

todos

Pascal Huber

19 December 2013

Contents

1	Configurations	1
1.1	TODO Change passwords	1
1.2	TODO Colors in git-output	1
2	Emacs	1
2.1	Repair yasnippet config <2013-12-16 Mon>	1
2.2	Repair auto-pair config <2013-12-16 Mon>	1
2.3	Language evaluation in org mode (see http://zeekat.nl/articles/making-emacs-work-for-me.html#sec-10)	1
3	Arbeitszeiten	1
4	Aufgaben	2
4.1	TODO Go through tutorials and manual (find mistakes) . .	2
4.1.1	TODO Bemerkungen	2
4.1.2	TODO Notizen	2
4.1.3	TODO Fragen	3

1 Configurations

1.1 TODO Change passwords

Ask Christian how to do this and which passwords have to be changed.

1.2 TODO Colors in git-output

2 Emacs

2.1 Repair yasnippet config <2013-12-16 Mon>

2.2 Repair auto-pair config <2013-12-16 Mon>

2.3 Language evaluation in org mode (see <http://zeekat.nl/articles/making-emacs-work-for-me.html#sec-10>)

3 Arbeitszeiten

- 2013-12-16 Sat 16:30–2013-12-16 Mon 18:00
- 2013-12-18 Wed 17:30–2013-12-18 Wed 19:56

4 Aufgaben

4.1 TODO Go through tutorials and manual (find mistakes)

4.1.1 TODO Bemerkungen

vielleicht eine Hinweis, wie man an das Manual kommt?

page 7 Letzter Satz: missing “of” after “... detailed specification”

page 11 Erster Satz: es heisst `examples/Argon/` nicht `example/Argon/`.

page 17 Verstehe nicht den Satz in der Klammer im Abschnitt *parallelepiped*

page 105 Dritter Satz fehlendes “s” in “exist”

page 105 Erhalte Warnung bei Aufruf von tremolo in Tutorial 14.1: **WARNING:**
Definition of unit system in the tremolo file is deprecated
and may not be supported in future versions of tremolo. Define
the unit system in the .potentials file instead.

page 107 oben, es fehlt “use a” in1 *Since that introduces a discontinuity, we also second potential, which ...*

4.1.2 TODO Notizen

- Overview

Das Tremolo Projekt besteht aus zwei Funktionalitaeten: a. sequentielle Simulation b. parallele Simulation

1. Different capabilities of tremolo
 - ensembles
 - integrators
 - thermostats
2. In-depth description of the different potentials
3. Detailed specification of the syntax of options in the parameter file.

- First steps

Start a tremolo simulation. Example: Go to `tremolo/examples/Argon/` and type `tremolo argon.tremolo`. This starts the simulation specified in the `*.tremolo` file.

- Ensembles and Thermostats

Es gibt unter anderem folgende Funktionalitaeten:

1. Propagators
2. Thermostats
3. Barostats

- **TODO** Tutorial

Kopie des Ordners `/tremolo/tutorial` befindet sich auf `~/playground/`.

- **TODO** 14.1 Optimizing an initial particle setup

1. Write a `*.tremolo`-file containing:
 - * defaultpath (has to be set!)
 - * projectname (all files will carry this name)

- * comment
 - * systemofunits
 - * base magnitudes for the system of units used.
2. Write a ***.potentials**-file containing the potentials.
 - (a) particles : Contains all particles in the simulation:
 - * particle_{type}
 - * element_{name}
 - * mass
 - * sigma, sigma14, epsilon, epsilo14
 - (b) potentials to be used in between particles

4.1.3 TODO Fragen

1. ☐ Was sind Ensembles?