

A17 - Soft #425

Project # 410 (Closed): Улучшение A17

Собрать старый интерфейс на риппере

25.05.2021 13:33 - Alexander Zlobin

Status:	Resolved	Start date:	25.05.2021
Priority:	Normal	Due date:	14.06.2021
Assignee:	Andrey Golovin	% Done:	100%
Category:			
Target version:			
Description			
Нужен старый интерфейс GMX-DFTB3, который можно запускать на риппере. - mpi - plumed Как вариант можете ределегировать Игорю			

History

#1 - 03.06.2021 10:54 - Andrey Golovin

Done:

export

```
LD_LIBRARY_PATH=${LD_LIBRARY_PATH}:/home/domain/data/prog-ripper/plumed-262-libtorch/lib/:/home/domain/data/prog-ripper/libtorch/lib:/home/domain/data/prog-ripper/lib
```

```
/home/domain/data/prog-ripper/gmx-5-dftb/bin/gmx
```

ldd gmx:

```
linux-vdso.so.1 (0x00007ffc9f3fc000)
```

```
libmpi.so.40 => /lib/x86_64-linux-gnu/libmpi.so.40 (0x00007f8da8f88000)
```

```
libpthread.so.0 => /lib/x86_64-linux-gnu/libpthread.so.0 (0x00007f8da8f65000)
```

```
libplumed.so => /home/domain/data/prog-ripper/plumed-262-libtorch/lib/libplumed.so (0x00007f8da8f5b000)
```

```
libdl.so.2 => /lib/x86_64-linux-gnu/libdl.so.2 (0x00007f8da8f55000)
```

```
libstdc++.so.6 => /lib/x86_64-linux-gnu/libstdc++.so.6 (0x00007f8da8d74000)
```

```
libm.so.6 => /lib/x86_64-linux-gnu/libm.so.6 (0x00007f8da8c23000)
```

```
libgomp.so.1 => /lib/x86_64-linux-gnu/libgomp.so.1 (0x00007f8da8be1000)
```

```
libgcc_s.so.1 => /lib/x86_64-linux-gnu/libgcc_s.so.1 (0x00007f8da8bc6000)
```

```
libc.so.6 => /lib/x86_64-linux-gnu/libc.so.6 (0x00007f8da89d4000)
```

```
/lib64/ld-linux-x86-64.so.2 (0x00007f8dab8e7000)
```

```
libopen-rte.so.40 => /lib/x86_64-linux-gnu/libopen-rte.so.40 (0x00007f8da891a000)
```

```
libopen-pal.so.40 => /lib/x86_64-linux-gnu/libopen-pal.so.40 (0x00007f8da886c000)
```

```
libhwloc.so.15 => /lib/x86_64-linux-gnu/libhwloc.so.15 (0x00007f8da8819000)
```

```
libplumedKernel.so => /home/domain/data/prog-ripper/plumed-262-libtorch/lib/libplumedKernel.so (0x00007f8da765f000)
```

```
libz.so.1 => /lib/x86_64-linux-gnu/libz.so.1 (0x00007f8da7643000)
```

```
libevent-2.1.so.7 => /lib/x86_64-linux-gnu/libevent-2.1.so.7 (0x00007f8da75ed000)
```

```
libutil.so.1 => /lib/x86_64-linux-gnu/libutil.so.1 (0x00007f8da75e8000)
```

```
libevent_pthreads-2.1.so.7 => /lib/x86_64-linux-gnu/libevent_pthreads-2.1.so.7 (0x00007f8da75e1000)
```

```
libudev.so.1 => /lib/x86_64-linux-gnu/libudev.so.1 (0x00007f8da75b5000)
```

```
libltdl.so.7 => /lib/x86_64-linux-gnu/libltdl.so.7 (0x00007f8da75aa000)
```

```
libtorch_cpu.so => /home/domain/data/prog-ripper/libtorch/lib/libtorch_cpu.so (0x00007f8d9f68d000)
```

libc10.so => /home/domain/data/prog-ripper/libtorch/lib/libc10.so (0x00007f8d9f60f000)

libmpi_cxx.so.40 => /lib/x86_64-linux-gnu/libmpi_cxx.so.40 (0x00007f8d9f5f1000)

libnuma.so.1 => /lib/x86_64-linux-gnu/libnuma.so.1 (0x00007f8d9f5e2000)

librt.so.1 => /lib/x86_64-linux-gnu/librt.so.1 (0x00007f8d9f5d7000)

libcudart.so.11.0 => /usr/local/cuda/lib64/libcudart.so.11.0 (0x00007f8d9f352000)

#2 - 03.06.2021 10:54 - Andrey Golovin

- *Status changed from New to Resolved*

- *% Done changed from 0 to 100*

#3 - 06.06.2021 18:01 - Alexander Zlobin

- *Status changed from Resolved to Feedback*

- *% Done changed from 100 to 50*

Illegal instruction (core dumped)

Не работает, как с плюмедом так и без

Папка

/home/domain/data/zlobin/2021/metadbench/test/tmp3/test-ripper-olddfbtb

#4 - 07.06.2021 12:46 - Andrey Golovin

можно путь для сборки tpr?

отбой, не надо. Выпадает явно раньше

#5 - 06.07.2021 09:40 - Alexander Zlobin

- *Status changed from Feedback to Resolved*

- *% Done changed from 50 to 100*

Все работает, использую, спасибо!