Possible bug with v-rescale thermostat and md-vv

I tried the md-vv integrator in release-4-5-patches (2859895) in concert with the v-rescale (Bussi) thermostat and found some weird heating behaviour on a 900-TIP3P system that was fine with the md integrator. (.mdp file below) Is/was this thermostat known to work with md-vv?

Attached a .tpr and a tarball of input and output.

With md-vv:

<table>
<thead>
<tr>
<th>Step</th>
<th>Time</th>
<th>Lambda</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.00000</td>
<td>0.00000</td>
</tr>
</tbody>
</table>

Energies (kJ/mol)

<table>
<thead>
<tr>
<th></th>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1.56788e+04</td>
<td>-2.52945e+02</td>
<td>-3.58017e+04</td>
<td>-3.73679e+03</td>
<td>-2.41127e+04</td>
</tr>
</tbody>
</table>

Kinetic En. Total Energy Conserved En. Temperature Pres. DC (bar)

9.86312e+03 | -1.42495e+04 | -1.42495e+04 | 4.39597e+02 | -1.54019e+02 |

Pressure (bar)

-5.69569e+04

Step Time Lambda

500 1.00000 0.00000

Energies (kJ/mol)

<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>8.23626e+03</td>
<td>-2.52945e+02</td>
<td>-1.74349e+04</td>
<td>-3.27515e+03</td>
<td>-1.27267e+04</td>
</tr>
</tbody>
</table>

Kinetic En. Total Energy Conserved En. Temperature Pres. DC (bar)

4.19512e+04 | 2.92245e+04 | 2.45247e+04 | 1.86976e+03 | -1.54019e+02 |

Pressure (bar)

2.97051e+04

Writing checkpoint, step 500000 at Mon Sep 3 23:15:57 2012

Energies (kJ/mol)

<table>
<thead>
<tr>
<th></th>
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<th></th>
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</thead>
<tbody>
<tr>
<td>1.01917e+04</td>
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<td>-1.51940e+04</td>
<td>-3.02693e+03</td>
<td>-8.28214e+03</td>
</tr>
</tbody>
</table>

Kinetic En. Total Energy Conserved En. Temperature Pres. DC (bar)

5.17784e+04 | 4.34963e+04 | 4.79009e+04 | 2.30775e+03 | -1.54019e+02 |

Pressure (bar)

3.82536e+04

Writing checkpoint, step 500000 at Mon Sep 3 23:15:57 2012
Statistics over 500001 steps using 50001 frames

Energies (kJ/mol)

<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>Energies</td>
<td>9.71441e+03</td>
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<td>-1.51389e+04</td>
<td>-3.03171e+03</td>
<td>-8.70917e+03</td>
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<tr>
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<td>5.25444e+04</td>
<td>4.38352e+04</td>
<td>4.10799e+04</td>
<td>2.34189e+03</td>
<td>-1.54019e+02</td>
</tr>
<tr>
<td>Pressure</td>
<td>3.73202e+04</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Obviously this is heating massively at the start and the thermostat is totally failing to deal with it. With integrator md:

Step  Time  Lambda
0  0.00000  0.00000

Energies (kJ/mol)

<table>
<thead>
<tr>
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<tr>
<td>Energies</td>
<td>1.56788e+04</td>
<td>-2.52945e+02</td>
<td>-3.58017e+04</td>
<td>-3.73679e+03</td>
<td>-2.41127e+04</td>
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<tr>
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<td>1.30540e+04</td>
<td>-1.10587e+04</td>
<td>-1.10587e+04</td>
<td>5.81814e+02</td>
<td>-1.54019e+02</td>
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<tr>
<td>Pressure</td>
<td>-1.29542e+04</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Step  Time  Lambda
500 1.00000  0.00000

Energies (kJ/mol)

<table>
<thead>
<tr>
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<th></th>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Energies</td>
<td>4.57027e+03</td>
<td>-2.52945e+02</td>
<td>-3.01897e+04</td>
<td>-4.38326e+03</td>
<td>-3.02556e+04</td>
</tr>
<tr>
<td></td>
<td>1.07502e+04</td>
<td>-1.95054e+04</td>
<td>-1.39359e+04</td>
<td>4.79135e+02</td>
<td>-1.54019e+02</td>
</tr>
<tr>
<td>Pressure</td>
<td>3.29939e+03</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Writing checkpoint, step 500000 at Wed Aug 29 01:54:51 2012

Energies (kJ/mol)

<table>
<thead>
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</tr>
</thead>
<tbody>
<tr>
<td>Energies</td>
<td>5.72530e+03</td>
<td>-2.52945e+02</td>
<td>-3.72877e+04</td>
<td>-4.50918e+03</td>
<td>-3.63246e+04</td>
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<tr>
<td></td>
<td>6.59347e+03</td>
<td>-2.97311e+04</td>
<td>-1.25805e+04</td>
<td>2.93870e+02</td>
<td>-1.54019e+02</td>
</tr>
<tr>
<td>Pressure</td>
<td>2.93870e+02</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Statistics over 500001 steps using 50001 frames

Energies (kJ/mol)

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</tr>
</thead>
<tbody>
<tr>
<td>5.74509e+03</td>
<td>-2.52945e+02</td>
<td>-3.72807e+04</td>
<td>-4.52328e+03</td>
<td>-3.63118e+04</td>
</tr>
</tbody>
</table>

Kinetic En. | Total Energy | Conserved En. | Temperature Pres. DC (bar) |
------------|--------------|---------------|---------------------------|
| 6.58722e+03 | -2.97246e+04 | -1.32539e+04 | 2.93591e+02 | -1.54019e+02 |

Pressure (bar)

-4.77602e+01

This looks fine.

Mark

: VARIOUS PREPROCESSING OPTIONS
    ; Preprocessor information: use cpp syntax.
    ; e.g.: -I/home/joe/roe -I/home/mary/roe
    include =
    ; e.g.: -DI_Want_Cookies -DMe_Too
    define = -DPOSRES

: RUN CONTROL PARAMETERS
    integrator = md-vv
    ; Start time and timestep in ps
    tinit = 0
    dt = 0.002
    nsteps = 500000
    ; For exact run continuation or redoing part of a run
    init_step = 0
    ; Part index is updated automatically on checkpointing (keeps files separate)
    simulation_part = 1
    ; mode for center of mass motion removal
    comm-mode = linear
    ; number of steps for center of mass motion removal
    nstcomm = 10
    ; group(s) for center of mass motion removal
    comm-grps =

: LANGEVIN DYNAMICS OPTIONS
    ; Friction coefficient (amu/ps) and random seed
    bd-fric = 91
    ld-seed = 1993

: ENERGY MINIMIZATION OPTIONS
    ; Force tolerance and initial step-size
    emtol = 100
    emstep = 0.01
    ; Max number of iterations in relax_shells
    niter = 20
    ; Step size (ps^2) for minimization of flexible constraints
    fcstep = 0
    ; Frequency of steepest descents steps when doing CG
nstcgsteep = 1000
nbfgs = 10

; TEST PARTICLE INSERTION OPTIONS
rtpi = 0.05

; OUTPUT CONTROL OPTIONS
; Output frequency for coords (x), velocities (v) and forces (f)
nstxout = 0
nstvout = 0
nstfout = 0

; Output frequency for energies to log file and energy file
nstlog = 500
nstenergy = 500
nstcalcenergy = 1

; Output frequency and precision for xtc file
nstxtcout = 0
xtc-precision = 1000

; This selects the subset of atoms for the xtc file. You can
; select multiple groups. By default all atoms will be written.
xtc-grps = System

; Selection of energy groups
energygrps =

; NEIGHBORSEARCHING PARAMETERS
; nblist update frequency
nstlist = 10

; ns algorithm (simple or grid)
ns_type = grid

; Periodic boundary conditions: xyz, no, xy
pbc = xyz
periodic_molecules = no

; nblist cut-off
rlist = 1.0

; long-range cut-off for switched potentials

; OPTIONS FOR ELECTROSTATICS AND VDW
; Method for doing electrostatics
coulombtype = PME
rcoulomb-switch = 0
rcoulomb = 1.0

; Relative dielectric constant for the medium and the reaction field
epsilon_r = 1
epsilon_rf = 1

; Method for doing Van der Waals
vdwtype = switch

; cut-off lengths
rvdw_switch = 0.8
rvdw = 0.9

; Apply long range dispersion corrections for Energy and Pressure
DispCorr = enerpres

; Extension of the potential lookup tables beyond the cut-off
table-extension = 1

; Seperate tables between energy group pairs
energygrp_table =

; Spacing for the PME/PPPM FFT grid
fourierspacing =

; FFT grid size, when a value is 0 fourierspacing will be used
fourierNx = 0
fourierNy = 0
fourierNz = 0

; Ewald/PME/PPPM parameters
pme_order = 4
ewald_rtol = 1e-6
ewald_geometry = 3d
epsilon_surface = 0
optimize_fft = no

03/20/2020
IMPLICIT SOLVENT ALGORITHM

implicit_solvent = no

OPTIONS FOR WEAK COUPLING ALGORITHMS

Temperature coupling
Tcoupl = v-rescale
Groups to couple separately
tc-grps = System
Time constant (ps) and reference temperature (K)
tau-t = 1
ref-t = xxx
Pressure coupling
Pcoupl = no
Pcoupltype = Isotropic
Time constant (ps), compressibility (1/bar) and reference P (bar)
tau-p = 1
compressibility = 4.5e-5
ref-p = 1.0
Scaling of reference coordinates, No, All or COM
refcoord_scaling = No
Random seed for Andersen thermostat
anderson_seed = 815131

OPTIONS FOR QMMM calculations
QMMM = no
Groups treated Quantum Mechanically
QMMM-grps =
QM method
QMmethod =
QMMM scheme
QMMMscheme = normal
QM basis set
QMbasis =
QM charge
QMcharge =
QM multiplicity
QMmult =
Surface Hopping
SH =
CAS space options
CASorbitals =
CASElectrons =
SAon =
SAoff =
SAsteps =
Scale factor for MM charges
MMChargeScaleFactor = 1
Optimization of QM subsystem
bOPT =
bTS =

SIMULATED ANNEALING

Type of annealing for each temperature group (no/single/periodic)
annealing =
Number of time points to use for specifying annealing in each group
annealing_npoints =
List of times at the annealing points for each group
annealing_time =
Temp. at each annealing point, for each group.
annealing_temp =

GENERATE VELOCITIES FOR STARTUP RUN

gen_vel = yes
gen-temp = xxx
gen-seed = 173529

OPTIONS FOR BONDS
constraints = all-bonds
constraint_algorithm = lincs
continuation = yes
; Use successive overrelaxation to reduce the number of shake iterations
Shake-SOR = no
shake-tol = 0.0001
; Number of iterations in the final step of LINCS. 1 is fine for
; normal simulations, but use 2 to conserve energy in NVE runs.
lincs_iter = 1
lincs-warnangle = 30
Constrained bonds to Morse potentials
morse = no

: ENERGY GROUP EXCLUSIONS
Pairs of energy groups for which all non-bonded interactions are excluded
energygrp_excl =

: WALLS
Number of walls, type, atom types, densities and box-z scale factor for Ewald
nwall = 0
wall_type = 9-3
wall_r_linpot = -1
wallAtomtype =
wall_density =
wall_ewald_zfac = 3

: COM PULLING
Pull type: no, umbrella, constraint or constant_force
pull = no

: NMR refinement stuff
Distance restraints type: No, Simple or Ensemble
disre = No
Force weighting of pairs in one distance restraint: Conservative or Equal
disre-weighting = Conservative
Use sqrt of the time averaged times the instantaneous violation
disre-mixed = no
disre-fc = 1000
disre-tau = 0
Output frequency for pair distances to energy file
nstdisreout = 100
Orientation restraints: No or Yes
orire = no
Orientation restraints force constant and tau for time averaging
orire-fc = 0
orire-tau = 0
orire-fitgrp =
Output frequency for trace(SD) and S to energy file
nstorireout = 100
Dihedral angle restraints: No or Yes
dihre = no
dihre-fc = 1000

: Free energy control stuff
free-energy = no
init-lambda = 0
delta-lambda = 0
foreign_lambda =
scale-alpha = 0
sc-power = 0
sc-sigma = 0.3
couple-moltype =
couple-lambda0 = vdw-q
couple-lambda1 = vdw-q
couple-intramol = no

; Non-equilibrium MD stuff
acc-grps =
accelerate =
freezegrps =
freezedim =
cos-acceleration = 0
deform =

; Electric fields
; Format is number of terms (int) and for all terms an amplitude (real)
; and a phase angle (real)
E-x =
E-xt =
E-y =
E-yt =
E-z =
E-zt =

; User defined thingies
user1-grps =
user2-grps =
userint1 = 0
userint2 = 0
userint3 = 0
userint4 = 0
userreal1 = 0
userreal2 = 0
userreal3 = 0
userreal4 = 0

Associated revisions
Revision 5f1fd720 - 01/15/2013 04:32 PM - Mark Abraham
Velocity-verlet integrators and v-rescale are broken

Added fatal error and suggestion to upgrade GROMACS version.

Fixes #1000

Change-id: l22653fafdf0fb2f11fa772fd95bc55fc072d8c

Revision b77fa706 - 04/19/2013 06:55 AM - Michael Shirts
Some changes for md-vv extracted from 4.6

a. Fixes for the pressure in MTTK with constraints + dispersion + rerun
   - Dispersion is correctly added in rerun
   - COM motion is removed only on the second half of the timestep.
   - Now can do md-vv + rerun with multiple threads.
   - Now gives exact kinetic energy reruns for everything except MTTK, where the iterative algorithm makes exact kinetic energy impossible when nstpcouple == 1.

b. md-vv works with v-rescale and berendsen

c. Fixes a bug when pressure control in md-vv when nstcalcenergy is not a multiple of nstpcouple or nsttcouple. This bug results in boxes slowly expanding to unphysical sizes because the virial is neglected in the second half of the md-vv calculation.

Also discovered that as part of the bug, global energies were being communicated where they did not need to be when nstpcouple and nsttcouple are > 1 in the case of md-vv, so redid some of the iteration counting and global communication to fix
this all together. In the process, this simplified some of the iteration counting.

Should fix bugs #1116, #1012, #1000, #1129 in redmine.

Change-id: I1b628d03ab588c29f2eb8789e61254da49c2b6f

History

#1 - 09/14/2012 12:29 PM - Mark Abraham
I looked at this again with a system with a single particle in a harmonic potential well, and found the same kind of problem - in release-4-5-patches, md with v-rescale was conservative, and md-vv was not conservative and the sampling was obviously skewed.

#2 - 09/14/2012 02:48 PM - Michael Shirts
Yes, as I mentioned, this is fixed in 4.6, and I just need to find the time to isolate the fix and pull in from release-4-6. There is very little time during the week for me.

#3 - 01/15/2013 12:09 AM - Mark Abraham
- Status changed from New to In Progress

https://gerrit.gromacs.org/2047 introduces a fatal error to "fix" this

#4 - 01/15/2013 12:28 AM - Michael Shirts
Quick thought on this -- is Berendsen already blocked by the 4.5 code? The same problem (and fixes in 4.6) should exist in both cases.

#5 - 01/17/2013 09:49 PM - Mark Abraham
Michael Shirts wrote:

Quick thought on this -- is Berendsen already blocked by the 4.5 code? The same problem (and fixes in 4.6) should exist in both cases.

Yes, REMD has blocked Berendsen for some time. My observations in August were that md-vv & v-rescale worked in release-4-6, but clearly that needs further checking now.

#6 - 02/09/2013 06:17 PM - Mark Abraham
- Target version changed from 4.5.6 to 4.5.7

Draft https://gerrit.gromacs.org/#/c/2101/ addresses this properly

#7 - 04/29/2013 06:44 PM - Mark Abraham
- Status changed from In Progress to Resolved
- Affected version set to 4.5.5

#8 - 12/16/2013 05:38 PM - Rossen Apostolov
- Status changed from Resolved to Closed

Files

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<thead>
<tr>
<th>File</th>
<th>Size</th>
<th>Last Modified</th>
<th>Author</th>
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<td>spc900_equil_NVT.tpr</td>
<td>79.2 KB</td>
<td>09/04/2012</td>
<td>Mark Abraham</td>
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<tr>
<td>spc900_equil_NVT.tgz</td>
<td>587 KB</td>
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<td>Mark Abraham</td>
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