The time step keyword

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Purpose

Set the time step for integration.

Grammar

• This keyword only requires a single parameter, which is the time step (in units of fs) for a run:

time_step value

Examples

To set the time step to 1 fs, add

time sten 1

before the run keyword.

Caveats

- There is also a **default value (1 fs)** for the time step. That is, if you forget to set one, a time step of 1 fs will be used.
- This keyword is **propagating**. That is, its effect will be passed from one run to the next. Most of the other keywords are **non-propagating**.

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