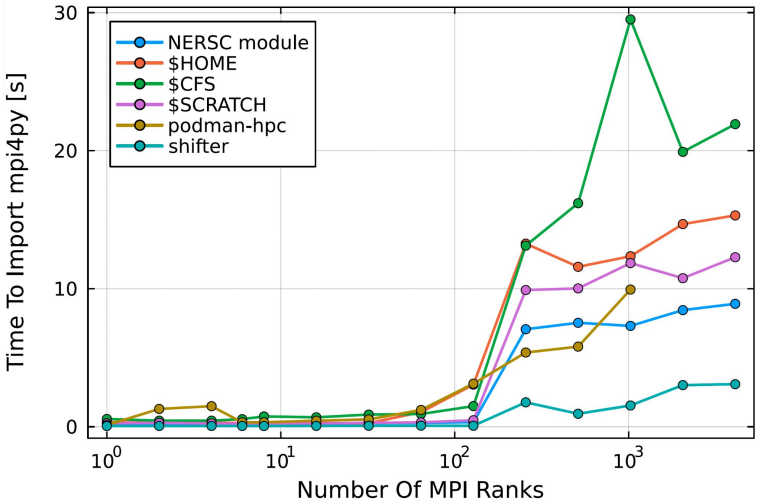
NERSC also supports podman-hpc

- NERSC built wrapper for podman (open source tool)
- All the benefits of shifter, but using OCI (Open Container Initiative) standard runtime
- A rootless containers enhances security, users can build images at NERSC

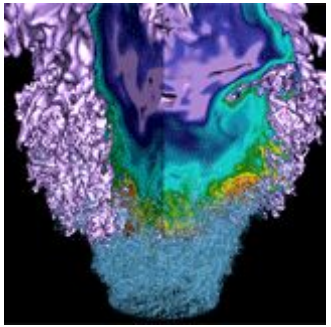
Performance Benchmark of Containers at NERSC

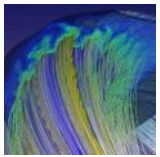
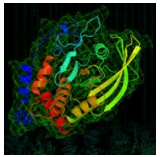
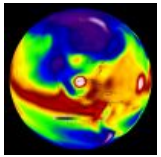
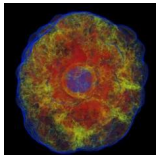
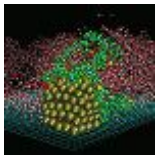
Scaling efficiency in scientific workflows with NERSC containers

- Enhances scaling efficiency of scientific workflows (reduced load times, even compared to optimized parallel file systems)
- Through encapsulation, containers introduce resilience in managing complex tasks
- At NERSC, Shifter and Podman-HPC offer scalable solutions supporting a wide range of research activities
- Containerized Checkpoint-Restart (C/R) mechanisms lead to faster and more reliable data processing, accelerating scientific discovery



Checkpoint-Restart (C/R)



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Checkpointing and Restarting (C/R)

- ***Checkpointing*** involves preserving the current state of a running process (jobs) by creating a checkpoint image file.
  - This includes capturing the memory, executing instructions, I/O status, and related data of the running process into a file
- ***Restarting*** the process is possible using the checkpoint file.
  - This enables the process to resume its execution from where it was saved (rather than from the beginning), either on the same or a different computer, seamlessly continuing its operation

It's a crucial capability in High-Performance Computing (HPC) due to complex and time-consuming computations. It can reduce startup times in applications and facilitates batch scheduler optimizations, including preemption

C/R: Benefits

HPC/NERSC Perspective

- **Enhanced Job Prioritization:** Potential preempting of less critical jobs for more urgent or time-sensitive tasks
- **Optimized Node Utilization:** Efficient backfilling, maximizing node usage, especially for large reservations
- **Uninterrupted Operations:** Run checkpointing jobs until system maintenance, ensuring minimal disruption
- **Enhanced Reliability:** Potentially checkpointing all jobs before unexpected power outages for system stability and job recovery

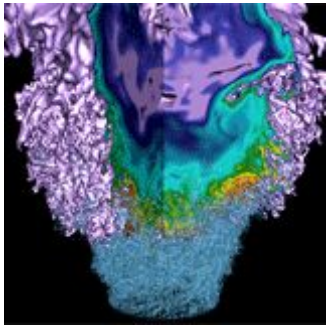
User Perspective

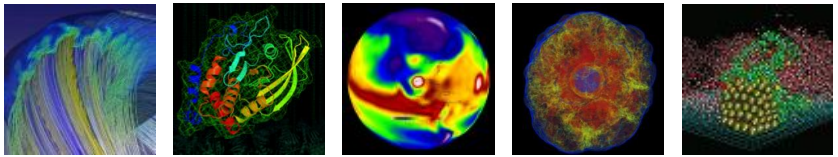
- **Extended Runtime:** Allow jobs to exceed walltime limits by resuming from checkpoints
- **Increased Throughput:** Leveraging gaps in the Slurm schedule to optimize job processing
- **Extended Interactivity:** Save and resume interactive sessions seamlessly (if it's time to go home to dinner, then checkpoint and restart the next day!)
- **Efficient Debugging**: Pause, identify errors, and restart jobs from specific checkpoints for iterative debugging

Challenges in C/R

- ***Complexity for User Transparency:*** Requires extensive effort to create a seamless experience for users during checkpointing and restarting processes
- ***MPI Support Challenges:*** Particularly intricate due to the combination of various MPI implementations (e.g., MPICH, OpenMPI) and networks (e.g., Slingshot, Infiniband), resulting in the need for multiple versions (MxN problem)
- DMTCP serves as a solution for overcoming these challenges
- For more details, refer to the NERSC documentation

DMTCP: Distributed MultiThreaded CheckPointing





NERSC documentation, DMTCP website, DMTCP github

DMTCP: Simplifying Checkpoint-Restart

An open-source tool offering seamless checkpoint and restart functionalities for distributed applications across clusters, grids, cloud environments etc

Preserves Application State Seamlessly

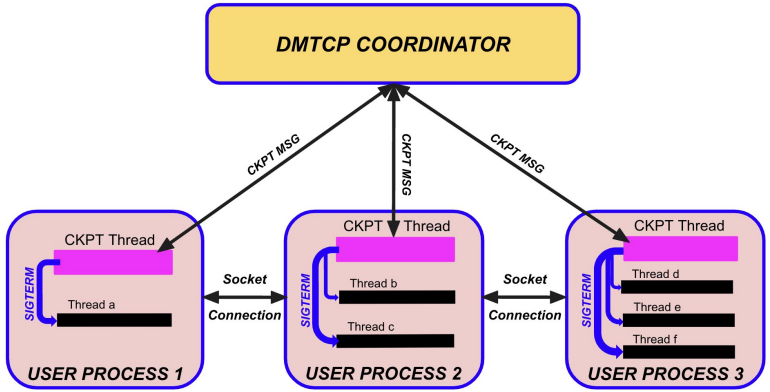
- **No Code or Kernel Modifications:** Stores complex threaded or distributed applications without altering their code or the Linux kernel
- **Accessible to Users:** Doesn't require special system privileges, allowing operation without root access

User-Friendly Checkpointing

- **Seamless User-Space Operation:** Performs checkpoints without changing user code or system settings
- **Versatile Application Support:** Works with diverse applications like MPI, OpenMP, Python, C/C++, Fortran, shell scripts, and resource managers (e.g., Slurm)

How does DMTCP Work?

DMTCP Architecture: Coordinated Checkpointing



DMTCP Coordinator to Computation Ratio: One DMTCP coordinator manages one checkpointable DMTCP computation

Multiple Checkpointable Computations: Multiple coordinators can handle separate computations, each independently checkpointtable

Checkpoint Thread vs. User Thread: Only one of the DMTCP checkpoint thread or user thread can be active at any given time, not both concurrently

Fault Tolerance without Single Point of Failure: No single point of failure if checkpoint image files are backed up. Even if the coordinator fails, the system can restart from the last checkpoint

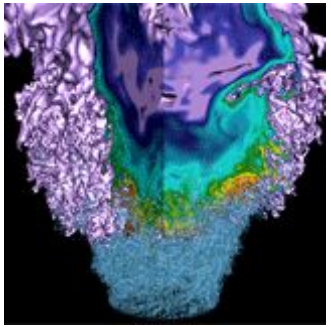
Preservation of Runtime Libraries: Runtime libraries are saved as part of the memory image. Applications continue using the same library API

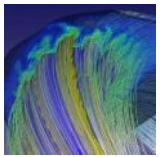
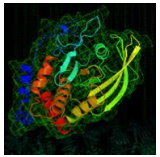
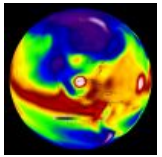
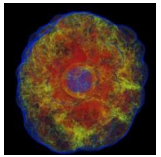
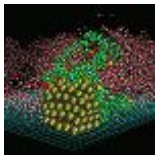
Inclusion of Linux Environment Variables: Linux environment variables are part of the memory image. Special DMTCP plugin needed to modify saved environment variables during checkpoint

User-Space Functionality: Entire process operates in user-space; no need for administrative privileges for its functioning

RESTART: same as ckpt, but in opposite order

Checkpoint/Restart (C/R) Jobs with DMTCP at Perlmutter



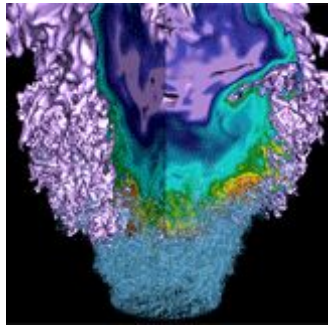






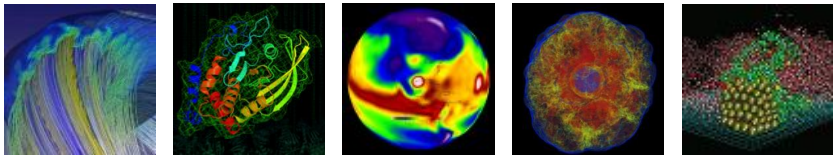
NERSC documentation

How does it work?

- NERSC CR Module (nersc_cr) manages Checkpoint/Restart (C/R) jobs
- Users can set the checkpoint interval with the -i option and submit their job either manual or automated way
- The batch system initiates job execution by allocating the requested nodes within available time frames, prioritizing higher-priority jobs
- As a part of automatic resubmission, the job runs until it receives signal USR1 (*--signal=B:USR1@60*) 60 seconds before it hits the allocated time limit
- Upon receiving the signal, the *func_trap* function gets executed, which in turn executes
  - *ckpt_command* if specified
  - Requeues the job and then updates remaining walltime for requeued job
- Steps 2-4 are repeated until the job completes or reaches the desired duration
- User checks the job results upon completion
- More details, NERSC documentation

Checkpoint/Restart (C/R) Jobs inside Container using DMTCP: Perlmutter





SHIFTER

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podman

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Requirements

- DMTCP cannot be checkpointed from outside the containers. It must be included within the container when it is build
- The simulation package can be built in many ways:
  - During the container's build process
  - After the container has been built, by linking the source code from elsewhere
  - Extend the functionality by building on top of an existing container, enabling quick experimentation with minimal modifications

  All methods have been tested and verified

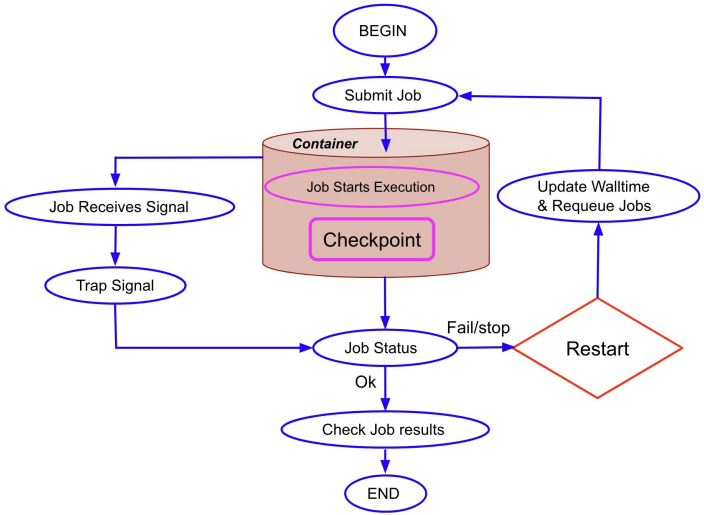
```
FROM my_application_container:latest

RUN git clone
https://github.com/dmtcp/dmtcp.git  \
   && cd dmtcp \
   && ./configure  && make \
   && make install
```

- In the context of Geant4, various versions can be directly sourced from the CernVM File System (CVMFS), facilitating easy access to multiple versions for testing and deployment

Automated C/R Strategies

- Users submit their job scripts, with the checkpoint interval (-i), incorporating DMTCP within containers, along with necessary software packages like Geant4, CP2K
- Custom batch scripts manage checkpoint-restart tasks, which isn't directly feasible within the container environment
- The script initiates checkpointing via *restart_job* function including a *start_coordinator* to initiate jobs and executes using *dmtcp_launch*, ensuring efficient job lifecycle management
- Upon receiving termination signals *(SIGTERM)*, the setup facilitates checkpointing, ensuring continuous job execution and effective resource utilization
- This method ensures efficient handling of Checkpoint/Restart processes, aligning with the specific needs of HPC environments, leading to the successful completion of jobs



Manual C/R Strategies

- Initial job submissions include checkpointing to set a baseline for potential restarts
- Users actively monitor job progress through output and error logs to detect interruptions
- Checkpoint files act as job snapshots, enabling precise recovery from disruptions
- Manual intervention allows for restarting jobs using these checkpoints, ensuring progress continuity
- The manual C/R process is a cycle of submission, monitoring, checkpointing, and restarting as needed
- This approach gives users direct control to address specific computational challenges within the job lifecycle

Results

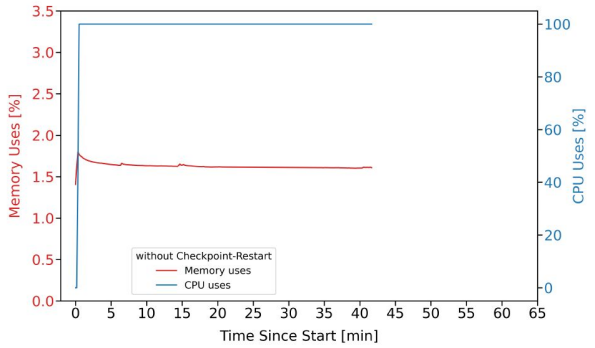
- Geant4 is a crucial tool for High Energy Physics (HEP) research, has been thoroughly tested and has passed the assessments
- Tested across multiple Geant4 versions (10.5, 10.7, 11.0) covering diverse simulation environments and particle interactions
- Performed tests using Shifter and Podman-HPC container images
- Each job, regardless of complexity, was preempted and then successfully resumed, highlighting the C/R mechanism's robustness
- Planning to extend our research into additional fields such as material science, with ongoing tests using CP2K

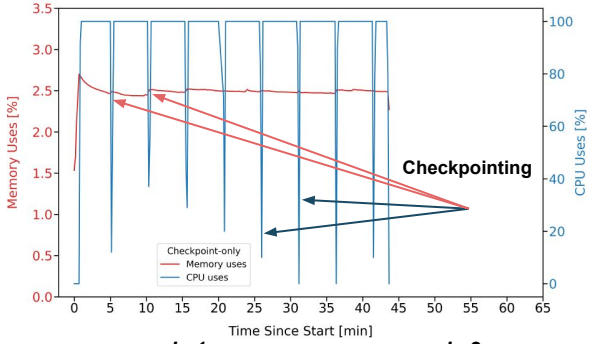
Results

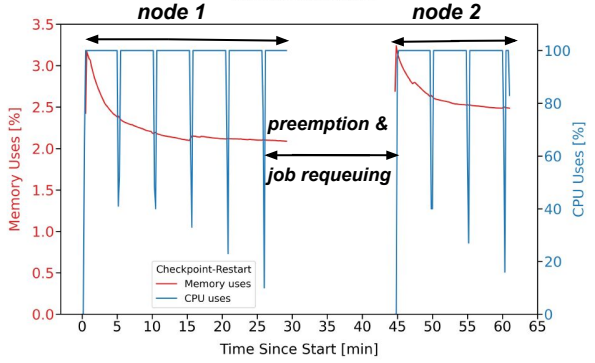
Impact of C/R on resource utilization

- ***Without C/R:*** The normal operational regime shows consistent CPU use and effective memory management
- ***Checkpoint-Only:*** Regular peaks in memory usage at checkpoints, with corresponding declines in CPU utilization
- ***Checkpoint-Restart:*** Spikes in memory use during checkpoints followed by corresponding declines in CPU utilization. A gaps in memory and CPU utilization due to preemption and job requeuing. We can see job has restarted in the different node afterward

C/R techniques exhibit a slight increase in computation time and memory usage (< 1%) because of DMTCP and associated file loading; however, this approach greatly reduces time and resource use by resuming the task from the last checkpoint state, enhancing efficiency







Future Directions

- Extend HEP-based simulation strategies to material science, enhancing research applications
- Plan to broaden testing with various material science software, including CP2K, VASP, BerkeleyGW, and LAMMPS
- Explore the use of MANA (MPI-Agnostic Network-Agnostic) for checkpointing to improve efficiency in MPI applications
- Leverage MANA's split-process approach for more streamlined and robust computational workflow management

Conclusion

- The study showcases the effectiveness of checkpoint-restart techniques using DMTCP in High-Performance Computing environments
- Demonstrated utility across HPC platforms including container technologies like Shifter and Podman-HPC
- This method is particularly valuable in complex, lengthy HPC computations, significantly reducing time and cost associated with process restarts
- Implementation in diverse simulations including HEP, medical science, and material science (test ongoing), showcasing versatility
- Highlights a critical advancement in efficient and reliable computational methodologies
- Confirms the effectiveness of the technique and opens new opportunities in computational science

Thank You

Some DMTCP Commands

dmtcp_coordinator -- coordinates checkpoints between multiple processes.

Example: `-i, --interval`: Time interval between automatic checkpoints (sec)

`--exit-on-last`: Auto-exits when the last client disconnects

dmtcp_launch -- Start a process under DMTCP control

Example: `-i, --interval`: Time interval between automatic checkpoints (sec)

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

dmtcp_restart -- Restart processes from a checkpoint image.

Example: `-h, --coord-host`: Specifies the hostname where `dmtcp_coordinator` is running

`-i, --interval`: Time interval between automatic checkpoints (sec)

dmtcp_command -- Send a command to the dmtcp_coordinator remotely

Example: `-s --status`: Prints status message

`-k --kill`: Kills all nodes

`-q --quit`: Kills all nodes and quits

For more details, refer to the DMTCP website, NERSC documentation

C/R Jobs with DMTCP CR Module: Perlmutter

Sample Job Script: Manual submission and resubmission

Original script

```
#!/bin/bash
#SBATCH -J test_cr
#SBATCH -q debug
#SBATCH -N 1
#SBATCH -C cpu
#SBATCH -t 00:07:00
#SBATCH -o %x-%j.out
#SBATCH -e %x-%j.err

#user settings
export OMP_PROC_BIND=spread
export OMP_PLACES=threads
export OMP_NUM_THREADS=2


./g4.sh
```

run.sh

```
#!/bin/bash
#SBATCH -J test_cr
#SBATCH -q debug
#SBATCH -N 1
#SBATCH -C cpu
#SBATCH -t 00:07:00
#SBATCH -o %x-%j.out
#SBATCH -e %x-%j.err
#SBATCH --time-min=00:05:30

#user settings
export OMP_PROC_BIND=spread
export OMP_PLACES=threads
export OMP_NUM_THREADS=2

#for c/r with dmtcp
module load dmtcp nersc_cr

#Checkpointing once every 5 min (change
interval as needed)
start_coordinator -i 300

#running under dmtcp control
dmtcp_launch -j ./g4.sh
```

restart.sh

```
#!/bin/bash
#SBATCH -J test_cr
#SBATCH -q debug
#SBATCH -N 1
#SBATCH -C cpu
#SBATCH -t 00:07:00
#SBATCH -o %x-%j.out
#SBATCH -e %x-%j.err
#SBATCH --time-min=00:05:30

#user settings
export OMP_PROC_BIND=spread
export OMP_PLACES=threads
export OMP_NUM_THREADS=2

#for c/r with dmtcp
module load dmtcp nersc_cr

#Checkpointing once every 5 min (change
interval as needed)
start_coordinator -i 300

#restarting from dmtcp checkpoint files
./dmtcp_restart_script.sh
```

To run:

```
sbatch run.sh
```

To restart:

```
sbatch restart.sh
```

C/R Jobs with DMTCP CR Module: Perlmutter

Sample Job Script: Auto resubmission

```
#!/bin/bash

# SLURM Job Submission Directives
#SBATCH -J test_cr       # Job name: test_cr
#SBATCH -q debug         # Queue name: debug
#SBATCH -N 1             # Number of nodes: 1
#SBATCH -C cpu           # Node type: CPU
#SBATCH -t 00:07:00      # Time limit: 7 minutes
#SBATCH -e %x-%j.err     # Standard error file format
#SBATCH -o %x-%j.out     # Standard output file format
#SBATCH --time-min=00:05:30 # Minimum time: 5 min 30 sec

#SBATCH --signal=B:USR1@60   # Send USR1 signal 60s before time limit
#SBATCH --requeue            # Enable job requeuing
#SBATCH --open-mode=append   # Open output files in append mode

# Load necessary modules for checkpoint/restart
module load dmtcp nersc_cr

# Start DMTCP coordinator for checkpointing every 5 minutes
start_coordinator -i 300
```

New for C/R jobs with DMTCP Automatic resubmission

```
# Checkpoint/Restart Logic
if [[ $(restart_count) == 0 ]]; then
   # First run of the job

   # Set OpenMP environment variables
   export OMP_PROC_BIND=spread
   export OMP_PLACES=threads
   export OMP_NUM_THREADS=2

   # Launch the user's application under DMTCP control
   dmtcp_launch -j ./my_g4.sh &
elif [[ $(restart_count) > 0 ]] && [[ -e dmtcp_restart_script.sh ]];
then
   # Restarting the job

   # Execute the restart script
   ./dmtcp_restart_script.sh &
else
   # If unable to restart, print error message and exit
   echo "Failed to restart the job, exit" ; exit
fi

# Requeuing Logic
ckpt_command=ckpt_dmtcp     # Command for additional checkpointing
requeue_job func_trap USR1 # Requeue job upon receiving USR1 signal

# Wait for all background processes to finish
wait
```

To run: `sbatch run.sh`

- The *requeue_job* function captures the specified signal (e.g., USR1) and then executes the *func_trap* function upon its reception
- The *func_trap* function initiates checkpointing, prepares inputs for the next job, requeues the job, and updates remaining walltime

C/R Jobs with DMTCP within Container: Perlmutter

Sample Job Script: Manual submission and resubmission

Original script

```
#!/bin/bash
#SBATCH -J G4_test_cont
#SBATCH -q debug
#SBATCH -N 1
#SBATCH -C cpu
#SBATCH -t 01:00:00
#SBATCH -o %x-%j.out
#SBATCH -e %x-%j.err
#SBATCH --time-min=00:06:00

## Additional directives...
#SBATCH --module=cvmfs
#SBATCH
--image=mtimalsina/geant4_dmtcp:9Nov2023

# Set the DMTCP_COORD_HOST variable
#to identify hosts or manage checkpoints
export DMTCP_COORD_HOST =$(hostname)

# Launch the job within the Shifter container
shifter --module=cvmfs
--image=mtimalsina/geant4_dmtcp:9Nov2023
/bin/bash ./my_g4.sh
```

run.sh

```
#!/bin/bash
#SBATCH -J G4_test_cont
#SBATCH -q debug
#SBATCH -N 1
#SBATCH -C cpu
#SBATCH -t 00:30:00
#SBATCH -o %x-%j.out
#SBATCH -e %x-%j.err
#SBATCH --time-min=00:06:00

## Additional directives...
#SBATCH --module=cvmfs
#SBATCH --image=mtimalsina/geant4_dmtcp:9Nov2023

# Set the DMTCP_COORD_HOST variable
#to identify hosts or manage checkpoints
export DMTCP_COORD_HOST =$(hostname)

# Launch the job within the Shifter container
shifter --module=cvmfs
--image=mtimalsina/geant4_dmtcp:9Nov2023
/bin/bash ./test-checkpoint.sh
```

test-checkpoint.sh

```
#!/bin/bash
dmtcp_launch --interval 300 ./my_g4.sh
```

restart.sh

```
#!/bin/bash
#SBATCH -J G4_test_cont
#SBATCH -q debug
#SBATCH -N 1
#SBATCH -C cpu
#SBATCH -t 00:30:00
#SBATCH -o %x-%j.out
#SBATCH -e %x-%j.err
#SBATCH --time-min=00:06:00

## Additional directives...
#SBATCH --module=cvmfs
#SBATCH --image=mtimalsina/geant4_dmtcp:9Nov2023

# Set the DMTCP_COORD_HOST variable
#to identify hosts or manage checkpoints
export DMTCP_COORD_HOST =$(hostname)

# Launch the job within the Shifter container
shifter --module=cvmfs
--image=mtimalsina/geant4_dmtcp:9Nov2023
/bin/bash ./dmtcp_restart_script.sh
```

Checkpoint image file

To run:

```
sbatch run.sh
```

To restart:

```
sbatch restart.sh
```

C/R Jobs with DMTCP within Container: Perlmutter

To run:

```
sbatch run.sh
```

```
#!/bin/bash

# Slurm directives for job properties
#SBATCH -J test-g4-cr       # Job name
#SBATCH -q regular          # Queue
#SBATCH -N 1                # Number of nodes
#SBATCH -C cpu              # CPU architecture
#SBATCH -t 01:00:00         # Wall clock time
#SBATCH -e %x-%j.err        # Error file
#SBATCH -o %x-%j.out        # Output file

#SBATCH --time-min=00:45:00     # Minimum time allocation
#SBATCH --comment=01:05:00      # Comment
#SBATCH --signal=SIGTERM@60     # Signal handling for termination
#SBATCH --requeue               # Requeue job if terminated
#SBATCH --open-mode=append      # Append mode for output files

## Additional directives...
#SBATCH --module=cvmfs                                  # Load module
#SBATCH --image=mtimalsina/geant4_dmtcp:Dec2023   # Container image

# Set the DMTCP_COORD_HOST variable
export DMTCP_COORD_HOST =$(hostname)

# Requeue function to resubmit the job on SIGTERM
function requeue () {
   echo "Got Signal. Going to requeue"
   scontrol requeue ${SLURM_JOB_ID}
}

# Trap SIGTERM to trigger requeue function
trap requeue SIGTERM

# Launch the job within the Shifter container
shifter --module=cvmfs --image=mtimalsina/geant4_dmtcp:Dec2023
/bin/bash ./test-auto.sh &

wait
```

Basic slurm directives

New for C/R jobs with DMTCP automatic resubmission

--comment sbatch flag is used to specify the desired walltime and to track the remaining walltime for the job after pre-termination

Export hostname to restart the job

Requeue function to resubmit the job

Trap signal (SIGTERM) to trigger requeue function

Launch the job within the Shifter container

C/R Jobs with DMTCP within Container: Perlmutter

test-auto.sh

```
#!/bin/bash

export DMTCP_COORD_HOST=$(hostname)
source my_env_setup.sh

# Function to restart or initiate the job
function restart_job() {
    start_coordinator -i 300

    if [[ $(restart_count) == 0 ]]; then
        # Initial job launch
        dmtcp_launch --join-coordinator -i 300 ./my_g4.sh
        echo "Initial launch successful."
    elif [[ $(restart_count) > 0 ]] && [[ -e $PWD/dmtcp_restart_script.sh ]];then
        # Restart the job
        echo "Restarting the job..."
        echo "Executing: $PWD/dmtcp_restart_script.sh"
        $PWD/dmtcp_restart_script.sh &
        echo "Restart initiated."

    else
        echo "Failed to restart the job, exiting." exit
    fi

    # Set up trap for checkpointing on termination signal
    trap ckpt_dmtcp SIGTERM
}

# Execute the function to restart the job
restart_job

# Wait for the job to complete or terminate
wait
```

This script provides functions for managing and monitoring SLURM jobs, including time tracking, signal trapping, job requeuing, and integration with DMTCP for checkpoint/restart functionality. It converts time to human-readable format, calculates remaining time for job scheduling, updates job comments accordingly, and manages job requeuing based on the remaining time

This function sets up and manages a job using DMTCP for checkpointing. It starts the job if it's the initial run. Or restarts it from a checkpoint if it's a subsequent run. Additionally, it configures a trap to automatically checkpoint the job when a termination signal is received

Your simulation code

Users can choose the checkpoint interval with the -i option.

C/R Jobs with DMTCP within Container: Perlmutter

```bash
#!/bin/bash

# Slurm directives for job properties
#SBATCH -J test-g4-cr-podman            # Job name
#SBATCH -q regular                      # Queue
#SBATCH -N 1                            # Number of nodes
#SBATCH -C cpu                          # CPU architecture
#SBATCH -t 01:00:00                     # Wall clock time
#SBATCH -e %x-%j.err                    # Error file
#SBATCH -o %x-%j.out                    # Output file
#SBATCH --time-min=00:45:00             # Minimum time allocation
#SBATCH --comment=01:05:00              # Comment
##SBATCH --signal=B:USR1@60              # Signal (previously used)
#SBATCH --signal=SIGTERM@60             # Signal handling for termination
#SBATCH --requeue                       # Requeue job if terminated
#SBATCH --open-mode=append              # Append mode for output files
## Additional directives...
#SBATCH --module=cvmfs                          # Load module
#SBATCH --image=mtimalsina/geant4_dmtcp:Dec2023   # Container image

# Set the DMTCP_COORD_HOST variable
export DMTCP_COORD_HOST=$(hostname)

# Requeue function to resubmit the job on SIGTERM
function requeue () {
   echo "Got Signal. Going to requeue"
   scontrol requeue ${SLURM_JOB_ID}
}
# Trap SIGTERM to trigger requeue function
trap requeue SIGTERM
#requeue_job func_trap USR1

# Launch the job within the Shifter container
podman-hpc run --userns keep-id --rm -it --mpi \
   -e SLURM_JOBID=${SLURM_JOB_ID} \
   -v /cvmfs:/cvmfs \
   -v $(pwd):/podman-hpc \
   -w /podman-hpc \
   mtimalsina/geant4_dmtcp:Dec2023 \
   /bin/bash ./test-auto.sh &

wait
```

```bash
#!/bin/bash

# Ensure the checkpoint directory exists and has the correct permissions
chmod 755 /podman-hpc
export DMTCP_COORD_HOST=$(hostname)
source my_env_setup.sh

# Function to restart or initiate the job
function restart_job() {
   start_coordinator -i 300

   if [[ $(restart_count) == 0 ]]; then
       # Initial job launch
       dmtcp_launch --join-coordinator --i 300 ./my_g4.sh
       echo "Initial launch successful."
   elif [[ $(restart_count) > 0 ]] && [[ -e $PWD/dmtcp_restart_script.sh ]]; then
       # Restart the job
       echo "Restarting the job..."
       echo "Executing: $PWD/dmtcp_restart_script.sh"
       $PWD/dmtcp_restart_script.sh &
       echo "Restart initiated."

   else
       echo "Failed to restart the job, exiting."; exit
   fi

   # Set up trap for checkpointing on termination signal
   trap ckpt_dmtcp SIGTERM
}

# Execute the function to restart the job
restart_job

# Wait for the job to complete or terminate
wait
```

Significant modifications have been implemented in the ***shifter*** image script to ensure compatibility with ***podman-hpc***