# 自研多重网格算法小组

2025/07/14-2025/07/26

# 工作汇报

兰州大学

核科学与技术学院

2021级核物二班

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代码托管:

https://github.com/zhangxin8069/qcu.git; https://gitee.com/zhangxin8069/qcu.git;

https://github.com/zhangxin8069/PyQCU.git; https://gitee.com/zhangxin8069/PyQCU.git;

代码运行环境:

SNSC;COMPUTER-4060;X99;

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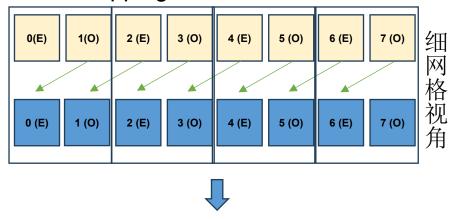
标签名	描述	提交信息
<b>♡</b> bug20	follow dev51, remember that ###Schmitt orthogonalization of complex space###:"null_vecs[i] -= torch.vdot(null_vecs[j].flatten(), null_vecs[i].flatten())/torch.vdot(null_vecs[j].flatten(), null_vecs[j].flatten())*null_vecs[j]", not "null_vecs[i] -=	Odfdf7e
<b>♡</b> dev51	follow bug19, 1. rename some var in PyQCU/pyqcu/ascend/dslash_parity.py:eye -> I; 2. referring to PyQCU/test/test-dev51-ASCEND-*, PyQCU/pyqcu/ascend/inverse.py:cg & bicgstab & give_null_vecs done! ^_^	7f18ca4 <b>1</b> 2025-07-25 16:16
<sup>©</sup> bug19	follow stab18, remember that ###vdot(,)=dot(conj(),)###!!!,do not use vdot as same as dot!!!, debug PyQCU/pyqcu/ascend/inverse.py and some PyQCU/test/test-dev50-ASCEND-WILSON-* done. www~	d597c71 <b>3</b> 2025-07-24 23:20
Stab18	follow dev50, referring to PyQCU/extern/cuda/qcu/include/ lattice_* and PyQCU/extern/cuda/qcu/src/apply_*, add "VERBOSE" to the params of qcu(cuda), some test files of test5 have been added and optimized. ^_^	7b22552 <b>3</b> 2025-07-18 20:42
♥ dev50	follow bug18, referring to PyQCU/test/test-dev50-ASCEND-* and PyQCU/pyqcu/ascend/dslash_parity.py, the bug mentioned earlier occurred due to the lack of details in parity handling: 1. The eye item should not appear in wilson_eo and wilson_oe, it should be	4ce92f2 <b>1</b> 2025-07-17 21:23
<sup>©</sup> bug18	follow dev49, there is a bug in PyQCU/pyqcu/ascend/dslash_parity.py(refer to PyQCU/test/test-dev50-ASCEND-WILSON-PARITY.py and /PyQCU/test/test-bug18-ASCEND-WILSON-PARITY.log)	a12c8e4 <b>1</b> 2025-07-15 17:40

工作一:引入奇偶分离处理,回顾如下:

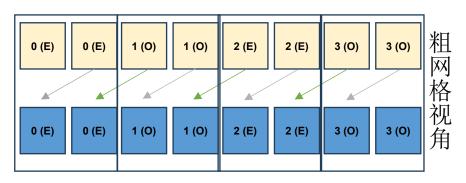
约定:

## 实际使用时为了粗化过程更加符合Dslash的数学特性 (实际引入了GMG的研究方法),将CLOVER项与 HOPPING项分开处理。

外禀非对角(称为Hopping项),以+1项为例,-1项同理



增加了外禀对角(称为Clover项),灰色标记的箭头



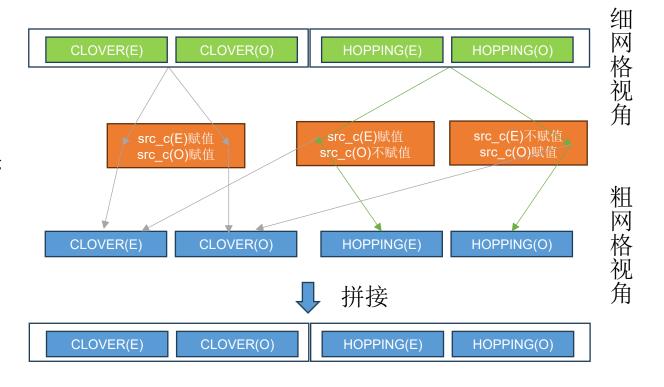
## <u>为了使粗化过程中细Hopping项产生的粗Hopping项与粗</u> Clover项分离,在此引入奇偶分离处理。



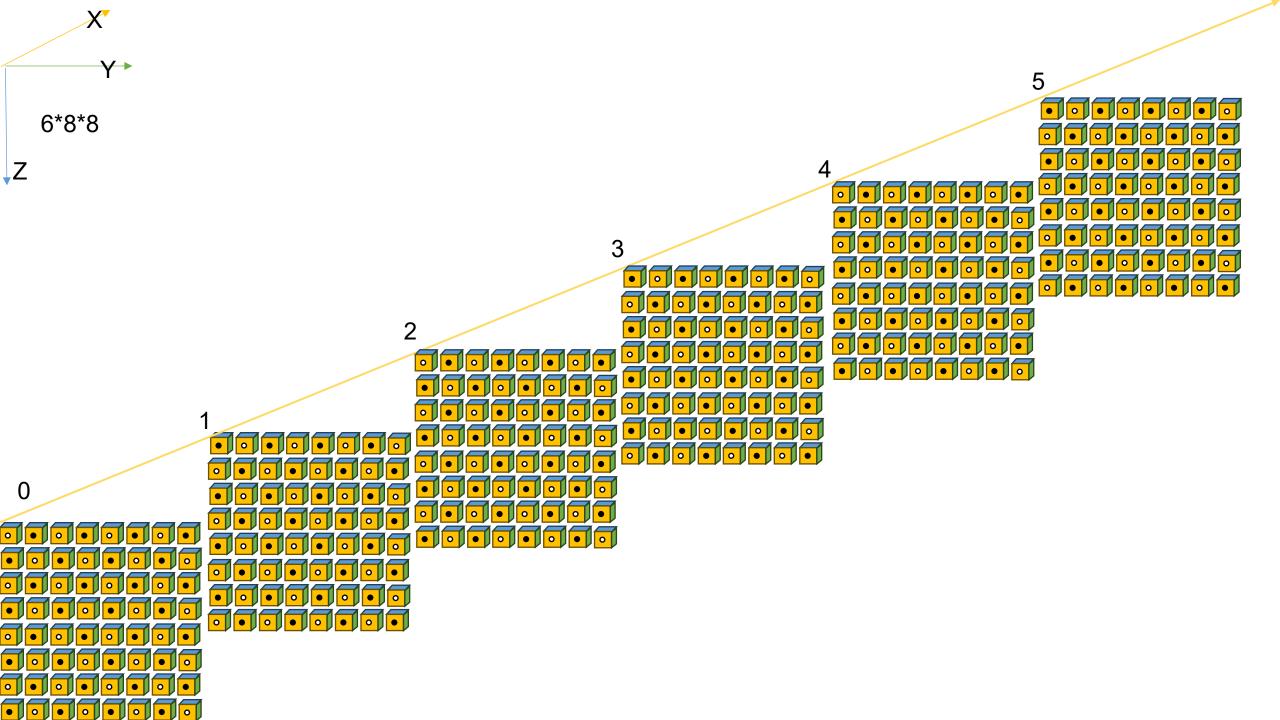
D\_c\*src\_c=R\*D\_f\*P\*src\_c=dest\_c 反复代入内禀单位的src\_c, 即for(xyzt): [1,0,0,0,0,0,0,0,0,0,0], [0,1,0,0,0,0,0,0,0,0,0], [0,0,1,0,0,0,0,0,0,0,0],

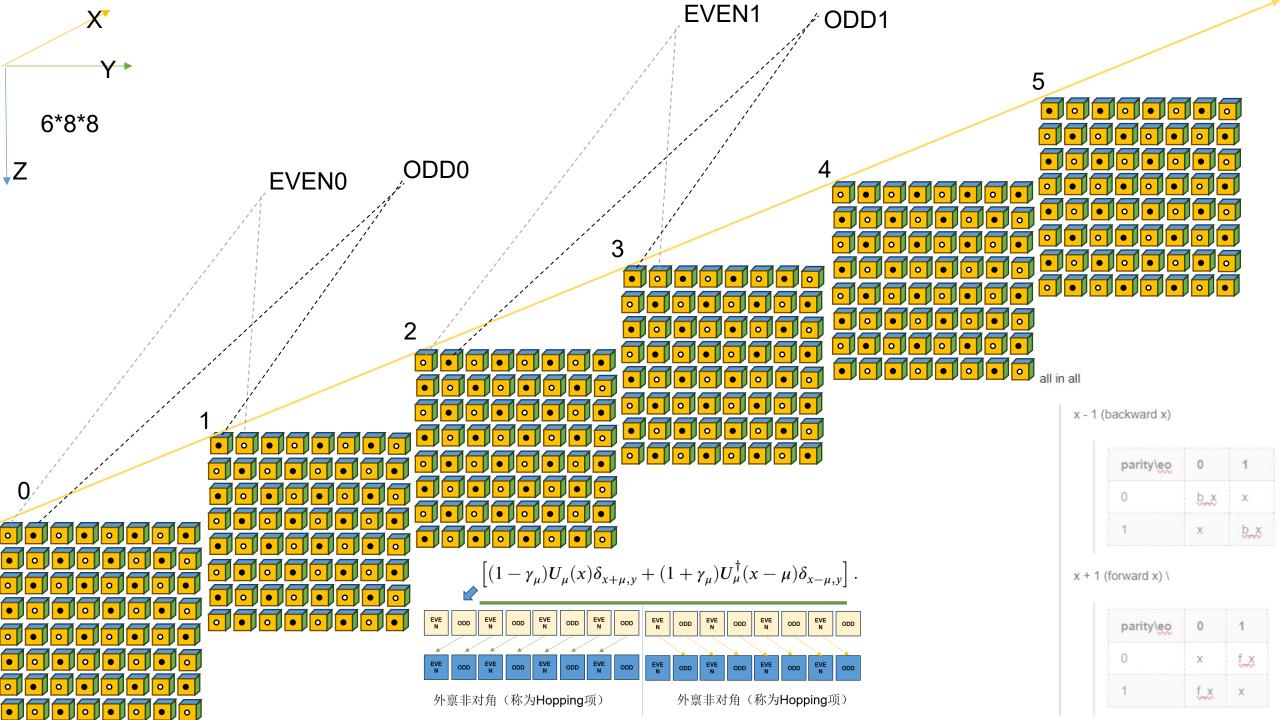
. .

来得到数值的显式的D\_c(SCSCTZYX)

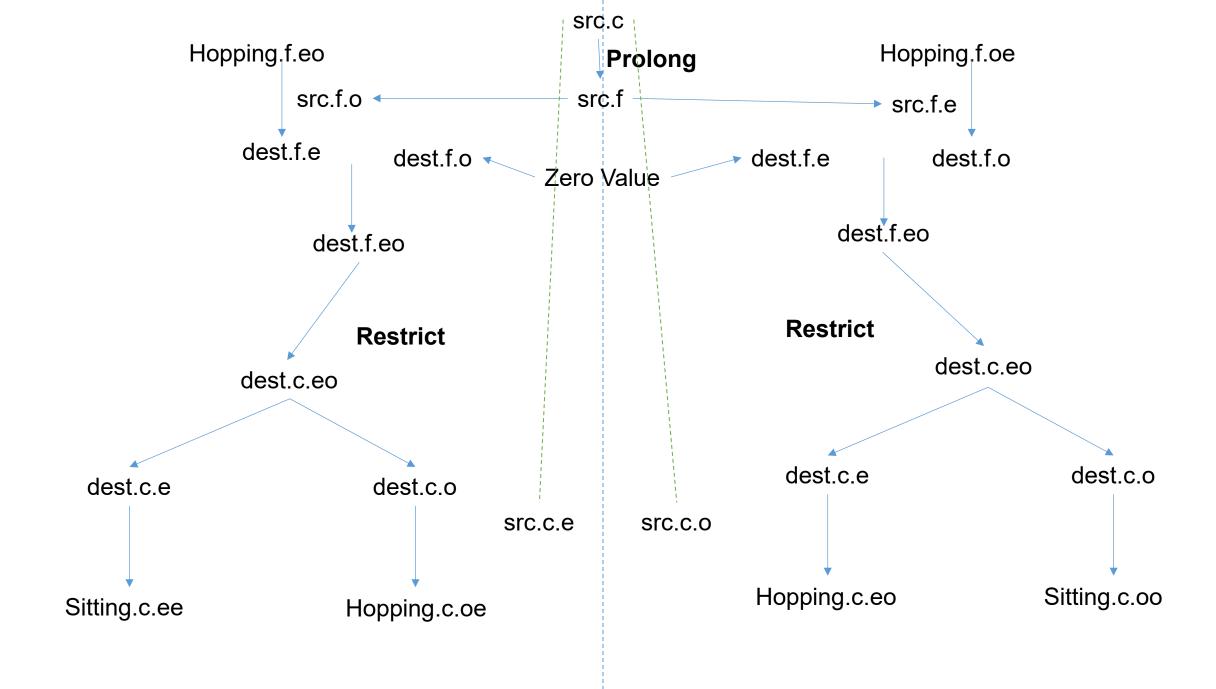


工作一:引入奇偶分离处理,思路如下:





工作一:引入奇偶分离处理,结果参考: bug18;dev50; 工作二:完成近核向量(零空间向量)构建,回顾参考"工作一:回顾",思路如下:



即寻找此Python实例没有加速比的原因

工作三: DEBUG以及参考wilson-mg(yht python版), 详情如下:

## PyQCU/test/mg\_example/bicgstab.py

bicgstab.py 2.60 KB

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```
# 计算步长 alpha

alpha = cp.vdot(cp.conj(r0), r) / cp.vdot(cp.conj(r0), Ap)

# print("alpha = ", alpha)

x += alpha * p
```

vdot(,)=dot(conj(),)

设  $\{v_1,v_2,\ldots,v_n\}$  是复数向量组,目标是构造正交组  $\{u_1,u_2,\ldots,u_n\}$ ,使得:

一键复制

$$u_k = v_k - \sum_{j=1}^{k-1} \mathrm{proj}_{u_j}(v_k), \quad$$
其中  $\mathrm{proj}_{u_j}(v_k) = rac{\langle u_j, v_k 
angle}{\langle u_j, u_j 
angle} u_j$ 

其中内积定义为(复共轭):

$$\langle x,y
angle = x^\dagger y = \sum_i \overline{x_i} y_i$$

原始数据

### PyQCU/test/mg\_example/mg.py

■ mg.py 24.26 KB

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```
# 生成近零空间向量

def near_null_vec(self, P_null_vec_coarse, coarse_dof, coarse_op):

for i in range(0, coarse_dof):

# 施密特正交化

for k in range(0, i):

P_null_vec_coarse[i, :, :, :] -= cp.vdot(cp.conj(P_null_vec_coarse[i, :, :, :]), P_null_vec_coarse[k, :, :, :])/cp.vdot(

cp.conj(P_null_vec_coarse[k, :, :, :]), P_null_vec_coarse[k, :, :, :])*P_null_vec_coarse[k, :, :, :]
```

工作三: DEBUG以及参考wilson-mg(yht python版), debug后完成了Null Space Vector的局域正交化, 结果参考:

bug20;

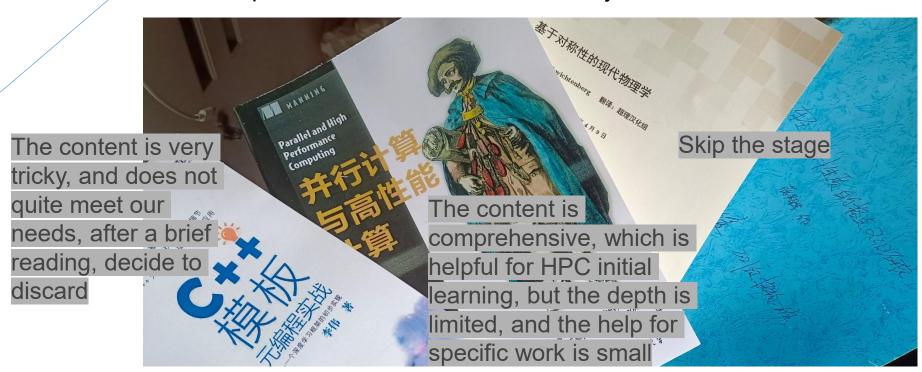
## 补充问题:

#### PyQCU/pyqcu/ascend/inverse.py

```
inverse.py 26.48 KB
                                                                                                                     原始数据按行查看
                                                                                                       一键复制
                                                                                                                                      历史
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149
            Orthonormal near-null space vectors
                                                                                <u>当使用此算法求解Null Space Vector时</u>
         \mathbf{n} \mathbf{n} \mathbf{n}
150
                                                                                ,tol的选择?
         dof = null vecs.shape[0] # Number of null space vectors
151
                                                                                太小时null vec趋近于零向量,
         null vecs = torch.rand like(null vecs)
152
                                                                                <u>太大时于随机向量无异(Av/v~=0.1,显然不近零)</u>
         for i in range(dof):
153
            # The orthogonalization of r
154
            if normalize:
155
                null_vecs[i] /= torch.norm(null_vecs[i]).item()
156
            for j in range(0, i):
157
                null_vecs[i] -= torch.vdot(null_vecs[j].flatten(), null_vecs[i].flatten())/torch.vdot(
158
                    null_vecs[j].flatten(), null_vecs[j].flatten())*null_vecs[j]
159
            if normalize:
160
                null_vecs[i] /= torch.norm(null_vecs[i]).item()
161
            # v=r-A^{-1}Ar
162
            null_vecs[i] -= bicgstab(b=matvec(null_vecs[i]), matvec=matvec, tol=tol*1000, max_iter=max_iter, x0=torch.zeros_like(null_vecs[i]),
163
                                    verbose=verbose) # tol needs to be bigger...
164
```

# Just pass.

- 1. Debug clover (multi version).--- a long time.
- 2. Test Performance.----- only a partial analysis of a single threaded program has been completed.
- 3. Improve wilson dslash.---- may more than a mouth.



# 希望大家一起讨论,指正

# 我的汇报到此结束谢谢大家!