FYS-4096 Computational Physics, exercise 7

Return your solution to project `exercise7` under your GitLab group for this course by Friday 5 AM.

Tag the final version with `final` keyword, and make sure to include a file `problems_solved` in the repository. The `problems_solved`-file should be a comma separated list of problems you have solved.

Problems

1. Python package with executable scripts (1 XP)

You can use your own implementation or the reference implementation for the code developed in `ex6`. Include the code in your Git repository for this exercise.

1. Modify the `setup.py` script. Include the argument

   ```
   scripts=['scripts/qdyn_laser',
            'scripts/plot_time_evolution'],
   ```

   for the `setuptools.setup` function we use in the script.

2. Make sure that your `install_requires` argument in `setup.py` reads

   ```
   install_requires=['numpy', 'scipy', 'h5py', 'matplotlib'],
   ```

3. Finally, the imports in your script `scripts/plot_time_evolution` should begin with `import matplotlib; matplotlib.use('TkAgg')` to make it work in the Taito supercluster.

2. Install the simulation code on Taito supercluster (2 XPs)

You should've received the username and password for logging into the Taito supercluster.

NEVER RUN SIMULATIONS ON THE LOGIN NODES! Always use either Taito-Shell or SLURM for running simulations.

0. Login to Taito once with ssh: `ssh username@taito.csc.fi`. This creates your home directory. Then exit with `exit`.
1. Send the git repository to Taito using, e.g., `scp`. Example usage: `scp -r mydir username@taito.csc.fi:~/`
2. Login to Taito with ssh: `ssh username@taito.csc.fi`.
3. See that your package arrived safely: `ls`

4. Load the pre-installed python environment: `ml python-env/intelpython3.5`
5. Install the simulation code and its dependencies using pip: `pip install --user -e .` If something goes wrong, removing the directory `~/.local` will delete all Python packages installed for your user.
6. Make sure your shell knows where to look for the Python packaces and the installed scripts by appending the following two lines at the end of `~/.bashrc`

   ```
   export PYTHONPATH=$HOME/.local/lib/python3.5/site-packages:$PYTHONPATH
   export PATH=$HOME/.local/bin:$PATH
   ```
7. Log out (`exit`) and login.

Verify your installation by logging into interactive Taito-Shell (from Taito) and trying to run your code:

```
$ ssh taito-shell
$ ml python-env/intelpython3.5
$ qdyn_laser ...
```

Leave your code installed on the machine. Its existence will be checked by an automatic grading system. You can remove it after you've received feedback for the exercise.

3. Launch a simulation with SLURM (2 XPs)

Create a batch job script that runs a simulation with the parameters '$\epsilon_{\max} = 0.11$', '$\omega_0 = 0.11$' and '$T_{\max} = 1000$'.

You should place the job script file in, e.g., `/wrk/<your taito username>/compphys_ex7/` and submit the job script to SLURM from within the same directory as the script. You may need to create this directory first.

Launch it via SLURM and wait for the simulation to finish. How much time did it take to run the code? Is it faster than on your PC? Write down your answers to `README.rst`.

4. Check for convergence (1 XP)

Launch multiple simulations and find parameters which quarantee convergence of your simulations with the same system parameters as in problem 3. Discuss your findings in `README.rst`.

5. Multiple simulations (4 XPs)

1. Launch multiple simulations with different laser electric field amplitudes ‘$\epsilon_{\text{max}} = 0.05 \ldots 0.11$‘ a.u. and different central frequencies ‘$\omega_0 = 0.02 \ldots 0.11$‘ a.u., but keep the pulse duration the same, ‘$T_{\text{max}} = 1000$‘ a.u. **Don't run more than a few hundred simulations in total!**
2. Go through all the simulations from step 1 and calculate their ground-state population at the end of the pulse, ‘$\left| \int_{-L}^{L} \mathrm{dx}\, \psi^*(x, t = 0)\psi(x, t = T_{\text{max}}) \right|^2$‘. What does this number describe? Answer to `README.rst`
3. Visualize the dependence of ground-state population (which you just calculated) on ‘ω_0‘ and ‘ϵ_{max}‘. Save your visualization script to `scripts/problem5_visualization.py`

6. Feedback (extra + 2 XPs)

Go provide some feedback via the following link:

https://www.webropolsurveys.com/S/DF9F7EC187FC87F9.par