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·GROMACS··checkpoint·····

Slurm ····· checkpoint·····
····· GROMACS 2026.4 · CPU thread-MPI ·····

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····· GROMACS ···· checkpoint ····· checkpoint ·····
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··checkpoint	·····	·····
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····· 1 ····· -maxh 0.8 ·· 48 ···GROMACS ····· 99% ····· checkpoint ·
····· 48 ·····2 CPU·2 GB ·····
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```
#!/usr/bin/env bash
#SBATCH --job-name=md-segment
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=2
#SBATCH --mem=2G
#SBATCH --time=01:00:00
#SBATCH --output=md-%j.out
set -euo pipefail
: "${RUN_DIR:?·····}" "${RUN_MODE:?fresh·resume}"
: "${SLURM_CPUS_PER_TASK:?Slurm···CPU·}"
[[ "$SLURM_CPUS_PER_TASK" =~ ^[1-9][0-9]*$ ]] || exit 2
[[ "$RUN_DIR" = /* ]] || exit 2
extra=()
case "$RUN_MODE" in
  fresh)
    : "${TPR:?·····TPR····}"
    [[ "$TPR" = /* ]] && test -s "$TPR"
    test ! -e "$RUN_DIR" && test ! -L "$RUN_DIR" || exit 2
    mkdir "$RUN_DIR"; cp "$TPR" "$RUN_DIR/run.tpr"
    (cd "$RUN_DIR"; sha256sum run.tpr > run.tpr.sha256)
    ;;
  resume)
    test -d "$RUN_DIR" && test ! -L "$RUN_DIR" || exit 2
    test -s "$RUN_DIR/run.cpt" && test -s "$RUN_DIR/run.tpr.sha256" || exit 2
    extra=(-cpi run.cpt -append)
    ;;
  *) exit 2 ;;
esac
cd "$RUN_DIR"
sha256sum -c run.tpr.sha256
mkdir -p attempts
attempt=$(mktemp -d "$PWD/attempts/segment.XXXXXX")
gmx --version > "$attempt/version.txt" 2>&1
/usr/bin/time -v -o "$attempt/time.txt" \
  gmx mdrun -s run.tpr -deffnm run -cpo run.cpt \
  -ntmpi 1 -ntomp "$SLURM_CPUS_PER_TASK" \
  -nb cpu -pme cpu -bonded cpu -update cpu -cpt 5 -maxh 0.8 \
  "${extra[@]}" > "$attempt/console.log" 2>&1
test -s run.cpt
printf '%s\n' SEGMENT_ENDED_CHECK_PROGRESS > "$attempt/status.txt"
```

····· RUN_MODE=fresh·RUN_DIR · TPR····· RUN_MODE=resume ·····GROMACS ·····
····· gmx mdrun -h ····· checkpoint ·····
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-cpi ····· checkpoint ····· checkpoint · GROMACS ·····
····· resume ····· run.cpt ····· checkpoint ····· che
ckpoint ····· GROMACS ····· checkpoint·····

··· SEGMENT_ENDED_CHECK_PROGRESS ····· checkpoint ····· Slurm ·
··md.log ·····checkpoint ····· checkpoint ····
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···· COMPLETED ·····
····· tpr ·····
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checkpoint ·····
·····
····· checkpoint·

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GROMACS 2026.4··mdrun···checkpoint·append·maxh https://manual.gromacs.org/current/onlinehelp/gmx-mdrun.html

Slurm··sbatch····· https://slurm.schedmd.com/sbatch.html