

## GROMACS - Feature #1026

### request for gen\_vel to work with multiple temperature coupling groups at different temperatures

10/30/2012 07:01 PM - Chris Neale

<b>Status:</b>	New
<b>Priority:</b>	Low
<b>Assignee:</b>	
<b>Category:</b>	
<b>Target version:</b>	
<b>Difficulty:</b>	uncategorized
<b>Description</b>	
<p>The output of grompp from v4.5.5 suggests that gen_vel only uses the first value given, although there is no error if multiple temperatures are listed. i.e. if I supply two temperatures to gen_vel, then I only get one message "Velocities were taken from a Maxwell distribution at X K, where X is the first listed temperature.</p> <p>Perhaps this is just an output issue with grompp. I was using the sd integrator.</p>	
<b>Related issues:</b>	
Related to GROMACS - Bug #1893: grompp fails to warn about .mdp values with t...	<b>Closed</b>

#### History

##### #1 - 11/01/2012 02:24 PM - Roland Schulz

I think this is a more general problem. Grompp accepts also multiple values for other variables (e.g. tinit or nsteps) and ignores them.

##### #2 - 12/30/2012 08:04 PM - Teemu Murtola

Is this a bug report about grompp silently accepting and ignoring some extra invalid input values (as the description suggests), or a request for it to actually do something with those values (like the title and the type suggest)?

If it is a bug report, then 5.0 could be the proper target version (and the type and title should be fixed). If we move to use the C++ options mechanism for parsing mdp options, this would likely get fixed more or less automatically.

##### #3 - 01/01/2013 03:43 AM - Chris Neale

This post was intended as an enhancement request. I did note a bug here, and that bug should probably be fixed, but I am not sure how useful it is to allow multiple temperature coupling groups and not allow multiple temperatures for velocity generation, so simply noting that the extra values are not used doesn't solve much beyond ensuring that the user knows what they are getting.

Please feel free to modify this into a bug or feature request as you see fit.

##### #4 - 11/17/2016 04:38 PM - Mark Abraham

- Related to Bug #1893: grompp fails to warn about .mdp values with the wrong type added

##### #5 - 11/17/2016 04:39 PM - Mark Abraham

The fix for [#1893](#) inadvertently made grompp complain when an mdp field had too many groups (as many users used to do for pressure coupling, which does not support groups).

The gen\_vel feature is still not implemented.