

Using Wolfram Mathematica on the HybriLIT Platform to Model Heavy Meson Properties in Effective QCD.

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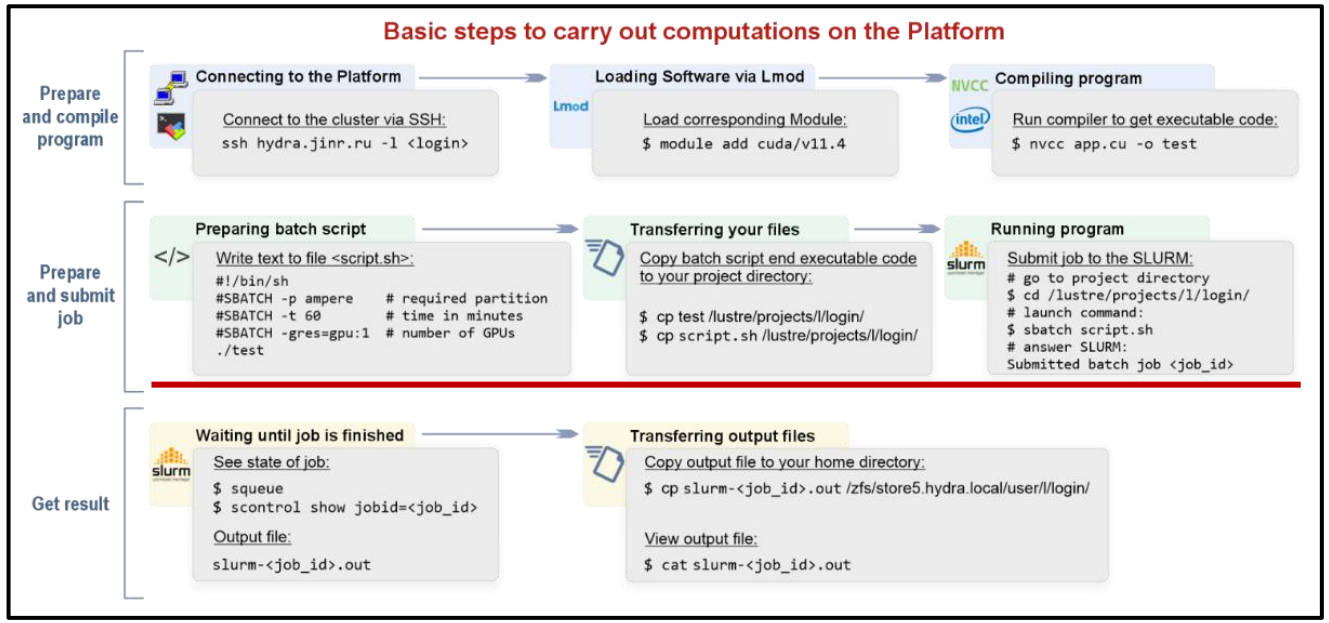
SLURM (Slurm Workload Manager)

Main SLURM workload manager commands:

- **sbatch** — command to submit an application/job to the queue;
- **squeue** — command to view the list of running applications/jobs in the queue;
- **sinfo** — command to view the status of compute nodes and queues. Compute nodes can be in one of the following states:

1. idle – the node is free/idle;
2. alloc – the node is in use by a process/allocated;
3. mix – the node is partially occupied and partially free;
4. down, drain, drng – the node is blocked/drained.

- **scancel** — command to cancel/remove an application/job from the queue.
- **scontrol** — used to view or modify the state of SLURM, including: jobs, nodes, and queues.



Prepare the program files with the **`_.m`** extension and a launch script with the **`_.sh`** extension.

→ Move the prepared files to the **`/lustre/projects/l/login`** directory

→ Submit a job to the **SLURM** workload manager

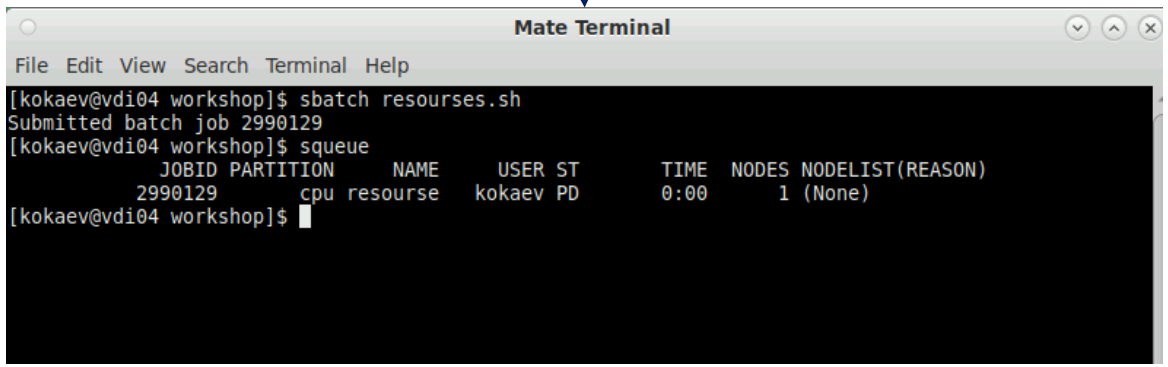
Task launch procedure

Example program **tutorial.m**

```
 (* 1. Initialization of constants and parameters *)
Nc = 3; Nf = 1;
pmin = 0.000001; pmax = 10.0;

(* Definition of physical functions *)
(* (phi, Equark, SolveMassGap, CalculateNorm, ...) *)

FuncSystemEquationAtT[T_, mq_, L_, D0_] := Module[{dm, m, M, Nv, fv},
(* Basic calculations (solving equations) *)
{T, m, 2*m, M, Nv, fv}
];

(* 2. Launching parallel computations *)
(* Checking sub-core availability and license count *)
slurmNTasks = ToExpression[Environment["SLURM_NTASKS"]];
slurmCpusPerTask = ToExpression[Environment["SLURM_CPUS_PER_TASK"]];
totalCores = slurmNTasks * slurmCpusPerTask;

licenseLimit = $MaxLicenseSubprocesses;
If[! NumericQ[licenseLimit], licenseLimit = Infinity];

nKernels = Min[totalCores - 1, licenseLimit];

LaunchKernels[nKernels];
Print[" KernelCount: ", $KernelCount];

(* 3. Preparation of the parameter grid *)
mqGrid = Range[1.1, 1.4, 0.05];
LGrid = Range[1.0, 2.0, 0.1];
D0Grid = Range[0.6, 1.4, 0.1];
grid = Flatten[Table[{mq, L, D0}, {mq, mqGrid}, {L, LGrid}, {D0, D0Grid}],2];

(* 4. Parallel parameter scanning *)
gridResults = ParallelMap[EvalPoint, grid, Method -> "CoarsestGrained"];

(* Searching for the best parameters and outputting the result *)
best = First@MinimalBy[gridResults, #[[2]] &];
Print["Best parameters: ", best[[1]]];

(* 5. Program termination *)
CloseKernels[]; (* Disabling parallel cores *)
Quit[];         (* Terminating the Mathematica kernel *)
```

Example of script text

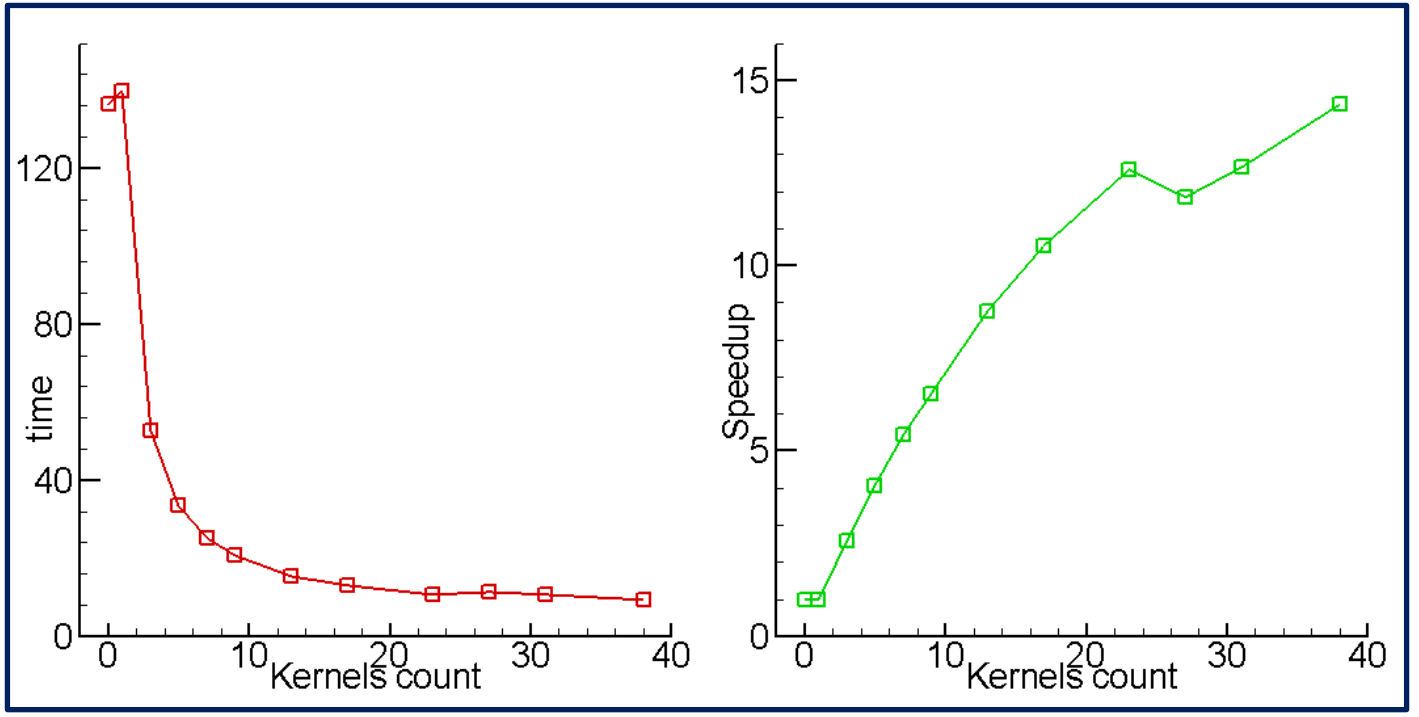
```
#!/bin/sh
#SBATCH -p cpu                          # queue to be used

#SBATCH --job-name=tutorial_task        # sets the job name in the queue
#SBATCH --output= tutorial_task _%j.out # sets the name of the standard output file
#SBATCH --error= tutorial_task _%j.err  # sets the name of the standard error output file

#SBATCH -t 10                           # reserved computation time (10 minutes)

#SBATCH --nodes=1                       # request the number of nodes per job
#SBATCH --ntasks=1                      # request the number of tasks
#SBATCH --cpus-per-task=1               # request 1 CPUs (processors) per task

module add Mathematica/v14.1            # load the Mathematica module
math -script tutorial.m                 # tutorial.m – the name of the file with the program
                                        listing
```



Launching a parallel task

```
#!/bin/sh
#SBATCH -p gpu_k80                      # queue to be used

#SBATCH --job-name=tutorial_task        # sets the job name in the queue
#SBATCH --output= tutorial_task _%j.out # sets the name of the standard output file
#SBATCH --error= tutorial_task _%j.err  # sets the name of the standard error output file

#SBATCH -t 10                           # reserved computation time (10 minutes)

#SBATCH --nodes=1                       # request the number of nodes per job
#SBATCH --ntasks=1                      # request the number of tasks
#SBATCH --cpus-per-task=40              # request 40 CPUs (processors) per task

module add Mathematica/v14.1            # load the Mathematica module
math -script tutorial.m                 # tutorial.m – the name of the file with the program listing
```

By changing the **`cpu-per-task`** parameter, you can request a larger number of physical processors per task.



Dependence of computation time and speedup on the number of cores