OpenMM Tutorial Sheet

Finding files:

```
$: cd examples
$: python testInstallation.py
```

If your installation ran without problems on your laptop:
> work on your laptop!
> Get the tutorial files from here:
https://www.mi.fu-berlin.de/w/CompMolBio/Resources

Things to add to the bashrc, if needed:

```
export PATH=/home/cocktail/ppxasjsm/local/bin:$PATH
export CPATH=/home/cocktail/ppxasjsm/local/include:$CPATH
export LIBRARY_PATH=/home/cocktail/ppxasjsm/local/lib:$LIBRARY_PATH
export LD_LIBRARY_PATH=$LIBRARY_PATH

export PYTHONPATH=$PYTHONPATH:/home/cocktail/ppxasjsm/local/lib/python2.7/site-packages/
export OPENMM_PLUGIN_DIR=/home/cocktail/ppxasjsm/local/lib/plugins
```

Solvation & Minimisation (93s on CPU):

```
$: python generateSolvatedAlanine.py
```

NVT equilibration:

Set temperature and number of equilibration steps
with 1000 equilibration steps it runs for 114.64s on CPU
Fill in the blanks for:
temperature =
nequib =

```
$: python nvtEquilibrate.py
```

Production:

If you have to run on CPU use low number of total steps if you want it to finish
Fill the blanks for:
max_iterations =
nsteps_per_iteration =

```
$: python production.py
```

add a pdbReporter and run for the second time:
https://simtk.org/api_docs/openmm/api4_1/python/classsimtk_1_1openmm_1_1app_1_1pdbreporter_1_1PDBReporter.html

REMD:

Runs for a very long time on CPU!

```
$: python REMD.py
```