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          Amber 11 SANDER                    2010
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| PMEMD implementation of SANDER, Release 11

| Run on 07/29/2017 at 10:04:58

  [-O]verwriting output

File Assignments:
|   MDIN: prod.in
|  MDOUT: prod16.out
| INPCRD: Q4QQ4-plus18-15.rst
|   PARM: Q4QQ4-plus18.parm7
| RESTRT: Q4QQ4-plus18-16.rst
|   REFC: Q4QQ4-plus18-15.rst
|  MDVEL: mdvel
|   MDEN: mden
|  MDCRD: Q4QQ4-plus18-16.crd
| MDINFO: mdinfo
|LOGFILE: logfile


 Here is the input file:

Constant pressure constant temperature production run
 &cntrl
  imin=0, irest=1, ntx=5,
  nstlim=1500000, dt=0.002,
  jfastw=4,
  ntc=2, ntf=2, ig=-1,
  ntb=2, ntp=1, taup=2.0,
  ntpr=1000, ntwx=1000,
  ntt=1, nrespa=1,
  temp0=310.0, iwrap=1,
 /


Note: ig = -1. Setting random seed based on wallclock time in microseconds
      and disabling the synchronization of random numbers between tasks
      to improve performance.


| Conditional Compilation Defines Used:
| DIRFRC_COMTRANS
| DIRFRC_EFS
| DIRFRC_NOVEC
```

| MPI
| PUBFFT
| FFTLOADBAL_2PROC
| BINTRAJ

| Largest sphere to fit in unit cell has radius =   40.299

| New format PARM file being parsed.
| Version =   1.000 Date = 06/19/17 Time = 10:07:50

| Note: 1-4 EEL scale factors are being read from the topology file.

| Note: 1-4 VDW scale factors are being read from the topology file.
| Duplicated   0 dihedrals

| Duplicated   0 dihedrals

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  1. RESOURCE   USE:
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 getting new box info from bottom of inpcrd

 NATOM =   67361 NTYPES =   12 NBONH =   44350 MBONA =   1188
 NTHETH =   24170 MTHETA =   1578 NPHIH =   5601 MPHIA =   3984
 NHPARM =   0 NPARM =   0 NNB   =   99259 NRES   =   21967
 NBONA =   1188 NTHETA =   1578 NPHIA =   3984 NUMBND =   13
 NUMANG =   30 NPTRA =   25 NATYP =   14 NPHB   =   1
 IFBOX =   1 NMXRS =   24 IFCAP =   0 NEXTRA =   0
 NCOPY =   0

| Coordinate Index Table dimensions: 18   16   18
| Direct force subcell size =   5.0176   5.0374   5.1955

    BOX TYPE: RECTILINEAR

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  2. CONTROL DATA FOR THE RUN
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default_name

General flags:
    imin   =   0, nmropt =   0

Nature and format of input:
    ntx   =   5, irest   =   1, ntrx   =   1

Nature and format of output:

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     ntxo    =       1, ntpr    =    1000, ntrx    =       1, ntwr    =    1600
     iwrap   =       1, ntwx    =    1000, ntwv    =       0, ntwe    =       0
     ioutfm  =       0, ntwprt  =       0, idecomp =       0, rbornstat=      0

Potential function:
     ntf     =       2, ntb     =       2, igb     =       0, nsnb    =      25
     ipol    =       0, gbsa    =       0, iesp    =       0
     dielc   =   1.00000, cut     =   8.00000, intdiel =   1.00000

Frozen or restrained atoms:
     ibelly  =       0, ntr     =       0

Molecular dynamics:
     nstlim  =   1500000, nscm    =      1000, nrespa  =         1
     t       =   0.00000, dt      =   0.00200, vlimit  =  20.00000

Berendsen (weak-coupling) temperature regulation:
     temp0   = 310.00000, tempi   =   0.00000, tautp   =   1.00000

Pressure regulation:
     ntp     =       1
     pres0   =   1.00000, comp    =  44.60000, taup    =   2.00000

SHAKE:
     ntc     =       2, jfastw  =       4
     tol     =   0.00001

| Intermolecular bonds treatment:
|     no_intermolecular_bonds =       1

| Energy averages sample interval:
|     ene_avg_sampling =    1000

Ewald parameters:
     verbose =       0, ew_type =       0, nbflag  =       1, use_pme =       1
     vdwmeth =       1, eedmeth =       1, netfrc  =       1
     Box X =   90.318   Box Y =   80.598   Box Z =   93.519
     Alpha =   90.000   Beta  =   90.000   Gamma =   90.000
     NFFT1 =   96       NFFT2 =   81       NFFT3 =   96
     Cutoff=    8.000   Tol   =0.100E-04
     Ewald Coefficient =  0.34864
     Interpolation order =    4

| PMEMD ewald parallel performance parameters:
|     block_fft =    0
|     fft_blk_y_divisor =    4
|     excl_recip =    0
|     excl_master =    0
|     atm_redist_freq =  320
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3. ATOMIC COORDINATES AND VELOCITIES

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default_name
 begin time read from input coords = 75693.600 ps

 Number of triangulated 3-point waters found: 0

    Sum of charges from parm topology file = -0.00000036
    Forcing neutrality...

| Dynamic Memory, Types Used:
| Reals 5564693
| Integers 2319777

| Nonbonded Pairs Initial Allocation: 959894

| Running AMBER/MPI version on 32 nodes
