Deflated solvers on GPUs

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Outline

- Motivation
- The Incremental EigCG
- Numerical experiments
- Conclusion

NVIDIA Kepler anatomy

K110B micro-architecture highlights

(Tesla K40m)

- 12GB RAM, BW up to 288GB/s
- 15 SMX units, 2880 cores (192 per SMX)
- $P_{theor.} = 1.43/4.29 GFlops$
- Dynamic parallelism, Hyper-Q, GPUdirect

Increased memory size $\rightarrow$ very essential for the deflated solvers!

The EigCG(nev, m) algorithm

- A. Stathopoulos and K. Orginos, SIAM J.Sci.Comput. 32 (2010) 439-462

$i = 0; V^m = []$; $r_0 = b - A\ x_0$; //search vectors and residual
for $j = 0, 1, ...$ **untill** $||r_j||/||r_0|| < tol$:
    Inside standard CG iteration:
        update the Lancz. matrix T_m and the Lancz. vector V_i^m
        if $i == m$: restart $V^{(2k)}$, set $i = 2 * nev$
        $i = i + 1$
    Update residual and solution
end for

Improving eigenvec. accuracy: the Incremental EigCG

- A. Stathopoulos and K. Orginos, SIAM J.Sci.Comput. 32 (2010) 439-462

$U = [], \quad H = []$ //accum. Ritz vectors
for $s = 1, \ldots, s_1$: //for s_1 RHS
    $x_0 = UH^{-1}U^H b_s$ //Galerkin proj.
    $[x_i, V, H] = eigCG(nev, m, A, x_0, b_i)$ //eigCG part
    $\bar{V} =$ orthogonalize V against U //(not strictly needed)
    $[U, H] =$RayleighRitz$[U, \bar{V}]$
end for

EigCG(nev, m) implementation in the QUDA library

create an eigenvector set: $V = [0 : m]$
start CG iterations
an extra iteration index: $i = 0$
load the Lanczos vectors: $V[i] \leftarrow r_i / ||r_i||$
construct the Lanczos matrix: T_m
if $i == m$:
  apply RR on T_m, $T_{m-1} \rightarrow Y_m, Y_{m-1}$ (nev lowest eigenpairs)
  QR factorize $Y_m, Y_{m-1}, \rightarrow Q =$orth$[Y_m, Y_{m-1}]$
  set $H = Q^{\dagger} T_m Q$ and apply RR on H : $HZ = Z\Lambda$
  restart V: $V = V(QZ)$
  reset $i = 2 * nev$ and rebuild T_m
end if
continue CG iterations until the next restart ($m - 2nev$ iters)

Eigenvectors in QUDA

- Main requirement is to keep QUDA functionality:
  - application of $\not{D}$
  - blas operations provided by QUDA
- Added extra attributes and members in spinor field classes:
  - ColorSpinorParam
  - ColorSpinorField
  - cudaColorSpinorField
- Allows to work with both the whole eigenvector set and individual eigenvectors

Eigenvectors in QUDA: cont.

```
class ColorSpinorParam : public LatticeFieldParam {

    ...
    int spinorset_dim;
    int spinorset_id;
    ...
};

class ColorSpinorField : public ColorSpinorParam {

    ...
    int spinorset_dim;
    int spinorset_id;
    int spinorset_volume;
    ...
    std::vector<ColorSpinorField*> spinorset;
    ...
};

class ColorSpinorField : public ColorSpinorParam {

    ...
    cudaColorSpinorField& SpinorsetItem(const int idx) const;
    ...
};
```

Eigenvectors in QUDA: cont.

- To create an eigenvector set:

```
cudaParam.create = QUDA_ZERO_FIELD_CREATE;
cudaParam.spinorset_dim = m;
cudaColorSpinorField *evects = new cudaColorSpinorField(cudaParam);
...
```

- To work with an individual eigenvector:

```
DiracMdagM m(dirac);
m(..., evects→SpinorsetItem(i), ...);
...
cDotProductCuda(evect→SpinorsetItem(i), evect→SpinorsetItem(j));
...
```

LA routines for the EigCG solver

- currently relies on MAGMA GPU library:
  - highly optimized lapack-like routines, $magma\_zgeqrf\_gpu(...), magma\_zunmqr(...),$ etc.
  - but no multi-process support

What kind of LA operations do we need?

- RR block:

if $i == m$:

1. $T_m Y = Y\Lambda$, $T_{m-1}\bar{Y} = \bar{Y}\bar{\Lambda}$ (at most m-dim eigenproblem)
2. $Q =$orth$[Y, \bar{Y}]$ ($2 * nev$ m-component vectors)
3. $H = Q^{\dagger} T_m Q$ ($2nev \times 2nev$ output matrix)
4. $HZ = Z\Lambda$ ($2nev$-dim eigenproblem)
5. $Q = (QZ)$ ($m \times 2nev$ output matrix)
6. $V = VQ$ (here we need multi-gpu!)

endif

What kind of LA operations do we need? cont.

- RR block:

if $i == m$:

1. $T_m Y = Y\Lambda$, $T_{m-1}\bar{Y} = \bar{Y}\bar{\Lambda}$ (magma_zheev_gpu())
2. $Q =$orth$[Y, \bar{Y}]$ (magma_zgeqrf_gpu())
3. $H = Q^{\dagger} T_m Q$ (magma_zunmr_gpu())
4. $HZ = Z\Lambda$ (magma_zheev_gpu())
5. $Q = (QZ)$ (magma_zgemm())
6. $V = VQ$ (here we need multi-gpu!)

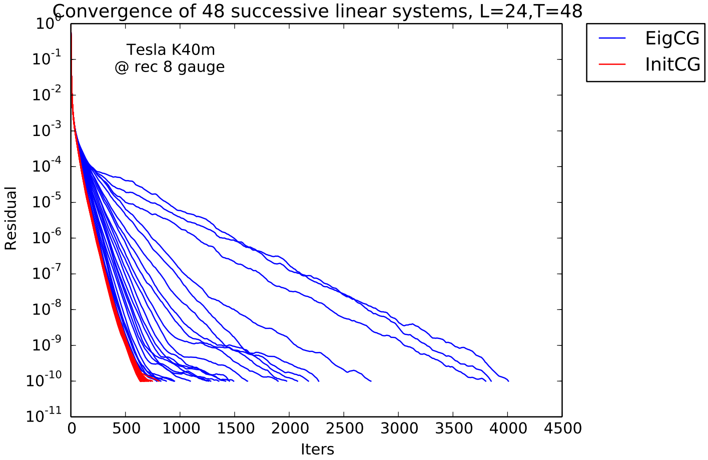
endif

Lattice setup

- Twisted mass fermion action
- Lattice volume: $24^3 \times 48$
- Two configurations:
  - $\kappa = 0.161231, \mu = 0.0085$
  - $\kappa = 0.163270, \mu = 0.0040$
- EigCG parameters: $nev = 8,\ m = 128,\ \ tol = 10^{-10}$
- Used 4-GPU K40m node @ JLAB and 2-GPU K40m node @ FNAL

Incremental EigCG convergence

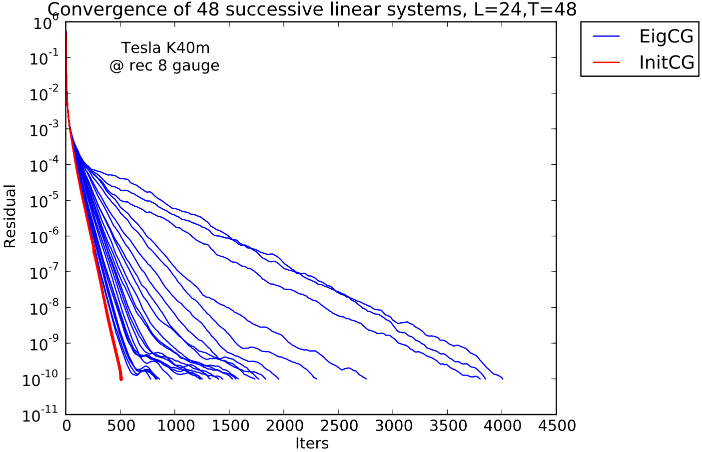
The degenerate twisted mass fermions, $\kappa = 0.163270, \mu = 0.0040$



Incremental EigCG convergence

The degenerate twisted mass fermions, $\kappa = 0.163270, \mu = 0.0040$

- InitCG restart at: $tol = 5 * 10^{-7}$



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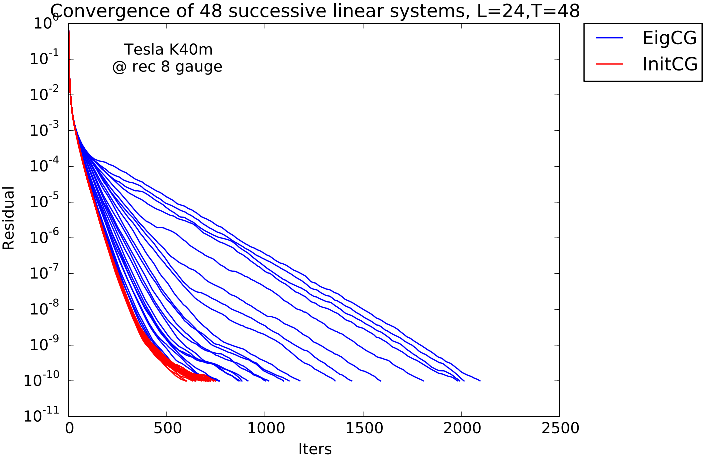

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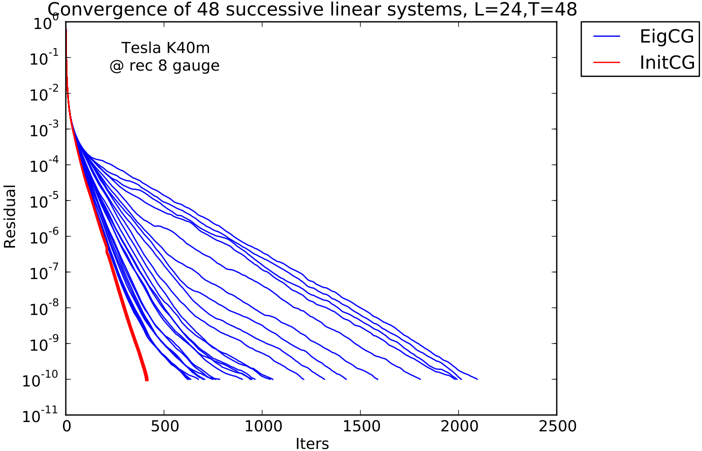
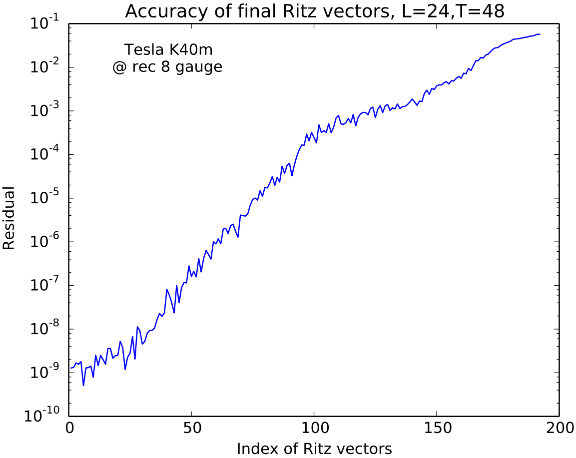


Eigenvectors accuracy

The degenerate twisted mass fermions, $\kappa = 0.163270, \mu = 0.0040$



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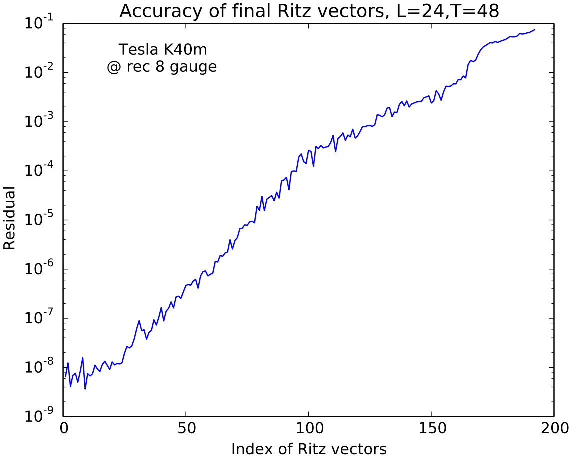

Conclusion

- Incremental EigCG efficiency:
  - essentially large scale application
  - $\times 8$ speedup in terms of iterations
  - $\times 6.5$ speedup in execution time for initCG stage
  - requires relaible updates with Reighley-Ritz for EigCG stage
- Future work:
  - EigBiCGstab
  - GMRES-DR