DEOM

FILE

This includes two-part(bose and fermi) of HEOM(Hierarchical equations of motion):

1. bose: boson bath and boson system
2. fermi: fermi bath and fermi system
3. docker: docker image builder
   1. dev: development environment with python, it will cause image size very huge.
   2. deom_mpi.sh: a bash shell help you to run the application.

and as the name of the folder indicate, 1d-corr means in that folder, you can calculate the equilibrium state of a given system, and calculate the correlation function of that. The sto_quad folder contains a stochastic algorithm to calculate quad system-bath coupling.

INSTALL

You should consider trying docker, docker image builder is in /docker folder. And note if you are in USTC, a harbor service that contains this image can be provided, you can contact us. (DO NOT ask me for docker hub things, too slow for me. If your internet condition is good enough, you can do it for me.)
In the /docker folder, we only provide Dockerfile, you have to download those software and modify version number.

1. eigen
2. folly
   1. googletest-release
   2. fmt
   3. gperftools
   4. jemalloc(get into trouble? click it!)
3. json11

DO NOT forget to modify the version number! Then you can build the image with `docker build -t deom_mpi:conda_dev .`, and you can run a container by deom_mpi.sh in /docker directory. You can change the deom_mpi:conda_dev to IMAGE: TAG you like but DO NOT forget to modify deom_mpi.sh after doing that. In docker container just build the application you need and then run it!

BRIEF

This is a HEOM calculator that utilizes the hashmap to do parallelize filter. Technical details is very simple: There are three things we need to do:

1. Store all density matrices
2. Look for the density matrix used
3. Calculate the super operator and calculate the $\dot rho^(n)_{/bf n}$

in step 1 and step 2 we will use an atomic hash map to do search things. In step 3, we can do it by using an embarrassingly parallel algorithm.

NOTE

We WON NOT provide input file samples in some applications due to that part of the work is not complete.

translation

English document is up to here, 下面是中文文档。

文件

这包括 HEOM（级联运动方程）的两部分（玻色和费米）：

1.bose：玻色子浴和玻色子系统 2. fermi：费米浴和费米系统 3. docker: docker 镜像构建器

1. dev：使用python开发环境，会导致图片体积很大。
2. deom_mpi.sh：一个帮助你运行应用程序的bash shell。

正如文件夹名称所示，1d-corr 表示在该文件夹中，您可以计算给定系统的平衡状态，并计算其相关函数。sto_quad 文件夹包含一个随机算法来计算四系统-环境耦合。

安装

您应该考虑尝试 docker，docker image builder 位于 /docker 文件夹中。请注意，如果您在中国科学技术大学，可以提供包含此图像的harbor服务，您可以联系我们。 （不要问我关于docker hub的事情，对我来说太慢了。如果你的互联网条件足够好，你可以帮我做。） 在 /docker 文件夹中，我们只提供 Dockerfile，您需要下载那些软件并修改版本号。

1. eigen
2. folly
   1. googletest-release
   2. fmt
   3. gperftools
   4. jemalloc(遇到麻烦？点击它！)
3. json11

不要忘记修改版本号！然后你可以使用`docker build -t deom_mpi:conda_dev .`构建镜像，你可以通过/docker目录下的deom_mpi.sh运行一个容器。您可以将 deom_mpi:conda_dev 更改为您喜欢的IMAGE: TAG，但不要忘记在执行此操作后修改 deom_mpi.sh。在 docker 容器中，只需构建您需要的应用程序，然后运行它！

简介

这是一个 HEOM 计算器，它利用 hashmap 进行并行化过滤。技术细节很简单： 我们需要做三件事：

1. 存储所有密度矩阵
2. 寻找使用的密度矩阵
3. 计算超算符，计算$\dot rho^(n)_{/bf n}$

在第 1 步和第 2 步中，我们将使用原子哈希映射来进行搜索。在第 3 步中，我们可以使用令人尴尬的并行算法来完成。

注意

由于部分工作未完成，我们不会在某些应用程序中提供输入文件示例。