http://manual.gromacs.org/documentation/2018.4/user-guide/mdp-options.html by Sobereva General information Default values are given in parentheses, or listed first among choices. The first option in the list is always the default option. Units are given in square brackets. The difference between a dash and an underscore is ignored. A <u>sample mdp file</u> is available. This should be appropriate to start a normal simulation. Edit it to suit your specific needs and desires. **Preprocessing** include directories to include in your topology. Format: -I/home/john/mylib -I../otherlib define defines to pass to the preprocessor, default is no defines. You can use any defines to control options in your customized topology files. Options that act on existing top file mechanisms include -DFLEXIBLE will use flexible water instead of rigid water into your topology, this can be useful for normal mode analysis. -DPOSRES will trigger the inclusion of posre.itp into your topology, used for implementing position restraints. Run control integrator (Despite the name, this list includes algorithms that are not actually integrators over time. <u>integrator=steep</u> and all entries following it are in this category) mdA leap-frog algorithm for integrating Newton's equations of motion. md-vv A velocity Verlet algorithm for integrating Newton's equations of motion. For constant NVE simulations started from corresponding points in the same trajectory, the trajectories are analytically, but not binary, identical to the <u>integrator=md</u> leap-frog integrator. The the kinetic energy, which is determined from the whole step velocities and is therefore slightly too high. The advantage of this integrator is more accurate, reversible Nose-Hoover and Parrinello-Rahman coupling integration based on Trotter expansion, as well as (slightly too small) full step velocity output. This all comes at the cost off extra computation, especially with constraints and extra communication in parallel. Note that for nearly all production simulations the <u>integrator=md</u> integrator is accurate enough. md-vv-avek A velocity Verlet algorithm identical to <u>integrator=md-vv</u>, except that the kinetic energy is determined as the average of the two half step kinetic energies as in the <u>integrator=md</u> integrator, and this thus more accurate. With Nose-Hoover and/or Parrinello-Rahman coupling this comes with a slight increase in computational cost. sd An accurate and efficient leap-frog stochastic dynamics integrator. With constraints, coordinates needs to be constrained twice per integration step. Depending on the computational cost of the force calculation, this can take a significant part of the simulation time. The temperature for one or more groups of atoms (tcgrps) is set with ref-t, the inverse friction constant for each group is set with tau-t. The parameter tcoupl is ignored. The random generator is initialized with ld-seed. When used as a thermostat, an appropriate value for <u>tau-t</u> is 2 ps, since this results in a friction that is lower than the internal friction of water, while it is high enough to remove excess heat NOTE: temperature deviations decay twice as fast as with a Berendsen thermostat with the same <u>tau-t</u>. bd An Euler integrator for Brownian or position Langevin dynamics, the velocity is the force divided by a friction coefficient (bd-fric) plus random thermal noise (ref-t). When bd-fric is 0, the friction coefficient for each particle is calculated as mass/<u>tau-t</u>, as for the integrator <u>integrator=sd</u>. The random generator is initialized with <u>ld-seed</u>. steep A steepest descent algorithm for energy minimization. The maximum step size is emstep, the tolerance is emtol. cg A conjugate gradient algorithm for energy minimization, the tolerance is <u>emtol</u>. CG is more efficient when a steepest descent step is done every once in a while, this is determined by nstcqsteep. For a minimization prior to a normal mode analysis, which requires a very high accuracy, GROMACS should be compiled in double precision. 1-bfgs A quasi-Newtonian algorithm for energy minimization according to the low-memory Broyden-Fletcher-Goldfarb-Shanno approach. In practice this seems to converge faster than Conjugate Gradients, but due to the correction steps necessary it is not (yet) parallelized. nm Normal mode analysis is performed on the structure in the tpr file. GROMACS should be compiled in double precision. tpi Test particle insertion. The last molecule in the topology is the test particle. A trajectory must be provided to mdrun -rerun. This trajectory should not contain the molecule to be inserted. Insertions are performed nsteps times in each frame at random locations and with random orientiations of the molecule. When nstlist is larger than one, nstlist insertions are performed in a sphere with radius rtpi around a the same random location using the same pair list. Since pair list construction is expensive, one can perform several extra insertions with the same list almost for free. The random seed is set with 1d-seed. The temperature for the Boltzmann weighting is set with <u>ref-t</u>, this should match the temperature of the simulation of the original trajectory. Dispersion correction is implemented correctly for TPI. All relevant quantities are written to the file specified with mdrun -tpi. The distribution of insertion energies is written to the file specified with mdrun -tpid. No trajectory or energy file is written. Parallel TPI gives identical results to single-node TPI. For charged molecules, using PME with a fine grid is most accurate and also efficient, since the potential in the system only needs to be calculated once per frame. tpic Test particle insertion into a predefined cavity location. The procedure is the same as for <u>integrator=tpi</u>, except that one coordinate extra is read from the trajectory, which is used as the insertion location. The molecule to be inserted should be centered at 0,0,0. GROMACS does not do this for you, since for different situations a different way of centering might be optimal. Also <u>rtpi</u> sets the radius for the sphere around this location. Neighbor searching is done only once per frame, nstlist is not used. Parallel integrator=tpic gives identical results to single-rank integrator=tpic. tinit (0) [ps] starting time for your run (only makes sense for time-based integrators) dt (0.001) [ps] time step for integration (only makes sense for time-based integrators) nsteps (0) maximum number of steps to integrate or minimize, -1 is no maximum (0) The starting step. The time at an step i in a run is calculated as: $t = \underline{tinit} + \underline{dt} * (\underline{init-step} + i)$. The freeenergy lambda is calculated as: $lambda = \underline{init-lambda} + \underline{delta-lambda} * (\underline{init-step} + i)$. Also non-equilibrium MD parameters can depend on the step number. Thus for exact restarts or redoing part of a run it might be necessary to set <u>init-step</u> to the step number of the restart frame. <u>gmx convert-tpr</u> does this automatically. simulation-part (0) A simulation can consist of multiple parts, each of which has a part number. This option specifies what that number will be, which helps keep track of parts that are logically the same simulation. This option is generally useful to set only when coping with a crashed simulation where files were lost. comm-mode Linear Remove center of mass translational velocity Angular Remove center of mass translational and rotational velocity around the center of mass Linear-acceleration-correction Remove center of mass translational velocity. Correct the center of mass position assuming linear acceleration over <u>nstcomm</u> steps. This is useful for cases where an acceleration is expected on the center of mass which is nearly constant over mdp:nstcomm steps. This can occur for example when pulling on a group using an absolute reference. None No restriction on the center of mass motion nstcomm (100) [steps] frequency for center of mass motion removal comm-grps group(s) for center of mass motion removal, default is the whole system Langevin dynamics bd-fric (0) [amu ps-1] Brownian dynamics friction coefficient. When bd-fric is 0, the friction coefficient for each particle is calculated as mass/ tau-t. ld-seed (-1) [integer] used to initialize random generator for thermal noise for stochastic and Brownian dynamics. When <u>ld-seed</u> is set to -1, a pseudo random seed is used. When running BD or SD on multiple processors, each processor uses a seed equal to <a>ld-seed plus the processor number. **Energy minimization** emtol (10.0) [kJ mol-1 nm-1] the minimization is converged when the maximum force is smaller than this value emstep (0.01) [nm] initial step-size nstcgsteep (1000) [steps] frequency of performing 1 steepest descent step while doing conjugate gradient energy minimization. nbfgscorr (10) Number of correction steps to use for L-BFGS minimization. A higher number is (at least theoretically) more accurate, but slower. **Shell Molecular Dynamics** When shells or flexible constraints are present in the system the positions of the shells and the lengths of the flexible constraints are optimized at every time step until either the RMS force on the shells and constraints is less than emtol, or a maximum number of iterations <u>niter</u> has been reached. Minimization is converged when the maximum force is smaller than <u>emtol</u>. For shell MD this value should be 1.0 at most. niter (20) maximum number of iterations for optimizing the shell positions and the flexible constraints. fcstep (0) [ps^2] the step size for optimizing the flexible constraints. Should be chosen as mu/(d2V/dq2) where mu is the reduced mass of two particles in a flexible constraint and d2V/dq2 is the second derivative of the potential in the constraint direction. Hopefully this number does not differ too much between the flexible constraints, as the number of iterations and thus the runtime is very sensitive to fcstep. Try several values! Test particle insertion rtpi (0.05) [nm] the test particle insertion radius, see integrators <u>integrator=tpi</u> and <u>integrator=tpic</u> Output control nstxout (0) [steps] number of steps that elapse between writing coordinates to output trajectory file, the last coordinates are always written nstvout (0) [steps] number of steps that elapse between writing velocities to output trajectory, the last velocities are always written nstfout (0) [steps] number of steps that elapse between writing forces to output trajectory. nstlog (1000) [steps] number of steps that elapse between writing energies to the log file, the last energies are always written nstcalcenergy (100) number of steps that elapse between calculating the energies, 0 is never. This option is only relevant with dynamics. This option affects the performance in parallel simulations, because calculating energies requires global communication between all processes which can become a bottleneck at high parallelization. nstenergy (1000) [steps] number of steps that else between writing energies to energy file, the last energies are always written, should be a multiple of <u>nstcalcenergy</u>. Note that the exact sums and fluctuations over all MD steps modulo <u>nstcalcenergy</u> are stored in the energy file, so <u>gmx energy</u> can report exact energy averages and fluctuations also when <u>nstenergy</u> > 1 nstxout-compressed (0) [steps] number of steps that elapse between writing position coordinates using lossy compression compressed-x-precision (1000) [real] precision with which to write to the compressed trajectory file compressed-x-grps group(s) to write to the compressed trajectory file, by default the whole system is written (if nstxout-compressed energygrps group(s) for which to write to write short-ranged non-bonded potential energies to the energy file (not supported on GPUs) **Neighbor searching** cutoff-scheme Verlet Generate a pair list with buffering. The buffer size is automatically set based on <u>verlet-buffer-</u> tolerance, unless this is set to -1, in which case rlist will be used. This option has an explicit, exact cutoff at <u>rvdw</u> equal to <u>rcoulomb</u>, unless PME or Ewald is used, in which case <u>rcoulomb</u> > <u>rvdw</u> is allowed. Currently only cut-off, reaction-field, PME or Ewald electrostatics and plain LJ are supported. Some gmx mdrun functionality is not yet supported with the <u>cutoff-scheme=Verlet</u> scheme, but <u>gmx grompp</u> checks for this. Native GPU acceleration is only supported with cutoff-scheme=Verlet. With GPU-accelerated PME or with separate PME ranks, gmx mdrun will automatically tune the CPU/GPU load balance by scaling recoulomb and the grid spacing. This can be turned off with mdrun -notunepme. cutoffscheme=Verlet is faster than cutoff-scheme=group when there is no water, or if cutoff-scheme=group would use a pair-list buffer to conserve energy. group Generate a pair list for groups of atoms. These groups correspond to the charge groups in the topology. This was the only cut-off treatment scheme before version 4.6, and is **deprecated since 5.1**. There is no explicit buffering of the pair list. This enables efficient force calculations for water, but energy is only conserved when a buffer is explicitly added. nstlist (10) [steps] >0 Frequency to update the neighbor list. When this is 0, the neighbor list is made only once. With energy minimization the pair list will be updated for every energy evaluation when nstlist is greater than 0. With cutoff-scheme=Verlet and verlet-buffer-tolerance set, nstlist is actually a minimum value and gmx mdrun might increase it, unless it is set to 1. With parallel simulations and/or non-bonded force calculation on the GPU, a value of 20 or 40 often gives the best performance. With <u>cutoff-scheme=group</u> and non-exact cut-off's, nstlist will affect the accuracy of your simulation and it can not be chosen freely. 0 The neighbor list is only constructed once and never updated. This is mainly useful for vacuum simulations in which all particles see each other. < 0 Unused. ns-type arid Make a grid in the box and only check atoms in neighboring grid cells when constructing a new neighbor list every <u>nstlist</u> steps. In large systems grid search is much faster than simple search. simple Check every atom in the box when constructing a new neighbor list every nstlist steps (only with cutoff-scheme=group cut-off scheme). pbc xyz Use periodic boundary conditions in all directions. no Use no periodic boundary conditions, ignore the box. To simulate without cut-offs, set all cut-offs and nstlist to 0. For best performance without cut-offs on a single MPI rank, set nstlist to zero and ns-type =simple. ху Use periodic boundary conditions in x and y directions only. This works only with ns-type = grid and can be used in combination with walls. Without walls or with only one wall the system size is infinite in the z direction. Therefore pressure coupling or Ewald summation methods can not be used. These disadvantages do not apply when two walls are used. periodic-molecules no molecules are finite, fast molecular PBC can be used yes for systems with molecules that couple to themselves through the periodic boundary conditions, this requires a slower PBC algorithm and molecules are not made whole in the output verlet-buffer-tolerance (0.005) [kJ/mol/ps] Useful only with the <u>cutoff-scheme-Verlet cutoff-scheme</u>. This sets the maximum allowed error for pair interactions per particle caused by the Verlet buffer, which indirectly sets <u>rlist</u>. As both <u>nstlist</u> and the Verlet buffer size are fixed (for performance reasons), particle pairs not in the pair list can occasionally get within the cut-off distance during <u>nstlist</u> -1 steps. This causes very small jumps in the energy. In a constant-temperature ensemble, these very small energy jumps can be estimated for a given cut-off and rlist. The estimate assumes a homogeneous particle distribution, hence the errors might be slightly underestimated for multi-phase systems. (See the <u>reference manual</u> for details). For longer pair-list life-time (<u>nstlist</u> -1) * dt the buffer is overestimated, because the interactions between particles are ignored. Combined with cancellation of errors, the actual drift of the total energy is usually one to two orders of magnitude smaller. Note that the generated buffer size takes into account that the GROMACS pair-list setup leads to a reduction in the drift by a factor 10, compared to a simple particle-pair based list. Without dynamics (energy minimization etc.), the buffer is 5% of the cut-off. For NVE simulations the initial temperature is used, unless this is zero, in which case a buffer of 10% is used. For NVE simulations the tolerance usually needs to be lowered to achieve proper energy conservation on the nanosecond time scale. To override the automated buffer setting, use <u>verlet-buffer-tolerance</u> =-1 and set <u>rlist</u> manually. rlist (1) [nm] Cut-off distance for the short-range neighbor list. With the <u>cutoff-scheme=Verlet</u> <u>cutoff-scheme</u>, this is by default set by the <u>verlet-buffer-tolerance</u> option and the value of <u>rlist</u> is ignored. **Electrostatics** coulombtype Cut-off Plain cut-off with pair list radius \underline{rlist} and Coulomb cut-off $\underline{rcoulomb}$, where $\underline{rlist} >= \underline{rcoulomb}$. Ewald Classical Ewald sum electrostatics. The real-space cut-off regulomb should be equal to rlist. Use e.g. rlist =0.9, rcoulomb =0.9. The highest magnitude of wave vectors used in reciprocal space is controlled by <u>fourierspacing</u>. The relative accuracy of direct/reciprocal space is controlled by <u>ewald-rtol</u>. NOTE: Ewald scales as $O(N^3/2)$ and is thus extremely slow for large systems. It is included mainly for reference - in most cases PME will perform much better. PME Fast smooth Particle-Mesh Ewald (SPME) electrostatics. Direct space is similar to the Ewald sum, while the reciprocal part is performed with FFTs. Grid dimensions are controlled with <u>fourierspacing</u> and the interpolation order with <u>pme-order</u>. With a grid spacing of 0.1 nm and cubic interpolation the electrostatic forces have an accuracy of 2-3*10^-4. Since the error from the vdw-cutoff is larger than this you might try 0.15 nm. When running in parallel the interpolation parallelizes better than the FFT, so try decreasing grid dimensions while increasing interpolation. P3M-AD Particle-Particle Particle-Mesh algorithm with analytical derivative for for long range electrostatic interactions. The method and code is identical to SPME, except that the influence function is optimized for the grid. This gives a slight increase in accuracy. Reaction-Field Reaction field electrostatics with Coulomb cut-off $\underline{rcoulomb}$, where $\underline{rlist} >= \underline{rvdw}$. The dielectric constant beyond the cut-off is <u>epsilon-rf</u>. The dielectric constant can be set to infinity by setting <u>epsilon-rf</u> =0. Generalized-Reaction-Field Generalized reaction field with Coulomb cut-off <u>recoulomb</u>, where <u>rlist</u> >= <u>recoulomb</u>. The dielectric constant beyond the cut-off is epsilon-rf. The ionic strength is computed from the number of charged (i.e. with non zero charge) charge groups. The temperature for the GRF potential is set with ref-t. Reaction-Field-zero In GROMACS, normal reaction-field electrostatics with <u>cutoff-scheme</u> = <u>cutoff-scheme=group</u> leads to bad energy conservation. <u>coulombtype=Reaction-Field-zero</u> solves this by making the potential zero beyond the cut-off. It can only be used with an infinite dielectric constant (epsilon-rf =0), because only for that value the force vanishes at the cut-off. <u>rlist</u> should be 0.1 to 0.3 nm larger than <u>rcoulomb</u> to accommodate for the size of charge groups and diffusion between neighbor list updates. This, and the fact that table lookups are used instead of analytical functions make <u>coulombtype=Reaction-Field-zero</u> computationally more expensive than normal reaction-field. Shift Analogous to vdwtype=Shift for vdwtype. You might want to use coulombtype=Reaction-Field-zero instead, which has a similar potential shape, but has a physical interpretation and has better energies due to the exclusion correction terms. Encad-Shift The Coulomb potential is decreased over the whole range, using the definition from the Encad simulation Switch Analogous to <u>vdwtype=Switch</u> for <u>vdwtype</u>. Switching the Coulomb potential can lead to serious artifacts, advice: use <u>coulombtype=Reaction-Field-zero</u> instead. User gmx mdrun will now expect to find a file table.xvg with user-defined potential functions for repulsion, dispersion and Coulomb. When pair interactions are present, gmx mdrun also expects to find a file tablep.xvg for the pair interactions. When the same interactions should be used for non-bonded and pair interactions the user can specify the same file name for both table files. These files should contain 7 columns: the x value, f(x), -f'(x), g(x), -g'(x), h(x), -h'(x), where f(x) is the Coulomb function, g(x) the dispersion function and h(x) the repulsion function. When <u>vdwtype</u> is not set to User the values for g, -g', h and -h' are ignored. For the non-bonded interactions x values should run from 0 to the largest cut-off distance + table-extension and should be uniformly spaced. For the pair interactions the table length in the file will be used. The optimal spacing, which is used for non-user tables, is 0.002 nm when you run in mixed precision or 0.0005 nm when you run in double precision. The function value at x=0 is not important. More information is in the printed manual. PME-Switch A combination of PME and a switch function for the direct-space part (see above). recoulomb is allowed to be smaller than <u>rlist</u>. This is mainly useful constant energy simulations (note that using PME with <u>cutoff-scheme</u> = <u>cutoff-scheme=Verlet</u> will be more efficient). PME-User A combination of PME and user tables (see above). recoulomb is allowed to be smaller than rlist. The PME mesh contribution is subtracted from the user table by gmx mdrun. Because of this subtraction the user tables should contain about 10 decimal places. PME-User-Switch A combination of PME-User and a switching function (see above). The switching function is applied to final particle-particle interaction, i.e. both to the user supplied function and the PME Mesh correction part. coulomb-modifier Potential-shift-Verlet Selects Potential-shift with the Verlet cutoff-scheme, as it is (nearly) free; selects None with the group cutoff-scheme. Potential-shift Shift the Coulomb potential by a constant such that it is zero at the cut-off. This makes the potential the integral of the force. Note that this does not affect the forces or the sampling. None Use an unmodified Coulomb potential. With the group scheme this means no exact cut-off is used, energies and forces are calculated for all pairs in the pair list. rcoulomb-switch (0) [nm] where to start switching the Coulomb potential, only relevant when force or potential switching is used rcoulomb (1) [nm] distance for the Coulomb cut-off epsilon-r (1) The relative dielectric constant. A value of 0 means infinity. epsilon-rf (0) The relative dielectric constant of the reaction field. This is only used with reaction-field electrostatics. A value of 0 means infinity. Van der Waals vdwtype Cut-off Plain cut-off with pair list radius <u>rlist</u> and VdW cut-off <u>rvdw</u>, where <u>rlist</u> $\geq = rvdw$. PME Fast smooth Particle-mesh Ewald (SPME) for VdW interactions. The grid dimensions are controlled with fourierspacing in the same way as for electrostatics, and the interpolation order is controlled with pmeorder. The relative accuracy of direct/reciprocal space is controlled by ewald-rtol-li, and the specific combination rules that are to be used by the reciprocal routine are set using <u>lj-pme-comb-rule</u>. Shift This functionality is deprecated and replaced by <u>vdw-modifier</u> = Force-switch. The LJ (not Buckingham) potential is decreased over the whole range and the forces decay smoothly to zero between rvdw-switch and rvdw. The neighbor search cut-off rlist should be 0.1 to 0.3 nm larger than rvdw to accommodate for the size of charge groups and diffusion between neighbor list updates. Switch This functionality is deprecated and replaced by <u>vdw-modifier</u> = Potential-switch. The LJ (not Buckingham) potential is normal out to <u>rvdw-switch</u>, after which it is switched off to reach zero at <u>rvdw</u>. Both the potential and force functions are continuously smooth, but be aware that all switch functions will give rise to a bulge (increase) in the force (since we are switching the potential). The neighbor search cutoff <u>rlist</u> should be 0.1 to 0.3 nm larger than <u>rvdw</u> to accommodate for the size of charge groups and diffusion between neighbor list updates. Encad-Shift The LJ (not Buckingham) potential is decreased over the whole range, using the definition from the Encad simulation package. User See user for <u>coulombtype</u>. The function value at zero is not important. When you want to use LJ correction, make sure that <u>rvdw</u> corresponds to the cut-off in the user-defined function. When <u>coulombtype</u> is not set to User the values for the f and -f' columns are ignored. vdw-modifier Potential-shift-Verlet Selects Potential-shift with the Verlet cutoff-scheme, as it is (nearly) free; selects None with the group cutoff-scheme. Potential-shift Shift the Van der Waals potential by a constant such that it is zero at the cut-off. This makes the potential the integral of the force. Note that this does not affect the forces or the sampling. None Use an unmodified Van der Waals potential. With the group scheme this means no exact cut-off is used, energies and forces are calculated for all pairs in the pair list. Force-switch Smoothly switches the forces to zero between <u>rvdw-switch</u> and <u>rvdw</u>. This shifts the potential shift over the whole range and switches it to zero at the cut-off. Note that this is more expensive to calculate than a plain cut-off and it is not required for energy conservation, since Potential-shift conserves energy just as well. Potential-switch Smoothly switches the potential to zero between <u>rvdw-switch</u> and <u>rvdw</u>. Note that this introduces articifically large forces in the switching region and is much more expensive to calculate. This option should only be used if the force field you are using requires this. rvdw-switch 0. [nm] where to start switching the LJ force and possibly the potential, only relevant when force or potential switching is used rvdw (1) [nm] distance for the LJ or Buckingham cut-off DispCorr no don't apply any correction EnerPres apply long range dispersion corrections for Energy and Pressure Ener apply long range dispersion corrections for Energy only **Tables** table-extension (1) [nm] Extension of the non-bonded potential lookup tables beyond the largest cut-off distance. The value should be large enough to account for charge group sizes and the diffusion between neighbor-list updates. Without user defined potential the same table length is used for the lookup tables for the 1-4 interactions, which are always tabulated irrespective of the use of tables for the non-bonded interactions. The value of tableextension in no way affects the values of rlist, recoulomb, or rvdw. energygrp-table When user tables are used for electrostatics and/or VdW, here one can give pairs of energy groups for which seperate user tables should be used. The two energy groups will be appended to the table file name, in order of their definition in energygrps, seperated by underscores. For example, if energygrps = Na Cl Sol and energygrp-table = Na Na Cl, gmx mdrun will read table_Na_Na.xvg and table_Na_Cl.xvg in addition to the normal table.xvg which will be used for all other energy group pairs.

me-(ier-ny ier-nz (0) Highest magnitude of wave vectors in reciprocal space when using Ewald. Grid size when using PME or P3N These values override fourierspacing per direction. The best choice is powers of 2, 3, 5 and 7. Avoid large primes.
wald	order (4) Interpolation order for PME. 4 equals cubic interpolation. You might try 6/8/10 when running in parallel and simultaneously decrease grid dimension.
	(1e-5) The relative strength of the Ewald-shifted direct potential at recoulomb is given by ewald-rtol . Decreasing this will give a more accurate direct sum, but then you need more wave vectors for the reciprocal sum. d-rtol-lj (1e-3) When doing PME for VdW-interactions, ewald-rtol-lj is used to control the relative strength of the dispersion potential at rvdw in the same way as ewald-rtol controls the electrostatic potential.
J-pr	(Geometric) The combination rules used to combine VdW-parameters in the reciprocal part of LJ-PME. Geometric rules are much faster than Lorentz-Berthelot and usually the recommended choice, even when the resofthe force field uses the Lorentz-Berthelot rules. Geometric Apply geometric combination rules
valo	Lorentz-Berthelot Apply Lorentz-Berthelot combination rules d-geometry 3d
	The Ewald sum is performed in all three dimensions. The reciprocal sum is still performed in 3D, but a force and potential correction applied in the <i>z</i> dimension to produce a pseudo-2D summation. If your system has a slab geometry in the <i>x-y</i> plane you can try to increase the <i>z</i> -dimension of the box (a box height of 3 times the slab height is usually ok) and use this option.
osi	(0) This controls the dipole correction to the Ewald summation in 3D. The default value of zero means it is turne off. Turn it on by setting it to the value of the relative permittivity of the imaginary surface around your infinite system. Be careful - you shouldn't use this if you have free mobile charges in your system. This value does not affect the slab 3DC variant of the long range corrections.
em	nperature coupling no No temperature coupling. berendsen
	Temperature coupling with a Berendsen-thermostat to a bath with temperature <pre>ref-t</pre> , with time constant <pre>tau-t</pre> . Several groups can be coupled separately, these are specified in the <pre>tc-grps</pre> field separated by spaces. <pre>nose-hoover</pre> <pre>Temperature coupling using a Nose-Hoover extended ensemble. The reference temperature and coupling</pre>
	groups are selected as above, but in this case <u>tau-t</u> controls the period of the temperature fluctuations at equilibrium, which is slightly different from a relaxation time. For NVT simulations the conserved energy quantity is written to energy and log file. andersen Temperature coupling by randomizing a fraction of the particles at each timestep. Reference temperature and coupling groups are selected as above. <u>tau-t</u> is the average time between randomization of each
	molecule. Inhibits particle dynamics somewhat, but little or no ergodicity issues. Currently only implemented with velocity Verlet, and not implemented with constraints. andersen-massive Temperature coupling by randomizing all particles at infrequent timesteps. Reference temperature and coupling groups are selected as above. tau-t is the time between randomization of all molecules. Inhibits particle dynamics somewhat, but little or no ergodicity issues. Currently only implemented with velocity
	Verlet. v-rescale Temperature coupling using velocity rescaling with a stochastic term (JCP 126, 014101). This thermostat similar to Berendsen coupling, with the same scaling using tau-t, but the stochastic term ensures that a proper canonical ensemble is generated. The random seed is set with ld-seed. This thermostat works correctly even for tau-t =0. For NVT simulations the conserved energy quantity is written to the energy and log file.
	(-1) The frequency for coupling the temperature. The default value of -1 sets nsttcouple equal to nstlist , unless nstlist <=0, then a value of 10 is used. For velocity Verlet integrators nsttcouple is set to 1.
rin	(10) The number of chained Nose-Hoover thermostats for velocity Verlet integrators, the leap-frog integrator=md integrator=md integrator only supports 1. Data for the NH chain variables is not printed to the edr file by defau but can be turned on with the print-nose-hoover-chains option. -nose-hoover-chain-variables no
c-gi	Do not store Nose-Hoover chain variables in the energy file. Yes Store all positions and velocities of the Nose-Hoover chain in the energy file. groups to couple to separate temperature baths
au−t ef−t	[ps] time constant for coupling (one for each group in tc-grps), -1 means no temperature coupling
res	sure coupling no No pressure coupling. This means a fixed box size.
	Exponential relaxation pressure coupling with time constant <pre>tau-p</pre> . The box is scaled every <pre>nstpcouple</pre> steps. It has been argued that this does not yield a correct thermodynamic ensemble, but it is the most efficient way to scale a box at the beginning of a run. Parrinello-Rahman Figure 1.1. Figure 1.1. Figure 2.1. Fi
	Extended-ensemble pressure coupling where the box vectors are subject to an equation of motion. The equation of motion for the atoms is coupled to this. No instantaneous scaling takes place. As for Nose-Hoover temperature coupling the time constant taup is the period of pressure fluctuations at equilibrium. This is probably a better method when you want to apply pressure scaling during data collection, but beware that you can get very large oscillations if you are starting from a different pressure. For simulation where the exact fluctation of the NPT ensemble are important, or if the pressure coupling time is very sho it may not be appropriate, as the previous time step pressure is used in some steps of the GROMACS implementation for the current time step pressure.
	Martyna-Tuckerman-Tobias-Klein implementation, only useable with integrator=md-vv or integrator=md-vv or integrator=md-vv or <a href="integrato</td></tr><tr><td>coup</td><td>isotropic scaling, and only works without constraints. Specifies the kind of isotropy of the pressure coupling used. Each kind takes one or more values for compressibility and ref-p. Only a single value is permitted for tau-p. isotropic</td></tr><tr><td></td><td>Isotropic pressure coupling with time constant tau-p. One value each for compressibility and ref-p is required. semiisotropic Pressure coupling which is isotropic in the x and y direction, but different in the z direction. This can be useful for membrane simulations. Two values each for compressibility and ref-p are required, for x/y and z directions respectively.</td></tr><tr><td></td><td>anisotropic Same as before, but 6 values are needed for xx, yy, zz, xy/yx, xz/zx and yz/zy components, respectively. When the off-diagonal compressibilities are set to zero, a rectangular box will stay rectangular. Beware the anisotropic scaling can lead to extreme deformation of the simulation box. surface-tension</td></tr><tr><td>st<sup>,</sup></td><td>Surface tension coupling for surfaces parallel to the xy-plane. Uses normal pressure coupling for the z-direction, while the surface tension is coupled to the x/y dimensions of the box. The first ref-p value is the reference surface tension times the number of surfaces bar nm, the second value is the reference z-pressur bar. The two compressibility values are the compressibility in the x/y and z direction respectively. The value for the z-compressibility should be reasonably accurate since it influences the convergence of the surface-tension, it can also be set to zero to have a box with constant height.</td></tr><tr><td>au-r</td><td>(-1) The frequency for coupling the pressure. The default value of -1 sets nstpcouple equal to nstlist , unless nstpcouple is set to 1. (1) [ps] The time constant for pressure coupling (one value for all directions).
ompi ef-r	[bar^-1] The compressibility (NOTE: this is now really in bar^-1) For water at 1 atm and 300 K the compressibility is 4.5e-5 bar^-1. The number of required values is implied by pcoupltype. [bar] The reference pressure for coupling. The number of required values is implied by pcoupltype.
efco	The reference coordinates for position restraints are not modified. Note that with this option the virial and pressure will depend on the absolute positions of the reference coordinates.
	The reference coordinates are scaled with the scaling matrix of the pressure coupling. Scale the center of mass of the reference coordinates with the scaling matrix of the pressure coupling. The vectors of each reference coordinate to the center of mass are not scaled. Only one COM is used, even whethere are multiple molecules with position restraints. For calculating the COM of the reference coordinate
imu iece eque	in the starting configuration, periodic boundary conditions are not taken into account. ulated annealing lated annealing is controlled separately for each temperature group in GROMACS. The reference temperature is wise linear function, but you can use an arbitrary number of points for each group, and choose either a single ence or a periodic behaviour for each group. The actual annealing is performed by dynamically changing the ence temperature used in the thermostat algorithm selected, so remember that the system will usually not
ıstar	Type of annealing for each temperature group
	No simulated annealing - just couple to reference temperature value. single A single sequence of annealing points. If your simulation is longer than the time of the last point, the temperature will be coupled to this constant value after the annealing sequence has reached the last time point.
nnea	The annealing will start over at the first reference point once the last reference time is reached. This is repeated until the simulation ends. A list with the number of annealing reference/control points used for each temperature group. Use 0 for groups that are not annealed. The number of entries should equal the number of temperature groups.
	List of times at the annealing reference/control points for each group. If you are using periodic annealing, the times will be used modulo the last value, <i>i.e.</i> if the values are 0, 5, 10, and 15, the coupling will restart at the Ops value after 15ps, 30ps, 45ps, etc. The number of entries should equal the sum of the numbers given in annealin npoints.
onfo	List of temperatures at the annealing reference/control points for each group. The number of entries should equathe sum of the numbers given in annealing-npoints. used? OK, let's use an example. Assume you have two temperature groups, set the group selections to annealing periodic, the number of points of each group to annealing-npoints = 3 4, the times to annealing-times a 6 0 2 4 6 and finally temperatures to annealing-temp = 298 280 270 298 320 320 298. The first group
etwe ps, i nd tl ne su	be coupled to 298K at 0ps, but the reference temperature will drop linearly to reach 280K at 3ps, and then linearly teen 280K and 270K from 3ps to 6ps. After this is stays constant, at 270K. The second group is coupled to 298K at increases linearly to 320K at 2ps, where it stays constant until 4ps. Between 4ps and 6ps it decreases to 298K, then it starts over with the same pattern again, <i>i.e.</i> rising linearly from 298K to 320K between 6ps and 8ps. Check immary printed by gmx grompp if you are unsure!
en−v	Do not generate velocities. The velocities are set to zero when there are no velocities in the input structure file.
	Generate velocities in gmx grompp according to a Maxwell distribution at temperature gen-temp, with random seed gen-seed. This is only meaningful with integrator integrator=md. (300) [K] temperature for Maxwell distribution
Son	(-1) [integer] used to initialize random generator for random velocities, when gen-seed is set to -1, a pseudo random seed is used.
ons	Controls which bonds in the topology will be converted to rigid holonomic constraints. Note that typical rigid water models do not have bonds, but rather a specialized [settles] directive, so are not affected by this keyword. No bonds converted to constraints.
	h-bonds Convert the bonds with H-atoms to constraints. all-bonds Convert all bonds to constraints.
	h-angles Convert all bonds to constraints and convert the angles that involve H-atoms to bond-constraints. all-angles Convert all bonds to constraints and all angles to bond-constraints.
ons	Chooses which solver satisfies any non-SETTLE holonomic constraints. LINCS LINCS LINear Constraint Solver. With domain decomposition the parallel version P-LINCS is used. The accurace in set with lines-order , which sets the number of matrices in the expansion for the matrix inversion. Aft the matrix inversion correction the algorithm does an iterative correction to compensate for lengthening does not be a solved to the description of the lengthening does not be a solved to the solved to the lengthening does not be a solved to the l
	to rotation. The number of such iterations can be controlled with lines-iter . The root mean square relative constraint deviation is printed to the log file every nstlog steps. If a bond rotates more than lines warnangle in one step, a warning will be printed both to the log file and to stderr . LINCS should not be used with coupled angle constraints. SHAKE SHAKE is slightly slower and less stable than LINCS, but does work with angle constraints. The relative
ont:	tolerance is set with shake-tol , 0.0001 is a good value for "normal" MD. SHAKE does not support constraints between atoms on different nodes, thus it can not be used with domain decompositon when int charge-group constraints are present. SHAKE can not be used with energy minimization. This option was formerly known as unconstrained-start.
	apply constraints to the start configuration and reset shells yes do not apply constraints to the start configuration and do not reset shells, useful for exact coninuation and reruns
	(0.0001) relative tolerance for SHAKE s-order (4) Highest order in the expansion of the constraint coupling matrix. When constraints form triangles, an additional expansion of the same order is applied on top of the normal expansion only for the couplings within
inc	such triangles. For "normal" MD simulations an order of 4 usually suffices, 6 is needed for large time-steps with virtual sites or BD. For accurate energy minimization an order of 8 or more might be required. With domain decomposition, the cell size is limited by the distance spanned by <pre>lincs-order</pre> +1 constraints. When one wants to scale further than this limit, one can decrease <pre>lincs-order</pre> and increase <pre>lincs-iter</pre> , since the accuracy does not deteriorate when (1+ <pre>lincs-order</pre> remains constant.
inc:	(1) Number of iterations to correct for rotational lengthening in LINCS. For normal runs a single step is sufficient but for NVE runs where you want to conserve energy accurately or for accurate energy minimization you might want to increase it to 2. S-warnangle (30) [deg] maximum angle that a bond can rotate before LINCS will complain
orse	bonds are represented by a harmonic potential yes
	bonds are represented by a Morse potential rgy group exclusions gygrp-excl Pairs of energy groups for which all non-bonded interactions are excluded. An example: if you have two energy groups Protein and SOL, specifying energygrp-excl = Protein Protein SOL SOL would give only the non-bonded interactions between the protein and the solvent. This is especially useful for speeding up energy
Val	calculations with mdrun -rerun and for excluding interactions within frozen groups. Is (0) When set to 1 there is a wall at z=0, when set to 2 there is also a wall at z=z-box. Walls can only be used wit pbc =xy. When set to 2 pressure coupling and Ewald summation can be used (it is usually best to use
all.	pbc =xy. When set to 2 pressure coupling and Ewald summation can be used (it is usually best to use semiisotropic pressure coupling with the x/y compressibility set to 0, as otherwise the surface area will change). Walls interact wit the rest of the system through an optional wall-atomtype. Energy groups wallo and wall1 (finwall =2) are added automatically to monitor the interaction of energy groups with each wall. The center of material motion removal will be turned off in the z-direction. -atomtype the atom type name in the force field for each wall. By (for example) defining a special wall atom type in the
	the atom type name in the force field for each wall. By (for example) defining a special wall atom type in the topology with its own combination rules, this allows for independent tuning of the interaction of each atomtype with the walls.
all-	-type 9-3 LJ integrated over the volume behind the wall: 9-3 potential
all·	-type 9-3
able	LJ integrated over the volume behind the wall: 9-3 potential LJ integrated over the wall surface: 10-4 potential LJ integrated over the wall surface: 10-4 potential direct LJ potential with the z distance from the wall
abl€	LJ integrated over the volume behind the wall: 9-3 potential 10-4 LJ integrated over the wall surface: 10-4 potential 12-6 direct LJ potential with the z distance from the wall user defined potentials indexed with the z distance from the wall, the tables are read analogously to the energygrp-table option, where the first name is for a "normal" energy group and the second name is wallo or wall, only the dispersion and repulsion columns are used
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able all-all-defined all-all-all-all-all-all-all-all-all-all	LJ integrated over the volume behind the wall: 9-3 potential 10-4 LJ integrated over the wall surface: 10-4 potential 12-6 direct LJ potential with the z distance from the wall suser defined potentials indexed with the z distance from the wall, the tables are read analogously to the substance from the wall, the tables are read analogously to the substance from the wall, only the dispersion and repulsion columns are used -r-linpot (-1) [nm] Below this distance from the wall the potential is continued linearly and thus the force is constant. Setting this option to a postive value is especially useful for equilibration when some atoms are beyond a wall. When the value is <=0 (<0 for wall-Lype =table), a fatal error is generated when atoms are beyond a wall. -density [nm^-3/nm^-2] the number density of the atoms for each wall for wall types 9-3 and 10-4 -ewald-zfac (3) The scaling factor for the third box vector for Ewald summation only, the minimum is 2. Ewald summation can only be used with mall =2, where one should use ewald-neometry = 3dc. The empty layer in the box serve to decrease the unphysical Coulomb interaction between periodic images. M pulling that where pulling coordinate are applicable, there can be more than one (set with pull-neometal) and multiple d mdp variables will exist accordingly. Documentation references to things like pull-neometal-vec should be stood to apply to to the applicable pulling coordinate.
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	Pull along an angle defined by four groups. The angle is defined as the angle between two vectors: the vector connecting the COM of the first group to the COM of the second group and the vector connecting the COM of the third group to the COM of the fourth group. angle-axis As <u>pull-coord1-geometry=angle</u> but the second vector is given by <u>pull-coord1-vec</u> . Thus, only the two
	groups that define the first vector need to be given. dihedral Pull along a dihedral angle defined by six groups. These pairwise define three vectors: the vector connecting the COM of group 1 to the COM of group 2, the COM of group 3 to the COM of group 4, and the COM of group 5 to the COM group 6. The dihedral angle is then defined as the angle between two planes: the plane spanned by the two first vectors and the plane spanned the two last vectors. coordl-groups The group indices on which this pull coordinate will operate. The number of group indices required is geometry dependent. The first index can be 0, in which case an absolute reference of pull-coordl-origin is used. With an absolute reference the system is no longer translation invariant and one should think about what to do with the center of mass motion.
pull-	center of mass motion. coord1-dim (Y Y Y) Selects the dimensions that this pull coordinate acts on and that are printed to the output files when pull-print-components = pull-coord1-start=yes. With pull-coord1-geometry = pull-coord1- geometry=distance, only Cartesian components set to Y contribute to the distance. Thus setting this to Y Y N results in a distance in the x/y plane. With other geometries all dimensions with non-zero entries in pull-coord1- yec should be set to Y, the values for other dimensions only affect the output.
pull- pull-	(0.0 0.0 0.0) The pull reference position for use with an absolute reference. coord1-vec (0.0 0.0 0.0) The pull direction. gmx grompp normalizes the vector. coord1-start no do not modify pull-coord1-init
pull-	add the COM distance of the starting conformation to <pre>pull-coordl-init</pre> <pre>coordl-init</pre> <pre>(0.0) [nm] / [deg] The reference distance at t=0.</pre>
pull-	(0) [nm/ps] / [deg/ps] The rate of change of the reference position. coord1-k (0) [kJ mol-1 nm-2] / [kJ mol-1 nm-1] / [kJ mol-1 rad-2] / [kJ mol-1 rad-1] The force constant. For umbrella pulling this is the harmonic force constant in kJ mol-1 nm-2 (or kJ mol-1 rad-2 for angles). For constant force pulling this is the force constant of the linear potential, and thus the negative (!) of the constant force in kJ mol-1 nm-1 (or kJ mol-1 rad-1 for angles). Note that for angles the force constant is expressed in terms of radians (while pull-coord1-init and pull-coord1-rate are expressed in degrees).
AW]	(pull-k1) [kJ mol-1 nm-2] / [kJ mol-1 nm-1] / [kJ mol-1 rad-2] / [kJ mol-1 rad-1] As pull-coord1-k , but for state B. This is only used when free-energy is turned on. The force constant is then (1 - lambda) * pull-coord1-k + lambda * pull-coord1-kB . H adaptive biasing No biasing.
awh-p	Adaptively bias a reaction coordinate using the AWH method and estimate the corresponding PMF. The PMF and other AWH data are written to energy file at an interval set by awh-nstout and can be extracted with the gmx awh tool. The AWH coordinate can be multidimensional and is defined by mapping each dimension to a pull coordinate index. This is only allowed if pull-coord1-type=external-potential and pull-coord1-potential-provider = awh for the concerned pull coordinate indices.
awh-s	The applied biasing potential is the convolution of the bias function and a set of harmonic umbrella potentials (see awh-potential=umbrella below). This results in a smooth potential function and force. The resolution of the potential is set by the force constant of each umbrella, see awh1-dim1-force-constant . The potential bias is applied by controlling the position of an harmonic potential using Monte-Carlo sampling. The force constant is set with awh1-dim1-force-constant . The umbrella location is sampled using Monte-Carlo every awh-nstsample steps. There are no advantages to using an umbrella. This option is mainly for comparison and testing purposes. Share-multisim NO AWH will not share biases across simulations started with gmx mdrun option -multidir. The biases will
awh-s	With gmx mdrun and option -multidir the bias and PMF estimates for biases with awhl-share-group >0 will be shared across simulations with the biases with the same awhl-share-group value. The simulations should have the same AWH settings for sharing to make sense. gmx mdrun will check whether the simulations are technically compatible for sharing, but the user should check that bias sharing physically makes sense.
awh-n awh-n	(-1) Random seed for Monte-Carlo sampling the umbrella position, where -1 indicates to generate a seed. Only used with awh-potential=umbrella . (100000) Number of steps between printing AWH data to the energy file, should be a multiple of nstenergy . (10) Number of steps between sampling of the coordinate value. This sampling is the basis for updating the bias and estimating the PMF and other AWH observables.
awh-n	(10) The number of coordinate samples used for each AWH update. The update interval in steps is awh-nstsample times this value. (1) The number of biases, each acting on its own coordinate. The following options should be specified for each bias although below only the options for bias number 1 is shown. Options for other bias indices are obtained by replacing '1' by the bias index. **error-init**
	(10.0) [kJ mol-1] Estimated initial average error of the PMF for this bias. This value together with the given diffusion constant(s) awh1-diffusion determine the initial biasing rate. The error is obviously not known a priori. Only a rough estimate of awh1-error-init is needed however. As a general guideline, leave awh1-error-init to its default value when starting a new simulation. On the other hand, when there is a priori knowledge of the PMF (e.g. when an initial PMF estimate is provided, see the awh1-user-data option) then awh1-error-init should reflect that knowledge.
	Each bias keeps a reference weight histogram for the coordinate samples. Its size sets the magnitude of the bias function and free energy estimate updates (few samples corresponds to large updates and vice versa). Thus, its growth rate sets the maximum convergence rate. By default, there is an initial stage in which the histogram grows close to exponentially (but slower than the sampling rate). In the final stage that follows, the growth rate is linear and equal to the sampling rate (set by awh-nstsample). The initial stage is typically necessary for efficient convergence when starting a new simulation where high free energy barriers have not yet been flattened by the bias. linear As awhl-growth=exp-linear but skip the initial stage. This may be useful if there is a priori knowledge (see awhl-growth=exp-linear but skip the initial stage. This is also the setting compatible with awhl-error-init) which eliminates the need for an initial stage. This is also the setting compatible with awhl-error-init) which eliminates the need for an initial stage. This is also the setting compatible with awhl-error-init) which eliminates the need for an initial stage. This is also the setting compatible with awhl-error-init) which eliminates the need for an initial stage.
awh1-	target=local-boltzmann. equilibrate-histogram no Do not equilibrate histogram. yes
	Before entering the initial stage (see awh1-growth=exp-linear), make sure the histogram of sampled weights is following the target distribution closely enough (specifically, at least 80% of the target region needs to have a local relative error of less than 20%). This option would typically only be used when awh1-share-group > 0 and the initial configurations poorly represent the target distribution. **target** **constant** The bias is tuned towards a constant (uniform) coordinate distribution in the defined sampling interval (defined by [awh1-dim1-start, awh1-dim1-end]). **cutoff** Similar to awh1-dim1-end]). **cutoff** Similar to awh1-target=constant , but the target distribution is proportional to 1/(1 + exp(F - awh1-target=cutoff)), where F is the free energy relative to the estimated global minimum. This provides a smooth switch of a flat target distribution in regions with free energy lower than the cut-off to a Boltzmann distribution in regions with free energy higher than the cut-off. **boltzmann** The target distribution is a Boltzmann distribution with a scaled beta (inverse temperature) factor given by awh1-target-beta-scaling . E.g., a value of 0.1 would give the same coordinate distribution as sampling with a simulation temperature scaled by 10. **local-boltzmann**
awh1-	Same target distribution and use of awh1-target-beta-scaling but the convergence towards the target distribution is inherently local i.e., the rate of change of the bias only depends on the local sampling. This local convergence property is only compatible with awh1-growth=linear , since for awh1-growth=exp-linear , since for <a href="mailto:awh1-growth=ex</td></tr><tr><td></td><td>Initialize the PMF and target distribution with default values. yes Initialize the PMF and target distribution with user provided data. For awh-nbias = 1, gmx mdrun will expect a file awhinit.xvg to be present in the run directory. For multiple biases, gmx mdrun expects files awhinit2.xvg , awhinit2.xvg , etc. The file name can be changed with the -awh option. The first awhinit2.xvg , etc. The file name can be changed with the -awh option.
	awhinit1.xvg, awhinit2.xvg, etc. The file name can be changed with the -awh option. The first awhl- ndim columns of each input file should contain the coordinate values, such that each row defines a point in coordinate space. Column awhl-ndim + 1 should contain the PMF value for each point. The target distribution column can either follow the PMF (column awhl-ndim + 2) or be in the same column as written by gmx awh. share-group 0 Do not share the bias.
awh1-	Share the bias and PMF estimates within and/or between simulations. Within a simulation, the bias will be shared between biases that have the same awhl-share-group index (note that the current code does not support this). With awhl-share-group index (note that the current code does not support this). With awhl-share-group index (note that the current code does not support this). With awhl-share-group index (note that the current code does not support this). With awhl-share-group index (note that the current code does not support this). With awhl-share-group index (note that the current code does not support this). With awhl-share-multisim=yes and gmx mdrun option -multidir the bias will also be shared across simulations. Sharing may increase convergence initially, although the starting configurations can be critical, especially when sharing between many biases. Currently, positive group values should start at 1 and increase by 1 for each subsequent bias that is shared.
awh1-	(1) [integer] Number of dimensions of the coordinate, each dimension maps to 1 pull coordinate. The following options should be specified for each such dimension. Below only the options for dimension number 1 is shown. Options for other dimension indices are obtained by replacing '1' by the dimension index. -dim1-coord-provider pull The module providing the reaction coordinate for this dimension. Currently AWH can only act on pull
awh1- awh1-	coordinates. diml-coord-index (1) Index of the pull coordinate defining this coordinate dimension. diml-force-constant (0) [kJ/mol/nm^2] or [kJ/mol/rad^2] Force constant for the (convolved) umbrella potential(s) along this coordinate dimension. diml-start (0.0) [nm]/[rad] Start value of the sampling interval along this dimension. The range of allowed values depends on the relevant pull geometry (see pull-coordl-geometry). For periodic geometries awhl-diml-start greater than awhl-diml-end is allowed. The interval will then wrap around from +period/2 to -period/2.
awh1- awh1-	diml-end (0.0) [nm]/[rad] End value defining the sampling interval together with awhl-diml-start. diml-period (0.0) [nm]/[rad] The period of this reaction coordinate, use 0 when the coordinate is not periodic. diml-diffusion (1e-5) [nm^2/ps]/[rad^2/ps] Estimated diffusion constant for this coordinate dimension determining the initial biasing rate. This needs only be a rough estimate and should not critically affect the results unless it is set to something very low, leading to slow convergence, or very high, forcing the system far from equilibrium. Not
awh1-	setting this value explicitly generates a warning. diml-cover-diameter (0.0)) [nm]/[rad] Diameter that needs to be sampled by a single simulation around a coordinate value before the point is considered covered in the initial stage (see awhl-growth=exp-linear). A value > 0 ensures that for each covering there is a continuous transition of this diameter across each coordinate value. This is trivially true for independent simulations but not for for multiple bias-sharing simulations (awhl-share-group >0). For a diameter = 0, covering occurs as soon as the simulations have sampled the whole interval, which for many sharing simulations does not guarantee transitions across free energy barriers. On the other hand, when the diameter >= the sampling interval length, covering occurs when a single simulation has independently sampled the whole interval.
These descri	e mdp parameters can be used enforce the rotation of a group of atoms, e.g. a protein subunit. The reference manualibes in detail 13 different potentials that can be used to achieve such a rotation. Tion No enforced rotation will be applied. All enforced rotation options will be ignored (and if present in the mdp file, they unfortunately generate warnings).
rot-n	Apply the rotation potential specified by rot-type0 to the group of atoms given under the rot-group0 option. agroups (1) Number of rotation groups.
rot-t	Name of rotation group 0 in the index file. Type 0 (iso) Type of rotation potential that is applied to rotation group 0. Can be of of the following: iso, iso-pf, pm, pm-pf, rm, rm-pf, rm2, rm2-pf, flex, flex-t, flex2, or flex2-t. The provided HTML representation of the following: iso, iso-pf, pm, pm-pf, rm, rm-pf, rm2, rm2-pf, flex, flex-t, flex2, or flex2-t.
	(1.0 0.0 0.0) Rotation vector, will get normalized. pivot0 (0.0 0.0 0.0) Pivot point (nm) for the potentials iso, pm, rm, and rm2.
rot-k rot-s	(0) Reference rotation rate (degree/ps) of group 0.
cot-e	(0.001) Minimum value (cutoff) of Gaussian function for the force to be evaluated (for the flexible axis potentials). 2ps0 (0.0001) Value of additive constant epsilon' (nm^2) for rm2* and flex2* potentials. 2it-method0 (rmsd) Fitting method when determining the actual angle of a rotation group (can be one of rmsd, norm, or potential). 2otfit-nsteps0
rot-p rot-n rot-n	(21) For fit type potential, the number of angular positions around the reference angle for which the rotation potential is evaluated. (0.25) For fit type potential, the distance in degrees between two angular positions. (100) Output frequency (in steps) for the angle of the rotation group, as well as for the torque and the rotation potential energy.
NMI	(1000) Output frequency for per-slab data of the flexible axis potentials, i.e. angles, torques and slab centers. R refinement no ignore distance restraint information in topology file
	simple (per-molecule) distance restraints. ensemble distance restraints over an ensemble of molecules in one simulation box. Normally, one would perform ensemble averaging over multiple subsystems, each in a separate box, using mdrun -multi. Supply topol0.tpr, topol1.tpr, with different coordinates and/or velocities. The environment variable GMX_DISRE_ENSEMBLE_SIZE sets the number of systems within each ensemble (usually equal to the mdrun
	multi value). e-weighting equal divide the restraint force equally over all atom pairs in the restraint conservative the forces are the derivative of the restraint potential, this results in an weighting of the atom pairs to the
	reciprocal seventh power of the displacement. The forces are conservative when disretau is zero. e-mixed no the violation used in the calculation of the restraint force is the time-averaged violation yes the violation used in the calculation of the restraint force is the square root of the product of the time-
disre	averaged violation and the instantaneous violation
nstdi	(100) [steps] period between steps when the running time-averaged and instantaneous distances of all atom pairs involved in restraints are written to the energy file (can make the energy file very large)
orire	(0) [kJ mol] force constant for orientation restraints, which is multiplied by a (possibly) different weight factor for each restraint, can be set to zero to obtain the orientations from a free simulation
orire	(0) [ps] time constant for orientation restraints running average. A value of zero turns off time averaging. e-fitgrp fit group for orientation restraining. This group of atoms is used to determine the rotation R of the system with respect to the reference orientation. The reference orientation is the starting conformation of the first subsystem. For a protein, backbone is a reasonable choice
nstor	(100) [steps] period between steps when the running time-averaged and instantaneous orientations for all
nstor Free free-	restraints, and the molecular order tensor are written to the energy file (can make the energy file very large) energy calculations energy no Only use topology A.
Free	energy calculations energy no Only use topology A. Interpolate between topology A (lambda=0) to topology B (lambda=1) and write the derivative of the Hamiltonian with respect to lambda (as specified with dhdl-derivatives), or the Hamiltonian differences with respect to other lambda values (as specified with foreign lambda) to the energy file and/or to dhdl.xvg, where they can be processed by, for example gmx bar. The potentials, bond-lengths and angles are interpolated linearly as described in the manual. When sc-alpha is larger than zero, soft-core potential are used for the LJ and Coulomb interactions.
Free Eree-	energy calculations energy no Only use topology A. Yes Interpolate between topology A (lambda=0) to topology B (lambda=1) and write the derivative of the Hamiltonian with respect to lambda (as specified with dhdl-derivatives), or the Hamiltonian differences with respect to other lambda values (as specified with foreign lambda) to the energy file and/or to dhdl.xvg, where they can be processed by, for example gmx bar. The potentials, bond-lengths and angles are interpolated linearly as described in the manual. When sc-alpha is larger than zero, soft-core potentials are used for the LJ and Coulomb interactions. Turns on expanded ensemble simulation, where the alchemical state becomes a dynamic variable, allowing jumping between different Hamiltonians. See the expanded ensemble options for controlling how expanded ensemble simulations are performed. The different Hamiltonians used in expanded ensemble simulations are defined by the other free energy options.
Free free- free- free- free-	energy calculations energy no Only use topology A. yes Interpolate between topology A (lambda=0) to topology B (lambda=1) and write the derivative of the Hamiltonian with respect to lambda (as specified with did inderivatives), or the Hamiltonian differences with respect to other lambda values (as specified with foreign lambda) to the energy file and/or to did it. xvg., where they can be processed by, for example gmx bar. The potentials, bond-lengths and angles are interpolated linearly as described in the manual. When ac-alpha is larger than zero, soft-core potential are used for the LJ and Coulomb interactions. deed Turns on expanded ensemble simulation, where the alchemical state becomes a dynamic variable, allowing jumping between different Hamiltonians. See the expanded ensemble options for controlling how expanded ensemble simulations are performed. The different Hamiltonians used in expanded ensemble simulations are defined by the other free energy options. lambda (-1) starting value for lambda (float). Generally, this should only be used with slow growth (i.e. nonzero deltalanbda). In other cases, init_lambda_state should be specified instead. Must be greater than or equal to 0. -lambda (0) increment per time step for lambda lambda-state (-1) starting value for the lambda state (integer). Specifies which column of the lambda vector (coul_lambdas, value_lambdas, tage_lambdas, tage_lambdas, tage_lambdas, fap_lambdas, should be used. This is a zero-based index: init_lambdas_nas_lambdas, tage_lambdas, tage_lambdas, fap_lambdas, should be used. This is a zero-based index: init_lambdas_nas_lambdas, tage_lambdas, tage_lambdas, fap_lambdas, tage_lambdas,
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Free free- free- delta init- fep-1	energy calculations ***energy calculations** **energy calculations** **Interpolate between topology A (lambda=0) to topology B (lambda=1) and write the derivative of the Hamiltonian with respect to hambda (as specified with India-intervolutions), or the Hamiltonian differences with respect to other lambda values (as specified with foreign lambda) to the energy file and/or to doubt a very where they can be processed by, for example guns hat. The potentials, bond-lengths and angles are interpolated internly as described in the manual. When are along is larger than zero, soft-core potential are used for the LJ and Coulomb interactions. **derd** **Interpolated discrete Hamiltonians. See the expanded ensemble options for controlling how expanded ensemble simulations are performed. The different Hamiltonians used in expanded ensemble simulations are defined by the other free energy options. **Jorebala** (-1) starting value for lambda (float). Generally, this should only be used with slow growth (i.e. nonzero del lambda). In other cases, inst_lambda arease should be specified instead. Must be greater than or equal to 0. -1.nembda** (0) increment per time step for lambda lambda arease should be specified instead. Must be greater than or equal to 0. -1.nembda** (1) starting value for the lambda state (integer). Specifies which column of the lambda vector (coul-lambda), should be used. This is a zero-based index; inst_lambda, arease al-audidas, lemostatus elambda; inst_lambda** [array] Zero, one or more lambda values for which Delta H values will be determined and written to didLxvg every marddel; steps. Values must be between 0 and 1. Free energy differences between different lambda values for which Delta H values will be determined and written to didLxvg every marddal; steps. Values must be between 0 and 1. Only the van der Waals inter
Free free- free- delta init- delta init-	energy calculations energy calculations only use topology A. Dolly use topology A. Interpolate between topology A (lambda=0) to topology B (lambda=1) and write the derivative of the Hamiltonian with respect to lambda (as specified with dutal-dar-ex-ext-exp) or the Hamiltonian differences with respect to other lambda values (as specified with foreign lambda) to the energy file andor to died 1. veg. where they can be processed by, for example gunx bar. The potentials, bond-lengths and angles are interpolated liment's as destrobed in the manual. When as-arlein is larger than zero, soft-core potential are used for the LI and Coulomb interactions. deed Turns on expanded ensemble simulation, where the alchemical state becomes a dynamic variable, allowing jumping between different Hamiltonians. See the expanded ensemble options for controlling how expanded ensemble simulations are performed. The different Hamiltonians used in expanded ensemble simulations are defined by the other free energy options. Jambda Lambda a fact (-1) starting value for lambda (float). Generally, this should only be used with slow growth (i.e., nonzero carlea lambda). In other cases, _init_lambda_arrance, should be specified instead. Must be greater than or equal in 0. Jambda at acte (-1) starting value for the lambda state (integer). Specifies which column of the lambda vector (carle lambda) and the properties of the lambda vector (carle lambda) and the properties of the lambda vector (carle lambda) and the properties of the lambda vector (carle lambda) and the properties of the lambda vector (carle lambda) and the properties of the lambda vector (carle lambda) and the properties of the lambda vector (carle lambda) and the properties of the lambda vector (carle lambda) and the properties of the lambda vector (carle lambda) and lambda—1 states have dif
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	Include either the total or the potential energy in the dhdl file. Ontions are 'no' 'notential' or 'total'. This
separ	Include either the total or the potential energy in the dhdl file. Options are 'no', 'potential', or 'total'. This information is needed for later free energy analysis if the states of interest are at different temperatures. If all states are at the same temperature, this information is not needed. 'potential' is useful in case one is using mdrun -rerun to generate the dhdl.xvg file. When rerunning from an existing trajectory, the kinetic energy will often not be correct, and thus one must compute the residual free energy from the potential alone, with the kinetic energy component computed analytically.
	The free energy values that are calculated (as specified with the foreign lambda and dhdl-derivatives settings) are written out to a separate file, with the default name dhdl.xvg . This file can be used directly with gmx bar .
lh-hi	The free energy values are written out to the energy output file (ener.edr, in accumulated blocks at every nstenergy steps), where they can be extracted with gmx energy or used directly with gmx bar. st-size (0) If nonzero, specifies the size of the histogram into which the Delta H values (specified with foreign lambda) and the derivative dH/dl values are binned, and written to ener.edr. This can be used to save disk space while calculating free energy differences. One histogram gets written for each foreign lambda and two for the dH/dl, at
lh-hi	every nstenergy step. Be aware that incorrect histogram settings (too small size or too wide bins) can introduce errors. Do not use histograms unless you're certain you need it. st-spacing (0.1) Specifies the bin width of the histograms, in energy units. Used in conjunction with dh-hist-size . This size limits the accuracy with which free energies can be calculated. Do not use histograms unless you're certain you need it.
ıstex	The number of integration steps beween attempted moves changing the system Hamiltonian in expanded ensemble simulations. Must be a multiple of nstcalcenergy , but can be greater or less than nstdhdl .
mc-s	No Monte Carlo in state space is performed. metropolis-transition Uses the Metropolis weights to update the expanded ensemble weight of each state. Min{1,exp(-(beta_new
	u_new - beta_old u_old)} barker-transition Uses the Barker transition critera to update the expanded ensemble weight of each state i, defined by exp(-beta_new u_new)/(exp(-beta_new u_new)+exp(-beta_old u_old)) wang-landau
	Uses the Wang-Landau algorithm (in state space, not energy space) to update the expanded ensemble weights. min-variance Uses the minimum variance updating method of Escobedo et al. to update the expanded ensemble weights Weights will not be the free energies, but will rather emphasize states that need more sampling to give every appropriate.
.mc−n	uncertainty. no No Monte Carlo in state space is performed. metropolis-transition
	Randomly chooses a new state up or down, then uses the Metropolis critera to decide whether to accept or reject: Min{1,exp(-(beta_new u_new - beta_old u_old)} barker-transition Randomly chooses a new state up or down, then uses the Barker transition critera to decide whether to accept or reject: exp(-beta_new u_new)/(exp(-beta_new u_new)+exp(-beta_old u_old))
.mc-s	Uses the conditional weights of the state given the coordinate (exp(-beta_i u_i) / sum_k exp(beta_i u_i) to decide which state to move to. metropolized-gibbs Uses the conditional weights of the state given the coordinate (exp(-beta_i u_i) / sum_k exp(beta_i u_i) to decide which state to move to, EXCLUDING the current state, then uses a rejection step to ensure detailed balance. Always more efficient that Gibbs, though only marginally so in many situations, such as when only the nearest neighbors have decent phase space overlap.
	(-1) random seed to use for Monte Carlo moves in state space. When lmc-seed is set to -1, a pseudo random seed is us emperature Temperature used for acceptance/rejection for Monte Carlo moves. If not specified, the temperature of the simulation specified in the first group of ref-t is used.
,l−ra	(0.8) The cutoff for the histogram of state occupancies to be reset, and the free energy incrementor to be changed from delta to delta * wl-scale. If we define the Nratio = (number of samples at each histogram) / (average number of samples at each histogram). wl-ratio of 0.8 means that means that the histogram is only considered flat if all Nratio > 0.8 AND simultaneously all 1/Nratio > 0.8.
	(0.8) Each time the histogram is considered flat, then the current value of the Wang-Landau incrementor for the free energies is multiplied by wl-scale. Value must be between 0 and 1. wl-delta (1.0) The initial value of the Wang-Landau incrementor in kT. Some value near 1 kT is usually most efficient, though sometimes a value of 2-3 in units of kT works better if the free energy differences are large.
/1 – Or	(no) Set Wang-Landau incrementor to scale with 1/(simulation time) in the large sample limit. There is significate vidence that the standard Wang-Landau algorithms in state space presented here result in free energies getting 'burned in' to incorrect values that depend on the initial state. when wl-oneovert is true, then when the incrementor becomes less than 1/N, where N is the mumber of samples collected (and thus proportional to the data collection time, hence '1 over t'), then the Wang-Lambda incrementor is set to 1/N, decreasing every step. Once this occurs, wl-ratio is ignored, but the weights will still stop updating when the equilibration criteria set in lmc-weights-equil is achieved.
	(1) Controls the number of times that each Monte Carlo swap type is performed each iteration. In the limit of large numbers of Monte Carlo repeats, then all methods converge to Gibbs sampling. The value will generally no need to be different from 1.
	(-1) Limit Gibbs sampling to selected numbers of neighboring states. For Gibbs sampling, it is sometimes inefficient to perform Gibbs sampling over all of the states that are defined. A positive value of lmc-gibbsdelta means that only states plus or minus lmc-gibbsdelta are considered in exchanges up and down. A value of -1 means that all states are considered. For less than 100 states, it is probably not that expensive to include all states orced-nstart (0) Force initial state space sampling to generate weights. In order to come up with reasonable initial weights, the setting allows the simulation to drive from the initial to the final lambda state, with lmc-forced-nstart steps at each state before moving on to the next lambda state. If lmc-forced-nstart is sufficiently long (thousands of steps, perhaps), then the weights will be close to correct. However, in most cases, it is probably better to simply run the standard weight equilibration algorithms.
	(-1) Frequency of outputting the expanded ensemble transition matrix. A negative number means it will only be printed at the end of the simulation. *trized-transition-matrix* (no) Whether to symmetrize the empirical transition matrix. In the infinite limit the matrix will be symmetric, but will diverge with statistical noise for short timescales. Forced symmetrization, by using the matrix T_sym = 1/2
ninir	(T + transpose(T)), removes problems like the existence of (small magnitude) negative eigenvalues. (100) The min-variance strategy (option of lmc-stats is only valid for larger number of samples, and can get stuck if too few samples are used at each state. mininum-var-min is the minimum number of samples that each state that are allowed before the min-variance strategy is activated if selected.
	The initial weights (free energies) used for the expanded ensemble states. Default is a vector of zero weights. format is similar to the lambda vector settings in <pre>fep-lambdas</pre> , except the weights can be any floating point number. Units are kT. Its length must match the lambda vector lengths.
	Expanded ensemble weights continue to be updated throughout the simulation. Yes The input expanded ensemble weights are treated as equilibrated, and are not updated throughout the simulation.
	Expanded ensemble weight updating is stopped when the Wang-Landau incrementor falls below this value number-all-lambda Expanded ensemble weight updating is stopped when the number of samples at all of the lambda states is greater than this value.
	number-steps Expanded ensemble weight updating is stopped when the number of steps is greater than the level specifie by this value. number-samples Expanded ensemble weight updating is stopped when the number of total samples across all lambda states
simu'	Expanded ensemble weight updating is stopped when the number of total samples across all lambda states is greater than the level specified by this value. count-ratio Expanded ensemble weight updating is stopped when the ratio of samples at the least sampled lambda state and most sampled lambda state greater than this value. ated-tempering
sim-t	(no) Turn simulated tempering on or off. Simulated tempering is implemented as expanded ensemble sampling with different temperatures instead of different Hamiltonians. emp-low (300) [K] Low temperature for simulated tempering. emp-high
	(300) [K] High temperature for simulated tempering. ated-tempering-scaling Controls the way that the temperatures at intermediate lambdas are calculated from the temperature-lambdas part of the lambda vector.
	Linearly interpolates the temperatures using the values of temperature-lambdas , <i>i.e.</i> if sim-temp-low = 300, sim-temp-low and <a block"="" href="mailto:sim-temp-</td></tr><tr><td></td><td>Interpolates temperatures geometrically between <pre>sim-temp-low</pre> and <pre>sim-temp-high</pre>. The i:th state has temperature <pre>sim-temp-low</pre> * (sim-temp-high / sim-temp-low) raised to the power of (i/(ntemps-1)). This should give roughly equal exchange for constant heat capacity, though of course things simulations that involve protein folding have very high heat capacity peaks. exponential Interpolates temperatures exponentially between <pre>sim-temp-low</pre> and <pre>sim-temp-high</pre>. The i:th state has temperature <pre>sim-temp-low</pre> + (sim-temp-high - sim-temp-low)*((exp(temperature-lambdas))</pre></td></tr><tr><td>Non-</td><td>(i))-1)/(exp(1.0)-i)). •equilibrium MD graps groups for constant acceleration (e.g. Protein Sol) all atoms in groups Protein and Sol will experience constant</td></tr><tr><td></td><td>acceleration as specified in the accelerate line erate (0) [nm ps^-2] acceleration for acc-grps; x, y and z for each group (e.g. 0.1 0.0 0.0 -0.1 0.0 0.0 means that first group has constant acceleration of 0.1 nm ps-2 in X direction, second group the opposite).</td></tr><tr><td>Îreez</td><td>Groups that are to be frozen (<i>i.e.</i> their X, Y, and/or Z position will not be updated; <i>e.g.</i> Lipid sol). freezedim specifies for which dimension the freezing applies. To avoid spurious contibrutions to the virial and pressure due to large forces between completely frozen atoms you need to use energy group exclusions, this also saves computing time. Note that coordinates of frozen atoms are not scaled by pressure-coupling algorithms. dimensions for which groups in freezegrps should be frozen, specify <i>Y</i> or <i>N</i> for X, Y and Z and for each group</td></tr><tr><td>cos-a</td><td>(e.g. Y Y N N N N means that particles in the first group can move only in Z direction. The particles in the second group can move in any direction). (0) [nm ps^-2] the amplitude of the acceleration profile for calculating the viscosity. The acceleration is in the X direction and the magnitude is cos-acceleration cos(2 pi z/boxheight). Two terms are added to the energy file</td></tr><tr><td>lefor</td><td>(0 0 0 0 0 0) [nm ps-1] The velocities of deformation for the box elements: a(x) b(y) c(z) b(x) c(x) c(y). Each steethe box elements for which deform is non-zero are calculated as: box(ts)+(t-ts)*deform, off-diagonal elements as corrected for periodicity. The coordinates are transformed accordingly. Frozen degrees of freedom are (purposel also transformed. The time ts is set to t at the first step and at steps at which x and v are written to trajectory to</td></tr><tr><td></td><td>ensure exact restarts. Deformation can be used together with semiisotropic or anisotropic pressure coupling whe the appropriate compressibilities are set to zero. The diagonal elements can be used to strain a solid. The off-diagonal elements can be used to shear a solid or a liquid. **Tric fields**</td></tr><tr><td></td><td>ric-field-x ; electric-field-y ; electric-field-z</td></tr><tr><td></td><td>Here you can specify an electric field that optionally can be alternating and pulsed. The general expression for the field has the form of a gaussian laser pulse: <math display=">E(t) = E0 \exp\left(-(t-t0)^2/(2 \operatorname{sigma^2})\right) \cos(\operatorname{omega}(t-t0)) For example, the four parameters for direction x are set in the three fields of electric-field-x (and similar for and z) like
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