Multigrid for Wilson Clover Fermions in Grid

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DISCLAIMER

Everything I say about Grid here is my opinion only.

OUTLINE

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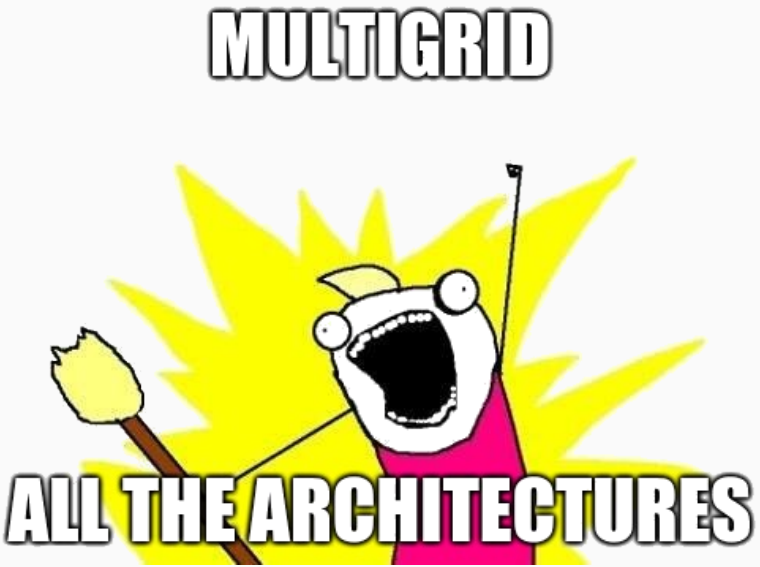
Motivation

Multigrid by now default solver algorithm for Wilson Clover fermions
Different architectures, different repositories

- DDalphaAMG library by Matthias Rottmann et al. (SSE only) [1303.1377], GitHub
- Xeon Phi implementation of DDalphaAMG by RQCD [1512.04506], [1710.07041]
- Chroma MG
- QUDA MG by Kate Clark et al. [0911.3191], GitHub
- New architectures? (see poster by Nils Meyer)

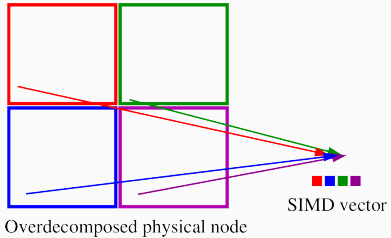
Plan: Unify in single implementation and have well-performing solver on all non-GPU architectures

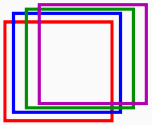
$\rightarrow$ Grid [1512.03487], GitHub


MULTIGRID
ALL THE ARCHITECTURES

Grid

- Data-parallel library (just like QDP++)
- Elegant high-level interface to QCD due to nested tensors + slim ET engine
- Satisfies all three major parallelism paradigms of CPUs
  - SIMD (big focus on site-fusing)
  - Threading with OpenMP (fork join model)
  - Message passing (MPI)
- User/Developer experience: QCD toolbox with lots of good stuff present
  - Almost like writing python/matlab code
  - Allows for rapid development





Basic building blocks for 2-level MG present [1611.06944]

```
template<class Fobj, class CComplex, int nbasis>
class Aggregation {
public:
  // ...
  Aggregation(GridBase *_CoarseGrid, GridBase *_FineGrid,
              int _checkerboard);
  void Orthogonalise();
  void CheckOrthogonal();
  void CreateSubspaceRandom(GridParallelRNG &RNG);
  void CreateSubspace(GridParallelRNG &RNG,
                      LinearOperatorBase<FineField> &hermop,
                      int nn = nbasis);
  void ProjectToSubspace(CoarseVector &CoarseVec,
                         const FineField &FineVec);
  void PromoteFromSubspace(const CoarseVector &CoarseVec,
                           FineField &FineVec);
};
```

```
template<class Fobj, class CComplex, int nbasis>
class CoarsenedMatrix :
public SparseMatrixBase<Lattice<iVector<CComplex, nbasis>>> {
public:
  // ...
  CoarsenedMatrix(GridCartesian &CoarseGrid);
  RealD M(const CoarseVector &in, CoarseVector &out);
  RealD Mdag(const CoarseVector &in, CoarseVector &out);
  void  Mdiag(const CoarseVector &in, CoarseVector &out);
  void  Mdir(const CoarseVector &in, CoarseVector &out,
             int dir, int disp);
  void  CoarsenOperator(GridBase *FineGrid,
                        LinearOperatorBase<Lattice<Fobj>> &linop,
                        Aggregation<Fobj, CComplex, nbasis> &Subspace);
};
```

But: No support for further coarsening. Requires from `CoarsenedMatrix`

- `Mdiag`
- `Mdir`

Implementation details

IMPLEMENTATION DETAILS – OVERVIEW

- Algorithmic goal: DDalphaAMG + variations
- Multilevel MG by enabling `CoarsenedMatrix` to be coarsened ✓
- Wuppertal iterative setup phase ✓
- Choice between GMRES/MR as smoother ✓
- Want to run MG preconditioner in lower precision than outer solver
  - ✓ Single precision MG / double precision outer solver trivial in Grid (`precisionChange`)
  - ? Half precision MG / double precision outer solver (no HP compute support)
- TODOs
  - Schwarz smoothing
  - Red-black preconditioning of coarse solver
  - Interface for simulation programs (Hadrons, Chroma, ...)

- MG requirement: need to preserve γ_5-hermiticity of D/chirality on coarser grids
- Grid's coarsening ecosystem is not (yet?) aware of internal dofs of a site spinor

```
typedef Lattice<iScalar<iVector<iVector<vComplex, Nc>, Ns> > >           FineVector;
typedef Lattice<iVector<iScalar<iScalar<vComplex> > >, nbasis> > CoarseVector;
```

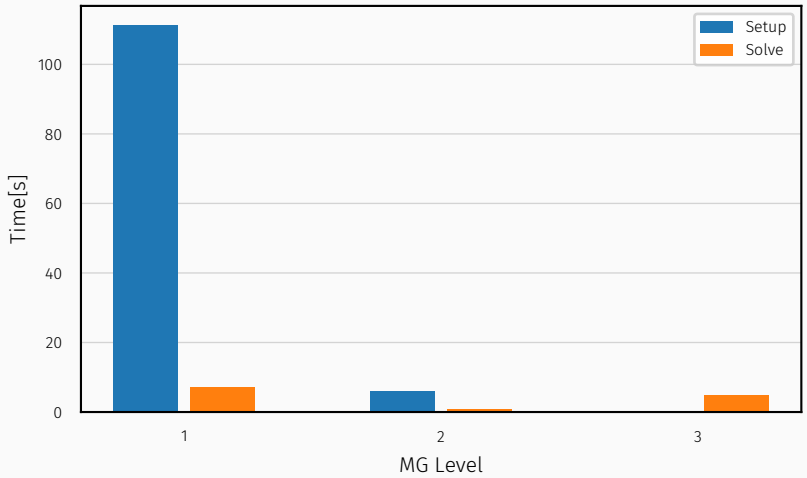
  ⟶ Forces us to do explicit chiral doubling of the null-space vectors, i.e., create $2N$ vectors out of N by using chiral projectors

$$v_i = \frac{1+\gamma_5}{2} v_{0,i}, \quad v_{i+N} = \frac{1-\gamma_5}{2} v_{0,i}$$

- Doubles memory requirement for null-space vectors w.r.t. DDalphaAMG for same coarse-grid size + means more work in setup
- Something in the pipeline ⟶ WIP

Performance

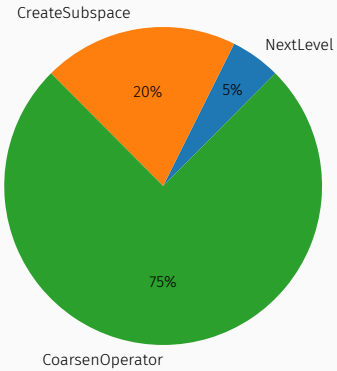
Runtime distribution using DDalphaAMG default parameters



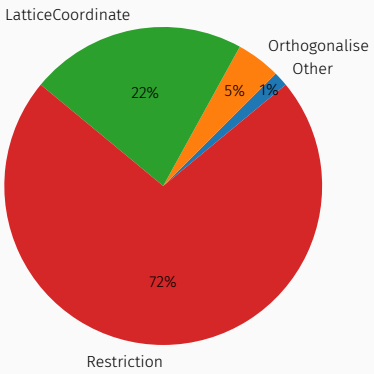
Clearly dominated by setup on finest level

Runtime distribution using DDalphaAMG default parameters: Setup

Setup



Setup – CoarsenOperator



Note: This is vanilla Grid code

PERFORMANCE – RESTRICTION OPERATOR

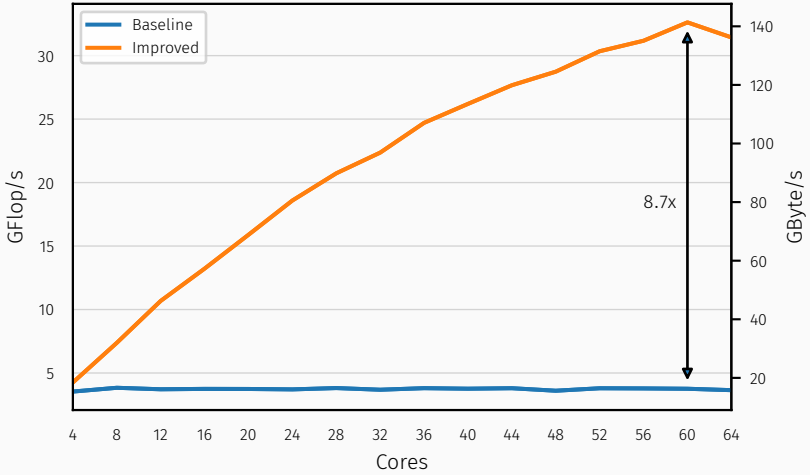
```
parallel_for(int sf=0; sf<fine->oSites(); sf++){
  // ...
  PARALLEL_CRITICAL
  for(int i=0; i<nbasis; i++)
    coarseData._odata[sc](i) = coarseData._odata[sc](i)
    + innerProduct(Basis[i]._odata[sf], fineData._odata[sf]);
  // ...
}
```

Baseline: Critical region is the problem, code basically runs serial

```
// ...
parallel_for(int sc=0; sc<coarse->oSites(); sc++) {
  for(auto sf : lookUpTable[sc]) {
    for(int i=0; i<nbasis; i++) {
      coarseData._odata[sc](i) = coarseData._odata[sc](i)
      + innerProduct(Basis[i]._odata[sf], fineData._odata[sf]);
    }
  }
}
```

Improvement: Do index calculation serially and thread calculation over coarse sites, not fine

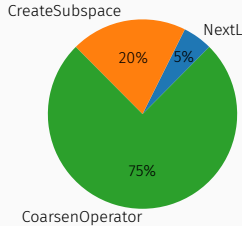
Implications on performance

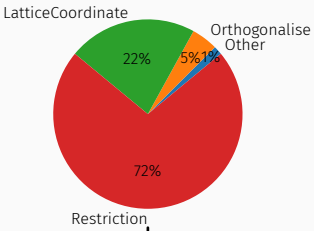


Lack of sustained memory bandwidth stems from irregular access pattern → WIP

PERFORMANCE – SETUP AFTER IMPROVEMENT OF RESTRICTION

Before



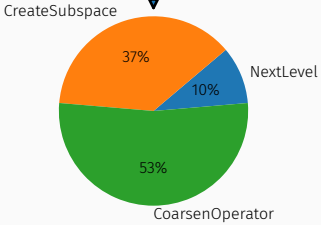


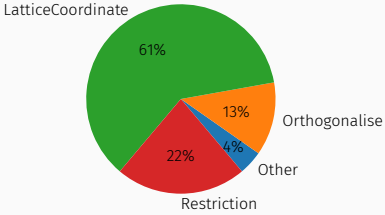
2.1x

Total MG setup:
2.0x

2.8x

After





Comparison with DDalphaAMG

A FIRST COMPARISON WITH DDALPHAAMG – TEST SETUP

- Fix GMRES as smoother
- DDalphaAMG supports vectorization with SSE, but only when even-odd preconditioning is on
- Grid MG supports all common SIMD extensions, but can't do even-odd preconditioning yet
- Could turn off SIMD for both, pointless
- Decided to let DDalphaAMG use SSE + even-odd and Grid MG use AVX
- Test setup (other parameters are DDalphaAMG defaults):

System	Lattice	Blocksize	Mass	Basis vectors	Smoother
8-core Broadwell	16^4	4^4	-0.25	20	GMRES

A FIRST COMPARISON WITH DDALPHAAMG – RESULTS

Setup iter	Outer Iter		Init Setup		Iter Setup		Solve		Total	
Repo	D	G	D	G	D	G	D	G	D	G
0	84	82	9.7	39.4	0	0	18.1	14.2	37	53
1	74	71	9.8	39.4	8.5	32.3	17.4	20.3	35	92
2	34	53	10.0	38.9	16.8	62.8	16.8	16.7	43	117
3	21	22	9.9	40.0	29.4	92.9	5.9	3.8	45	136
4	20	21	9.7	39.9	38.8	121	6.1	3.5	54	164
5	20	20	9.8	39.5	47.7	158	5.8	3.7	63	201
6	20	21	9.2	39.1	55.9	193	6.2	5.0	71	237
7	20	20	9.8	39.7	64.2	226	6.3	3.3	80	269
8	20	20	9.7	39.9	72.2	251	6.1	3.2	88	294
9	20	20	9.9	40.0	80.6	286	6.3	3.3	96	329
10	20	20	9.6	39.8	86.8	316	6.0	3.5	102	359

Conclusions

CONCLUSIONS & OUTLOOK

- Multilevel MG solver for Wilson Clover now present in Grid GitHub, PR pending
- But: Has some performance pitfalls that need to be resolved → WIP
- First comparison to DDalphaAMG: Solve time as expected, losing in setup
- Future directions:
  - Improve upon setup
  - Implement missing parts (Schwarz, Even-odd, ...)
  - Interface for simulation programs
  - Investigate multi-node behavior