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Performing Parameter Sweeps on Odyssey

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Goal

Use SLURM commands and the power of BASH shell scripts to perform effective parameter sweeps on Odyssey.

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Use SLURM commands and the power of BASH shell scripts to perform effective parameter sweeps on Odyssey.

Outline

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- ❑ Serial parameter sweeps
- ❑ Parallel parameter sweeps
  - Multiple jobs submission – Bash Shell Scripts
  - Multiple jobs submission – Job Arrays
  - Parallelization of serial applications
- ❑ Advanced topics – Submitting Multiple Jobs with Job Dependencies

Introduction / Purpose

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Parameter sweep applications are a class of applications in which the **same code is run multiple times using unique set of input parameter values**. This includes varying one parameter over a range of values, or varying multiple parameters over a large multidimensional space.

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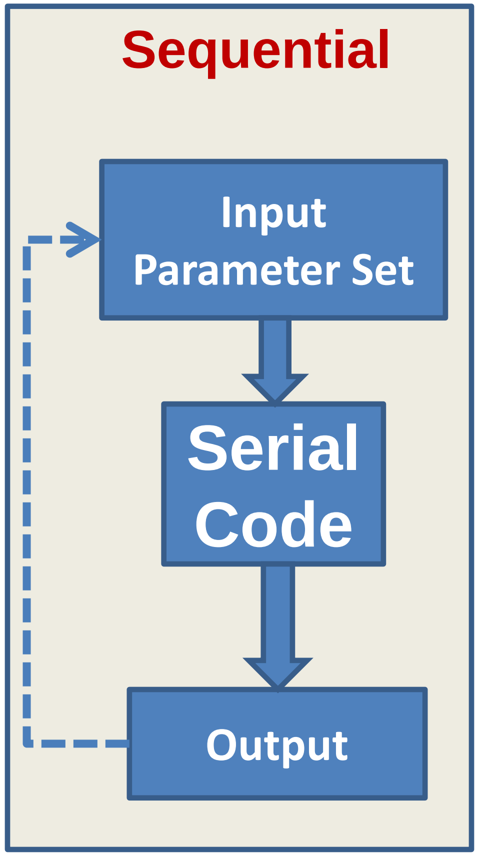
Parameter sweep applications are a class of applications in which the **same code is run multiple times using unique set of input parameter values**. This includes varying one parameter over a range of values, or varying multiple parameters over a large multidimensional space.



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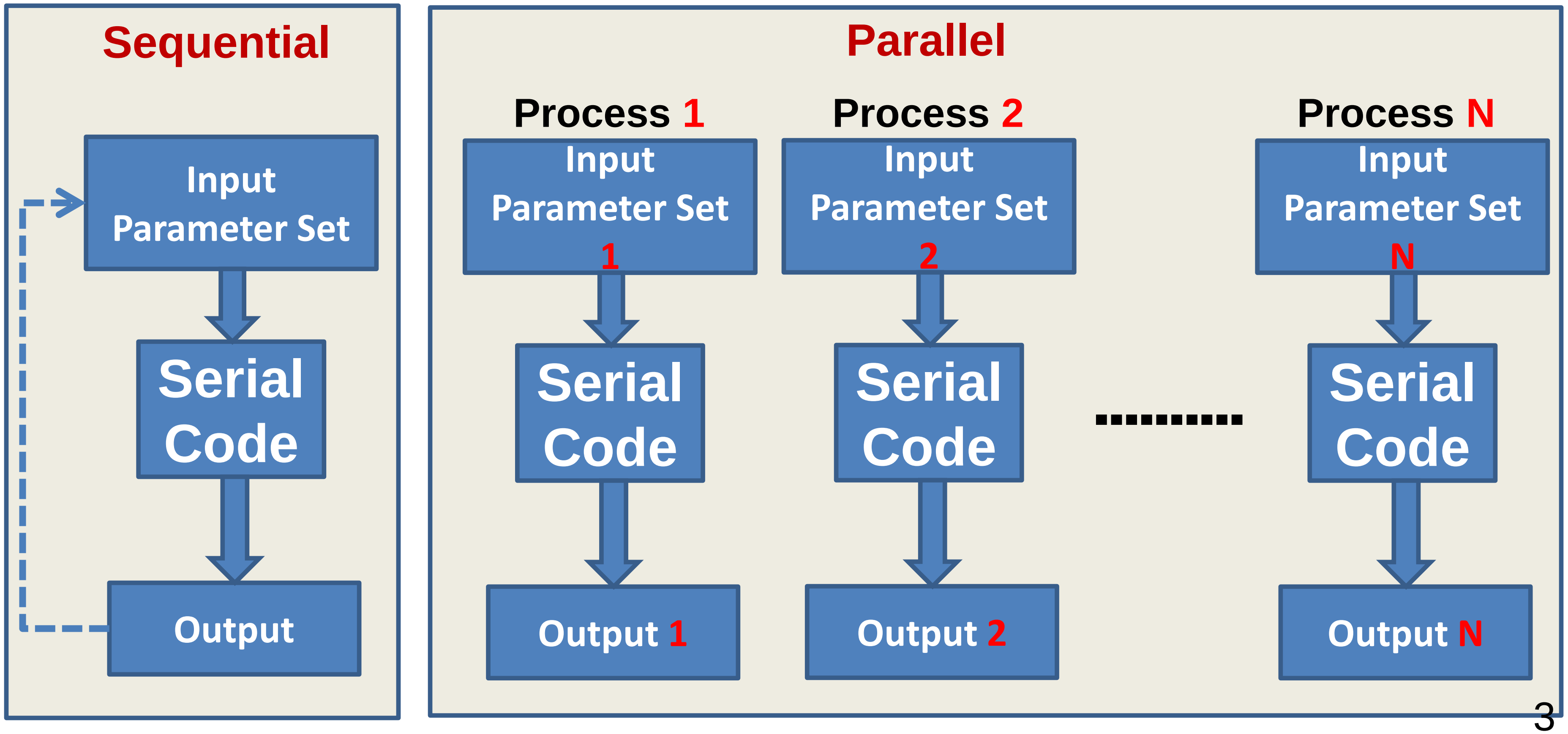

Serial Parameter Sweeps

Example: Serial Matlab program computing the sum of integers from 1 to N for **N = [100, 200, 300]**. N is a parameter passed to the program from the Matlab command line.

Serial Parameter Sweeps

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```
%=========================================
% Function: serial_sum( N )
%           Calculates integer sum from 1 to N
%=========================================
function s = serial_sum(N)
  s = 0;
  for i = 1:N
    s = s + i;
  end
  fprintf('Sum of numbers from 1 to %d is %d.\n', N, s);
end
```

Serial Parameter Sweeps

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serial_sum.sh: Bash shell script for running the serial code for each value of the parameter N (100, 200, and 300). Runs are performed in serial.

```
#!/bin/bash
parameter_list=( 100 200 300 )
i=0
for N in "${parameter_list[@]}"
do
    i=$(($i+1))
    echo "Iteration: $i"
    echo "Parameter value: $N"
    echo "Starting Matlab ..."
    matlab -nodesktop -nosplash -r "serial_sum($N);exit"
    echo "“
done
```

Serial Parameter Sweeps

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serial_sum.run: Batch-job submission script to submit the serial parameter sweep job.

```
#!/bin/bash
#SBATCH -J serial_sum
#SBATCH -o serial_sum.out
#SBATCH -e serial_sum.err
#SBATCH -p general
#SBATCH -n 1
#SBATCH -t 30
#SBATCH --mem=2000
sh serial_sum.sh
```

Serial Parameter Sweeps

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serial_sum.run: Batch-job submission script to submit the serial parameter sweep job.

```
#!/bin/bash
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#SBATCH -e serial_sum.err
#SBATCH -p general
#SBATCH -n 1
#SBATCH -t 30
#SBATCH --mem=2000
sh serial_sum.sh
```

Use

```
sbatch serial_sum.run
```

to submit the job to the queue.

Parallel Parameter Sweeps

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Submitting multiple jobs with the help of Bash shell scripts: Jobs are submitted simultaneously with separate parameter sets.

```
#!/bin/bash
parameter_list=( 100 200 300 )
i=0
job_name="parallel_sum"
for N in "${parameter_list[@]}"
do
    i=$(($i+1))
    echo "Submitting job $i ..."
    echo "Parameter value: $N"
    sbatch -J ${job_name}_${i}     \
           -o ${job_name}_${i}.out \
           -e ${job_name}_${i}.err \
           -p general              \
           -n 1                    \
           -t 30                   \
           --mem=2000              \
    --wrap="matlab -nodesktop -nosplash -r 'serial_sum($N);exit'"
    echo ""
    sleep 1
done
```

Parallel Parameter Sweeps

Submitting multiple jobs with the help of Job Arrays: Jobs are submitted simultaneously with different parameter sets. Parameter sets are read from separate input files for each job instance.

Parallel Parameter Sweeps

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<u>Submitting multiple jobs with the help of Job Arrays</u>: Jobs are submitted simultaneously with different parameter sets. Parameter sets are read from separate input files for each job instance.

```
%=======================================
% Function: serial_sum( infile )
%          Calculates integer sum from 1 to N
%=======================================
function s = serial_sum(infile)
  fid = fopen(infile,'r');
  m = fgets(fid);
  fclose(fid);
  N = sscanf(m,'%d');
  s = 0;
  for i = 1:N
    s = s + i;
  end
  fprintf('Sum of numbers from 1 to %d is %d.\n', N, s);
end
```

Parallel Parameter Sweeps

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Submitting multiple jobs with the help of Job Arrays: Jobs are submitted simultaneously with different parameter sets. Parameter sets are read from separate input files for each job instance.

Batch-job submission script for the array job

```
#!/bin/bash
#SBATCH -J parallel_sum
#SBATCH -o output_%a.out
#SBATCH -e error_%a.err
#SBATCH -p general
#SBATCH -n 1
#SBATCH -t 30
#SBATCH --mem=2000
#SBATCH --array=1-3
matlab -nodesktop -nosplash -r "serial_sum('input_${SLURM_ARRAY_TASK_ID}');exit"
```

Parallel Parameter Sweeps

Parallelization of serial applications: A typical parameter sweep application consists of a for loop which repeatedly executes the same code, usually in a function. A unique set of arguments is supplied to the function in each iteration.

Parallel Parameter Sweeps

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spar.m: serial Matlab script

```
%=========================================
% Matlab code for calling the function serial_sum
% with different parameter values (100, 200, 300)
%=========================================
parameter_list = [100, 200, 300];
N = 3;
for i = 1: N
   serial_sum(parameter_list(i));
end
exit;
```

Parallel Parameter Sweeps

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```
#!/bin/bash
#SBATCH -J serial
#SBATCH -o serial.out
#SBATCH -e serial.err
#SBATCH -p general
#SBATCH -n 1
#SBATCH -t 30
#SBATCH --mem=2000
matlab -nosplash -nodesktop -r "spar"
```

Parallel Parameter Sweeps

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Parallelization of serial applications: A typical parameter sweep application consists of a for loop which repeatedly executes the same code, usually in a function. A unique set of arguments is supplied to the function in each iteration.

ppar.m: parallel Matlab script using 3 Matlab workers with PCT

```
%======================================
% Parallel Matlab code for calling the function serial_sum
% with different parameter values (100, 200, 300)
%======================================
% create a local cluster object
pc = parcluster('local')
parpool(pc, 3)
parameter_list = [100, 200, 300];
N = 3;
parfor i = 1: N
  serial_sum(parameter_list(i));
end
delete(gcp);
exit;
```

Parallel Parameter Sweeps

Parallelization of serial applications: A typical parameter sweep application consists of a for loop which repeatedly executes the same code, usually in a function. A unique set of arguments is supplied to the function in each iteration.

```
#!/bin/bash
#SBATCH -J parallel
#SBATCH -o parallel.out
#SBATCH -e parallel.err
#SBATCH -p general
#SBATCH -n 3
#SBATCH -N 1
#SBATCH -t 30
#SBATCH --mem=2000
matlab-default -nosplash -nodesktop -r "ppar"
```

Job Dependencies

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Example: Submitting three jobs (step_1, step_2, step_3). Subsequent job starts if only the previous job has completed successfully.

```
#!/bin/bash
n_steps=3
for i in `seq 1 ${n_steps}`;
do
    echo "Iteration: $i"
    command="sbatch --dependency=afterok:$latest_id step_${i}.run"
    if [ $i = 1 ]; then
        command="sbatch step_${i}.run"
    fi
    latest_id=$($command | awk ' { print $4 }')
    echo "Successfully submitted job $latest_id."
done
```

Job Dependencies

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```
#!/bin/bash
n_steps=3
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do
    echo "Iteration: $i"
    command="sbatch --dependency=afterok:$latest_id step_${i}.run"
    if [ $i = 1 ]; then
        command="sbatch step_${i}.run"
    fi
    latest_id=$($command | awk ' { print $4 }')
    echo "Successfully submitted job $latest_id."
done
```

Get Job ID