The ensemble keyword

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Purpose

- This keyword is used to set up an integration method (an integrator). The name of this keyword might be somewhat misleading, but is not very bad.

Grammar

- The number of parameters depends on the first parameter, which can be:

```
nve
nvt_ber
nvt_nhc
nvt_bdp
nvt_lan
npt_ber
heat_nhc
heat_bdp
heat_lan
```

- When the first parameter is `nve`, it means that the ensemble for the current run is NVE (micro-canonical). There is no need to further specify any other parameters. Therefore, the full command is

```
ensemble nve
```

- When the first parameter is `nvt_ber`, it means that the ensemble for the current run is NVT (canonical) generated by using the Berendsen (ber) method. In this case, one needs to specify an initial target temperature `T_1`, a final target temperature `T_2`, and a parameter `T_coup` which reflects the strength of the coupling between the system and the thermostat. The full command is

```
ensemble nvt_ber T_1 T_2 T_coup
```

The target temperature (not the instant system temperature) will vary linearly from `T_1` to `T_2` during a run.

- When the first parameter is `nvt_nhc`, it is similar to the case of `nvt_ber`, but using the Nose-Hoover chain (nhc) method.
- When the first parameter is `nvt_bdp`, it is similar to the case of `nvt_ber`, but using the Bussi-Donadio-Parrinello (bdp) method.
- When the first parameter is `nvt_lan`, it is similar to the case of `nvt_ber`, but using the Langevin (lan) method.

- When the first parameter is `npt_ber`, it means that the ensemble for the current run is NPT (isothermal–isobaric) generated by using the Berendsen (ber) method. In this case, apart from the same parameters as in the case of `nvt_ber`, one needs to further specify the pressure components in three directions `Px`, `Py`, and `Pz`, and a pressure coupling constant `P_coup`. The full command is

```
ensemble npt_ber T_1 T_2 T_coup Px Py Pz P_coup
```

- When the first parameter is `heat_nhc`, it means heating a source region and simultaneously cooling a sink region using local Nose-Hoover chain thermostats. The full command is

```
ensemble heat_nhc T T_coup delta_T label_source label_sink
```

The target temperatures in the source region with label `label_source` and the sink region with label `label_sink` are `T+delta_T` and `T-delta_T`, respectively. Therefore, the temperature difference between the two regions is twice of `delta_T`. In the command above, the parameter `T_coup` has the same meaning as in the case of `nvt_nhc`.

- When the first parameter is `heat_bdp`, it is similar to the case of `heat_nhc`, but using the Bussi-Donadio-Parrinello (bdp) method.
- When the first parameter is `heat_lan`, it is similar to the case of `heat_nhc`, but using the Langevin (lan) method.
- About the units and parameter values.
  - The units of temperature and pressure for this keyword are K and GPa, respectively.
  - The temperature coupling constant in the Berendsen method can be any positive number less than or equal to 1 and we recommend a value in the range of $[0.01, 1]$. A larger number results in a faster control of the temperature. The temperature coupling constant (the relaxation time) in the Nose-Hoover chain, BDP, and Langevin methods is in units of the time step and is recommended to be in the range of $[10, 1000]$. Here, a larger number results in a slower control of the temperature.
  - The pressure coupling constant in the Berendsen method should be a small positive number in the unit system adopted by `GPUMD`. We recommend a value in the range of $[0.0001, 0.01]$. For a stiffer material (such as diamond or graphene), one should use a smaller value.
  - In practice, all these parameters should be determined by try and error.

Examples

See the tutorials.

Caveats

- One should use one and only one instance of this keyword for each run.