http://linux.about.com/od/commands/l/blcmdl1\_grep.htm

#Coordinates and Velocity

grep -A 8 "Cartesian coordinates" MD\_log > coords.txt

grep -v "Cartesian coordinates" coords.txt > coords2.txt

grep -A 8 "Velocities" MD\_log > vel.txt

grep -v "Velocities" vel.txt > vel2.txt

#Potential Energy

grep "ETOT" MD\_log > PE.txt

sstr=a

found=0

while IFS= read -r line

do

case $line in

\*"$sstr"\*) : do whatever; found=1 ;;

esac

done < file

if [ $found -eq 0 ]

then

: do something else

fi