Manual fixes

Pascal Huber

20 January 2014

Contents

1 TODO Fix all things in the Tremolo-Tutorial that are obvious **1**
1.1 Gemachte Aenderungen: 1
1.2 **TODO** Noch zu machende Aenderungen: 3

2 DONE Check 1.6: Box parameters: What happens for different values in *.parameters and *.data? **4**

3 TODO [ ] Check 1.2: Check 0.0005 and 0.005. **4**

4 DONE Create new branch for that. **4**

DEADLINE: *2014-01-23 Thu*

- Created branch **manual-fix** in tremolo directory.

1 TODO Fix all things in the Tremolo-Tutorial that are obvious

SCHEDULED: *2014-01-20 Mon*

1.1 Gemachte Aenderungen:

Page 108 *Visuals shall be created every 5 time units or 10 iteration steps, whereas the particle data shall be written every 500 time units or 10*

iteration steps.
"Visuals **(argon.vis.##.[xyz,pdb,data])** shall be created . . . "

Page 109 *The optimized particle positions are written to argon.data.999.*
"The optimized particle positions are written to argon.data.999 **9**."

Page 110 *For this example we can still ignore the extra lines.*
"For this example we can still ignore the extra lines **at the top of the file**."

Page 111 *Take a look at the velocity distribution in the argon.histogram file*
"*Plot a histogram displaying the velocity distribution contained in the argon.histogram file*."

Page 112 *1.4 An alternative: The Nose-Hoover-thermostat*
"1.4 An alternative: The Nosé-Hoover-thermostat"

Page 112 *Thus, when using the Nosé-Hoover-thermostat considerations with respect to equilibration are imperative.*
"Thus, when using the Nosé-Hoover-thermostat, considerations with respect to equilibration are imperative." (Komma hinzugefuegt)

Page 113 *We begin by modifying the the optimization of the sample . . .*
"We begin by modifying **the** optimization of the sample. . . "

Page 114 *Again we work in the =argon.parameter= file and enter the thermostat after (or in place of) the thermostat:*
Again we work in the `argon.parameter` file and enter the **barostat** after (or in place of) the thermostat:

Page 115 *So go ahead and change the domain in the appropriate line*
"So go ahead and change the domain in the appropriate line **of the argon.parameters** file."

Page 115 *Change the extpressure value.*
"Change the **Pressure** value."

Page 118 *. . . but this time additionally to the external pressure we also support a custom stress tensor, . . .*
". . . but this time additionally to the external pressure we also support a custom stress tensor σ, . . . " Die Spannung mit σ zu bezeichnen, scheint Standard zu sein: Wikipedia(Stress)

Page 119 *The strain is defined as the length change ...*
"The strain ϵ is defined as the length change ..."

Page 120 *Add a 100 [t] relaxation time at the beginning ($\sigma = 0$).*
"Add a 100 [t] relaxation time ($\sigma = 0$) at the beginning **of the simulation by inserting an additional line in the =stresstensor= section of the =graphene.parameters= file.**"

Page 121 *As stated earlier the potential should not be cut off but has to to fit the linked cell structure of the domain.* "As stated earlier the potential should not be cut off but has **to** fit the linked cell structure of the domain."

Page 125 *TODO* entfernt (kann keinen Buchstabendreher entdecken).

1.2 TODO Noch zu machende Aenderungen:

Page 110 *For the integration of the particle trajectories we choose a standard verlet algorithm with a time step of 0.005 custom time units.*

Kann nicht beurteilen, ob deltaT=0.5e-3 oder deltaT=5e-3 richtig ist.
Output fuer die Geschwindigkeitsverteilung in Kapitel 1.2:
Geschwindigkeitsverteilung bei deltaT=0.5e-3
Geschwindigkeitsverteilung bei deltaT=5e-3

Page 114 Letzter Punkt in Exercises 14.5.1: Optimierung ist nicht moeglich fuer `constraint=isotropic`, wenn nur eine /secondary axis= geaendert wird.

Page 114 Das Listing unterscheidet sich vom File im `/tutorials/`-Ordner. Beispielsweise: `ensemble=NPE` im Listing und `ensemble=NPT` im File im Ornder `6sim_npt`

Page 115 *Should you attempt to start it right away, you will receive an error message.*
Ich erhalte keine Fehlermeldung, allerdings die Warnung: `Attention: BOX statement in .data file overwrites domain size data in .parameters file suggest correcting moment and angular moment with Max.-Boltz. distribution`

Page 115 Dritter Punkt in Exercises 14.6.1: *In the* `constraintmap` *change one of the secondary axis entries. Check and compare the new box values.*

Hier muss auch der `type` der `constraintmap` geaendert werden. Darueber hinaus muessen bei den sekundaeren Achsen immer Paare geaendert werden.

Page 122 Die Simulation ist fehlerhaft: Die meisten Partikel verlassen das Gebiet. Das `*.generalmeas` file enthaelt nur Nullen.

Page 129 Erhalte die folgenden Fehlermeldungen: `Error: Cannot open file: /home/neuen/tremolo/tutorial/12eam.external`
`Error: Cannot open file: /home/neuen/tremolo/tutorial/12eam.exttypes`
In den Kapiteln 14.1 bis 14.11 habe ich diese Meldungen nicht finden koennen.

2 DONE Check 1.6: Box parameters: What happens for different values in *.parameters and *.data?

`SCHEDULED:` *2014-01-20 Mon* `CLOSED:` *2014-01-20 Mon 18:11*
Erhalte die folgende Fehlermeldung, wenn die Werte der Box in `*.parameters` und in `*.data` nicht uebereinstimmen:
`Attention: BOX statement in .data file overwrites domain size data in .parameters file suggest correcting moment and angular moment with Max.-Boltz. distribution.`

3 TODO [ ] Check 1.2: Check 0.0005 and 0.005.

`SCHEDULED:` *2014-01-20 Mon*

4 DONE Create new branch for that.

`SCHEDULED:` *2014-01-20 Mon* `CLOSED:` *2014-01-19 Sun 13:12*