A Lockstep Parallel xTB-GFN2 Implementation

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Abstract—Abstract.

I. Introduction

A. Paper overview

II. Methods

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$$a + b = \gamma \tag{1}$$

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Fig. 1: A circle representing the Sun.

In Fig. 1 you can see a common representation of the Sun, which is a star that is located at the center of the solar system.

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TABLE I: The Planets of the Solar System and Their Average Distance from the Sun

Planet	Distance (million km)
Mercury	57.9
Venus	108.2
Earth	149.6
Mars	227.9
Jupiter	778.6
Saturn	1,433.5
Uranus	2,872.5
Neptune	4,495.1

In Table I, you see the planets of the solar system and their average distance from the Sun. The distances were calculated with (1) that we presented in Section II.

III. Parallel Computing

Find out how large nbf can get, aka how many iterations the loops in electro can be. Based on that we would choose between the cpu or gpu version, or only use the cpu version if iterations are at most < 100k or such.

IV. Lockstep Parallel Electrostatics and Self-Consistent-Charges

```python
def electro(nbf, H0, P, dq, dqsh, atomicGam, shellGam,
jmat, shift):

  es = get_isotropic_electrostatic_energy(dq, dqsh,
atomicGam, shellGam, jmat, shift)

  k = 0
  h = 0.0
  for i in range(nbf):
    for j in range(i):
      h += P[i,j] * H0[k]
      k += 1
    h += P[i,i] * H0[k] * 0.5
    k += 1

  scc = es + 2.0 * h * evtoau
  return es, scc
```

Pseudo code for a lockstep implementation.

```python
def electro(nbf, H0, P, dq, dqsh, atomicGam, shellGam,
jmat, shift):
  es = get_isotropic_electrostatic_energy(dq, dqsh,
atomicGam, shellGam, jmat, shift)

  h_dev = sycl_malloc(number_of_blocks * block_size)

  ######### KERNEL ##########
  idx = block * blocksize + thread

  if (thread < block):
    h_dev[idx] = P[idx] * H0[idx]
```

```
if (thread == block):
    h_dev[idx] = P[idx] * H0[idx] * 0.5

# barrier
reduce(h_dev)
###########################

# copy hr from device to host
h = sycl_move(h_dev)

scc = es + 2.0 * h * evtoau
return es, scc
```

REFERENCES