# Non-blocking Preconditioned Conjugate Gradient Methods for Extreme-scale Computing

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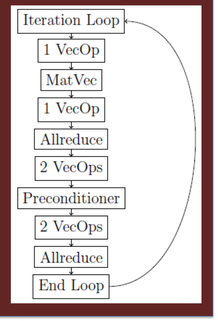
## Abstract

To achieve the best performance on extreme-scale systems we need to develop more scalable method variations. For PCG, dot products limit scalability because they are a synchronization point. Non-blocking methods provide potential to hide most of the cost of the allreduce and avoid synchronization cost due to performance variation across cores.

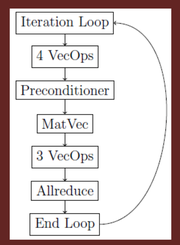
## Preconditioned Conjugate Gradient Method (PCG)

- Iterative algorithm for solving large sparse systems of linear equations.
- Preconditioners accelerate convergence.
- Can rearrange PCG to:
  - •Reduce communication latency using a single allreduce (L56PCG, PIPECG).
  - •Overlap communication and computation using non-blocking allreduces (NBPCG, PIPECG).
- Optimizations introduce vector operations and initialization costs.

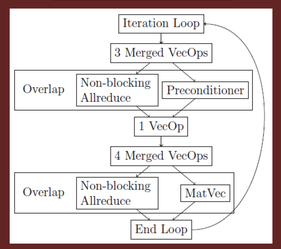



## Scalable Conjugate Gradient Methods

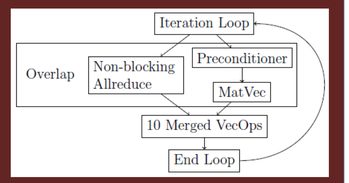
### L56PCG[1]




### NBPCG




### PIPECG[2]




- Each method equivalent to PCG in exact arithmetic.
- Implemented custom solvers in PETSc.

## Non-blocking Allreduce

**Current Approaches:**

**1. MPI_Test:** MPI_Test calls during computation give MPI control of process so it can make progress on allreduce, but requires code modifications.

**2. Progress Threads:** Dedicate one or more threads per node to communication.

**Future Approach:**

**3. Hardware Acceleration**: Executes non-blocking allreduce in hardware, allowing processors to focus on computation.

### MPI_Test Approach

```
MPI_Iallreduce(...);
for(...) {
  do_chunk_computation();
  if (timetotest) {
    MPI_Test(...);
  }
}
MPI_Wait(...);
```

### Ideal Approach

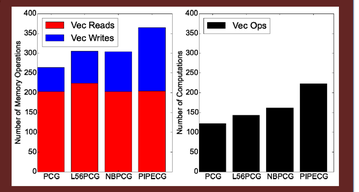
```
MPI_Iallreduce(...);
do_all_computation();
MPI_Wait(...);
```

## Merged Vector Operations

```
VecAYPX(p,beta,u);
VecAYPX(s,beta,w);
VecDot(p,s,&gamma);
```

```
for (i=0; i<n; i++) {
  p[i]     = u[i]+beta*p[i];
  s[i]     = w[i]+beta*s[i];
  gamma += p[i]*s[i];
}
```

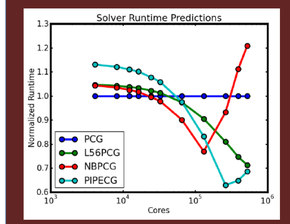
**Merging three vector operations allows us to use four vector reads instead of six. The number of vector writes and computations remains the same.**

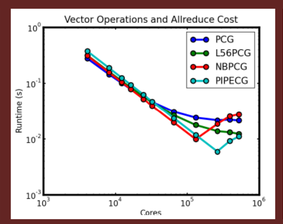


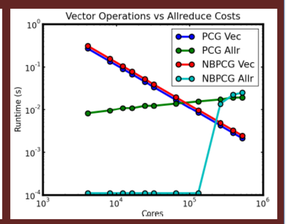

- Merging vector operations avoids cost of extra vector reads.
- Rearranged methods still require additional writes to memory.
- Requires additional computations, but these are cheap compared to memory accesses.
- PCG and L56PCG read some vectors from cache when multiple vectors fit in cache.

## Performance Modeling

- Determine memory access and compute costs with modified STREAM benchmark.
- Model communication with LogGOPS.
- Compute parameters with Netgauge.
- Analyze performance using strong scaling tests.




General Observations

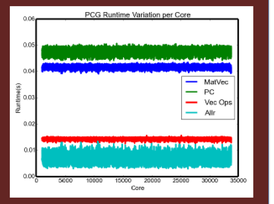
- Non-blocking methods should perform better than blocking methods as the vector operations cost decreases and allreduce cost increases.
- Non-blocking methods should perform well while the MatVec and/or PC have enough computation to hide allreduce cost.
- NBPCG initially should outperforms PIPECG due to lower vector operations cost.
- PIPECG should scale better due to overlapping cost of allreduce with computation of both the MatVec and PC.

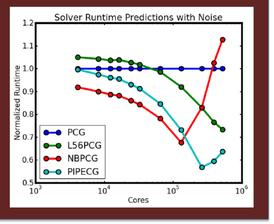
## Impact of Noise

Noise throughout PCG limits performance by causing all processes to wait for slowest process at sync points.

- Computational noise sources: Operating system processes, error correction, etc.
- Communication noise sources: Contention in network, varying distances between nodes, varying size/number of messages, etc.

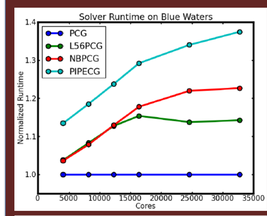
Performance models predict ability to minimize impact of noise may be a key advantage to non-blocking solvers.



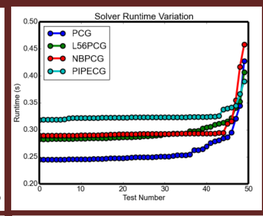




## Solver Performance Results

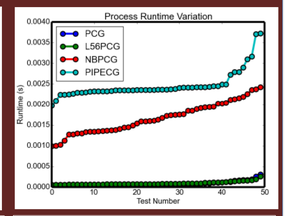
- Ran tests on Blue Waters on up to 32k cores using a 5-point 1-billion row Poisson matrix and block Jacobi ILU preconditioner.



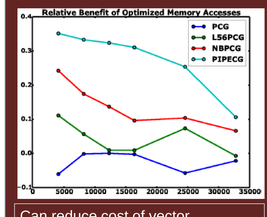

Currently non-blocking allreduce is not efficient enough to overcome increased vector operations cost. Blocking methods obtain improved performance at larger core counts as multiple vectors fit in cache.



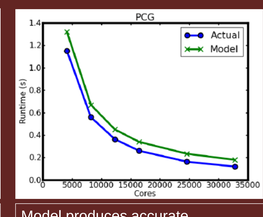

Runtimes can vary significantly between different runs. Non-blocking solvers produce more consistent results.



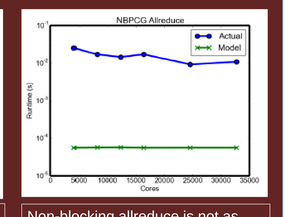

Non-blocking allreduce can allow different processes to make progress at different rates, minimizing the impact of noise. Blocking methods make progress in lockstep.




Can reduce cost of vector operations by over 30% using merged compared to separate vector operations.




Model produces accurate predictions for runtime for PCG.




Non-blocking allreduce is not as efficient as ideal model predicts. More detailed non-blocking allreduce models are needed.

## Conclusions

- Non-blocking solvers provide potential to improve performance at scale due to hiding cost of allreduce and avoiding synchronization.
- Current implementations cannot yet outperform standard PCG.
- Performance models show potential for NBPCG and PIPECG to be more scalable than PCG.
- Ability to minimize impact of noise may be key benefit.

[1]E. D'Azevedo, V. Eijkhout, and C. Romine. Lapack working note 56: Reducing communication costs in the conjugate gradient algorithm on distributed memory multiprocessors. Technical Report, 1993.

[2]P. Ghysels and W. Vanroose, Hiding global synchronization latency in the preconditioned Conjugate Gradient algorithm. Journal of Parallel Computing, Vol 40, Issue 7, 2014.

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