The Algorithmic Development of a Fully Asynchronous Conjugate Gradient Method

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About Me

- BS in Computer Science and Mathematics, University of Kansas
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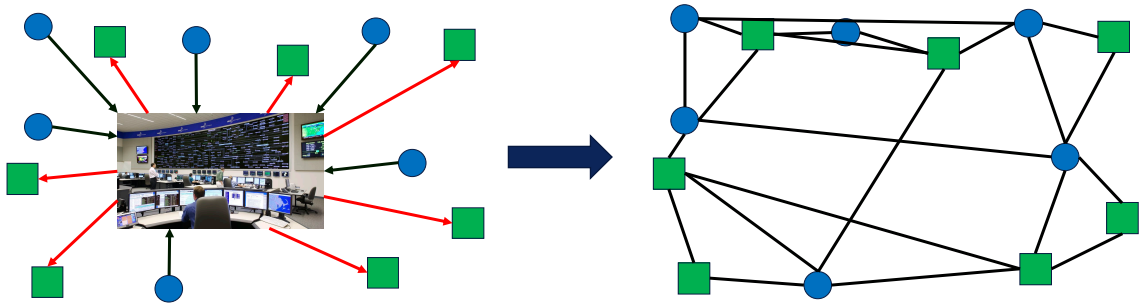
Motivation

- Modern decentralized computing environments
  - Spatially distributed
  - Low-power and/or heterogenous computational units (nodes)
- Lack of iterative solvers with desirable properties
  - Data locality
  - Asynchronous
  - Avoid global (all-to-all) communication
    - i.e. no dot products or MPI allreduce



Motivation

- Asynchronous Jacobi (ASJ) is too slow
  - Scales poorly for ill-conditioned matrices
  - Requires large number of iterations for even low accuracy
- Conjugate gradient (CG) is extremely fast
  - Strong convergence guarantees
  - Widely used in HPC
- But, CG requires synchronous all-to-all communication
  - We will try to remove this and make an asynchronous algorithm

Classical CG Method

Formulation (Hestenes & Stiefel, 1952)

- Solve the linear system $A\mathbf{x} = \mathbf{b}$, A symmetric positive-definite (SPD)
- Initialize $\mathbf{p}^{(0)} = \mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$, $\mathbf{x}^{(0)}$ arbitrary
- For $t = 0,1,2,\ldots$

1. Compute $\alpha^{(t)} = \dfrac{\|\mathbf{r}^{(t)}\|^2}{\langle \mathbf{p}^{(t)}, A\mathbf{p}^{(t)} \rangle}$
2. Update $\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} + \alpha^{(t)}\mathbf{p}^{(t)}$
3. Update $\mathbf{r}^{(t+1)} = \mathbf{r}^{(k)} - \alpha^{(t)}A\mathbf{p}^{(t)}$
4. Compute $\beta^{(t)} = \dfrac{\|\mathbf{r}^{(t+1)}\|^2}{\|\mathbf{r}^{(t)}\|^2}$
5. Update $\mathbf{p}^{(t+1)} = \mathbf{r}^{(t+1)} + \beta^{(t)}\mathbf{p}^{(t)}$

Matrix vector product and dot product

Dot product

- Need to compute a matrix-vector product and two dot products at each iteration

Classical CG Method

Distributed Memory Implementation

- Given an SPD, likely sparse, matrix $A \in \mathbb{R}^{m \times m}$ and vector $\mathbf{b} \in \mathbb{R}^m$
- Distribute rows of A over N agents by the partition $\mathcal{P} = \bigcup_{k=1}^{N} \mathcal{P}_k$
- Notation :
  - Denote by $A_{[k]}$ the $n_k := |\mathcal{P}_k|$ rows local to agent k
  - Denote by $\mathbf{v}_{[k]} \in \mathbb{R}^{n_k}$ the part of the vector $\mathbf{v} \in \mathbb{R}^m$ corresponding to the partition $\mathcal{P}_k$
  - Denote by $\mathbf{v}_k \in \mathbb{R}^m$ the copy of the global vector $\mathbf{v} \in \mathbb{R}^m$ on agent k
- Store local parts of all vectors and matrix: $\mathbf{x}_{[k]}^{(t)}$, $\mathbf{r}_{[k]}^{(t)}$, $\mathbf{p}_{[k]}^{(t)}$, and $A_{[k]}$
- Compute dot products using all-reduce and matrix-vector product using neighbor communication

Reducing the Impact of Communication in CG

Existing Approaches

- Pipelined CG
  - Communication hiding
    - Ghysels & Vanroose, 2014
    - Eller & Gropp, 2016
- s-step CG
  - Communication avoiding
    - Chronopoulos & Gear, 1989
    - Carson, 2020
- Pipelined s-step CG
  - Both communication avoiding and hiding
    - Tiwari & Vadhiyar, 2021
- Not truly asynchronous

Toward Asynchronous CG

CG as a Conjugate Directions Method

- What is a conjugate directions method (CD-method)?
  - Direction vectors $\mathbf{p}^{(t)}$ are chosen to be mutually conjugate (A-orthogonal)
  - That is, $\left\langle \mathbf{p}^{(t)}, \mathbf{p}^{(\ell)} \right\rangle_A = \left\langle \mathbf{p}^{(t)}, A\mathbf{p}^{(\ell)} \right\rangle = 0$ for $\ell \neq t$
  - Step size looks familiar:

$$\alpha^{(t)} = \frac{\left\langle \mathbf{r}^{(t)},\ \mathbf{p}^{(t)} \right\rangle}{\left\langle \mathbf{p}^{(t)},\ A\mathbf{p}^{(t)} \right\rangle}$$

- CG is a special case of the CD-method
  - Generate $\mathbf{p}^{(t)}$ by A-orthogonalization of the residual vectors $\mathbf{r}^{(t)}$
  - Leads to orthogonal residuals
  - Formulation used extensively by (Hestenes & Stiefel, 1952)

Towards Asynchronous CG

Algorithmic Requirements

- Aim to at least satisfy requirements of a CD-method
  - Direction vectors must be conjugate
- Direction vector should only use local and asynchronously received data
- Requires storage of some past direction vectors
- Need to compute A-product of the direction vector without more communication

Asynchronous s-Approximate CD Method (s-ACD)

Initialization

- Given:
  - SPD $A \in \mathbb{R}^{m \times m}$ partitioned over N agents as

$$A = \begin{bmatrix} A_{[1]} \\ \vdots \\ A_{[k]} \\ \vdots \\ A_{[N]} \end{bmatrix}$$

  - Vector $\mathbf{b} \in \mathbb{R}^m$
- Initialize on each agent k:
  - Solution vector $\mathbf{x}_k^{(0)} = \mathbf{0}$,
  - Residual vector and **local direction vector** $\mathbf{r}_k^{(0)} = \mathbf{p}_k^{(0)} = \mathbf{b}$

Asynchronous s-Approximate CD Method (s-ACD)

Algorithm

At iteration t_k of agent k,

1. Asynchronously share ***partial*** **local direction vector** $\mathbf{p}_{[k]}^{(t_k)}$ and ***partial*** $\boldsymbol{A}$**-product** $\mathbf{w}_k^{(t_k)} := A_{[k]}^T \mathbf{p}_{[k]}^{(t_k)}$
2. Receive available updates $\left\{\mathbf{w}_\ell^{(t_\ell)}, \mathbf{p}_{[\ell]}^{(t_\ell)}\right\}_{\ell \in \mathcal{U}_k}$ from other nodes
3. Define the **asynchronous direction vector** $\widetilde{\mathbf{p}}_k^{(t_k)} \in \mathbb{R}^m$ block-wise as

$$\widetilde{\mathbf{p}}_{k,[\ell]}^{(t_k)} = \begin{cases} \mathbf{p}_{[k]}^{(t_k)}, & \ell = k \\ \mathbf{p}_{[\ell]}^{(t_\ell)}, & \ell \in \mathcal{U}_k \\ \mathbf{0}_{n_\ell}, & else \end{cases}$$

- Allows us to compute the **exact matrix-vector product**

$$\widetilde{\mathbf{w}}_k^{(t_k)} := A\widetilde{\mathbf{p}}_k^{(t_k)} = \mathbf{w}_k^{(t_k)} + \sum_{\ell \in \mathcal{U}_k} \mathbf{w}_\ell^{(t_\ell)}$$

- An issue: The **asynchronous direction vector** $\widetilde{\mathbf{p}}_k^{(t_k)}$ is probably not conjugate to earlier directions!

Asynchronous s-Approximate CD Method (s-ACD)

Algorithm (cont.)

At iteration t_k of agent k (cont.),

4. Define the **s-conjugate direction vector** $\mathbf{d}_k^{(t_k)}$ recursively by $\mathbf{d}_k^{(0)} := \tilde{\mathbf{p}}_k^{(0)}$ and

$$\mathbf{d}_k^{(t_k)} := \tilde{\mathbf{p}}_k^{(t_k)} - \sum_{i=1}^{\min(s,\, t_k)} \operatorname{proj}_A\left(\tilde{\mathbf{p}}_k^{(t_k)}, \mathbf{d}_k^{(t_k-i)}\right) \mathbf{d}_k^{(t_k-i)}, \qquad t_k > 0$$

where the projection operator under the A-inner product is defined by

$$\operatorname{proj}_A(\mathbf{u}, \mathbf{v}) := \frac{\langle \mathbf{u}, A\mathbf{v} \rangle}{\langle \mathbf{v}, A\mathbf{v} \rangle}$$

Note, the **exact A-product** can be defined recursively by $A\mathbf{d}_k^{(0)} := \tilde{\mathbf{w}}_k^{(0)}$ and

$$A\mathbf{d}_k^{(t_k)} := \tilde{\mathbf{w}}_k^{(t_k)} - \sum_{i=1}^{\min(s,\, t_k)} \operatorname{proj}_A\left(\tilde{\mathbf{p}}_k^{(t_k)}, \mathbf{d}_k^{(t_k-i)}\right) A\mathbf{d}_k^{(t_k-i)}, \qquad t_k > 0$$

- Requires storing the s previous conjugate direction vectors and their A-products
- Ensures conjugacy against last s directions with ***no additional communication!***

Asynchronous s-Approximate CD Method (s-ACD)

Algorithm (cont.)

At iteration t_k of agent k (cont.),

5. Compute $\alpha_k^{(t_k)} := \dfrac{\left\langle \mathbf{r}_k^{(t_k)}, \mathbf{d}_k^{(t_k)} \right\rangle}{\left\langle \mathbf{d}_k^{(t_k)}, A\mathbf{d}_k^{(t_k)} \right\rangle}$
6. Update $\mathbf{x}_k^{(t_k+1)} := \mathbf{x}_k^{(t_k)} + \alpha_k^{(t_k)} \mathbf{d}_k^{(t_k)}$
7. Update $\mathbf{r}_k^{(t_k+1)} := \mathbf{r}_k^{(t_k)} - \alpha_k^{(t_k)} A\mathbf{d}_k^{(t_k)}$

- Note, if $\mathbf{r}_k^{(t_k)} = \mathbf{b} - A\mathbf{x}_k^{(t_k)}$, then

$$\mathbf{r}_k^{(t_k+1)} = \mathbf{b} - A\mathbf{x}_k^{(t_k)} - \alpha_k^{(t_k)} A\mathbf{d}_k^{(t_k)} = \mathbf{b} - A\left(\mathbf{x}_k^{(t_k)} - \alpha_k^{(t_k)} \mathbf{d}_k^{(t_k)}\right) = \mathbf{b} - A\mathbf{x}_k^{(t_k+1)}$$

- So, the residual is still correct!

Asynchronous s-Approximate CD Method (s-ACD)

Algorithm (cont.)

At iteration t_k of agent k (cont.),

8. Save the **s-conjugate direction vector** $\mathbf{d}_k^{(t_k)}$ and its A-product $\mathbf{v}_k^{(t_k)}$

9. Finally, compute the next **local direction vector** $\mathbf{p}_k^{(t_k+1)}$ using prior directions:

$$\mathbf{p}_k^{(t_k+1)} := \mathbf{r}_k^{(t_k+1)} - \sum_{i=0}^{\min(s,\, t_k)-1} \operatorname{proj}_A\left(\mathbf{r}_k^{(t_k+1)}, \mathbf{d}_k^{(t_k-i)}\right) \mathbf{d}_k^{(t_k-i)}$$

{ Since the new direction is conjugate to the prior s directions, we refer to it as the asynchronous s-approximate CD method }

Asynchronous s-Approximate CD Method (s-ACD)

High-Level Summary

1. Asynchronously communicate **partial local direction vectors** and **partial A-products**
   - Send **partial local direction vector** and **partial A-product**
   - Receive updates from some other agents
   - No update from an agent ⇔ update of all zeros
2. Construct the **asynchronous direction vector** and its exact **A-product**
   - Concatenate the sent and received **partial local direction vectors**
   - Sum the sent and received **partial A-products**
3. Compute the **conjugate direction vector** and its exact **A-product**
   - A-orthogonalize **asynchronous direction vector** against s previous **conjugate direction vectors**
4. Perform a local CG iteration using the **conjugate direction vector**
5. Compute next **local direction vector**
   - A-orthogonalize the **local residual vector** against previous and current **conjugate direction vectors**

Asynchronous s-Approximate CD Method (s-ACD)

Trade-offs

- Pros:
  - Only communicate once per iteration
  - No synchronization!
- Cons:
  - Send vectors rather than scalars
  - Store $2s$ additional vectors
  - Computing conjugate direction vectors

Asynchronous s-Approximate CD Method (s-ACD)

Final Notes

- Some issues remain:
  - Since direction vectors may differ between nodes, solution vector desyncs
  - Similarly, residual differs between nodes, so no clear stopping criteria
- A solution to both:
  - Send local solution vector $\mathbf{x}_k^{(t_k)}$ and local part of residual $\mathbf{r}_{[k]}^{(t_k)}$ at each iteration
  - Periodically restart the CD method
    - Average the solution vectors as $\tilde{\mathbf{x}}_k^{(t_k)} = \frac{1}{N}\sum_{\ell=1}^{N} \mathbf{x}_k^{(t_k)}$
    - Reconstruct residual vector $\tilde{\mathbf{r}}_k^{(t_k)}$ using most recent $\left\{\mathbf{r}_{[\ell]}^{(t_\ell)}\right\}$ like we did with asynchronous direction vectors
    - Restart the method with $\mathbf{x}_k^{(0)} = \tilde{\mathbf{x}}_k^{(t_k)}$ and $\mathbf{r}_k^{(0)} = \mathbf{p}_k^{(0)} = \tilde{\mathbf{r}}_k^{(t_k)}$
  - Experimentally found that restarting every ~15 iterations provided optimal speedup

Numerical Results

Test Problem

- 2D Poisson problem

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -f(x,y), \qquad (x,y) \in (0,1)\times(0,1)$$

- Homogeneous Dirichlet boundary conditions

$$u(x,0) = u(x,1) = 0, \qquad x \in [0,1]$$
$$u(0,y) = u(1,y) = 0, \qquad y \in [0,1]$$

- Discretized over a 20×20 grid of internal nodes, yields the linear system

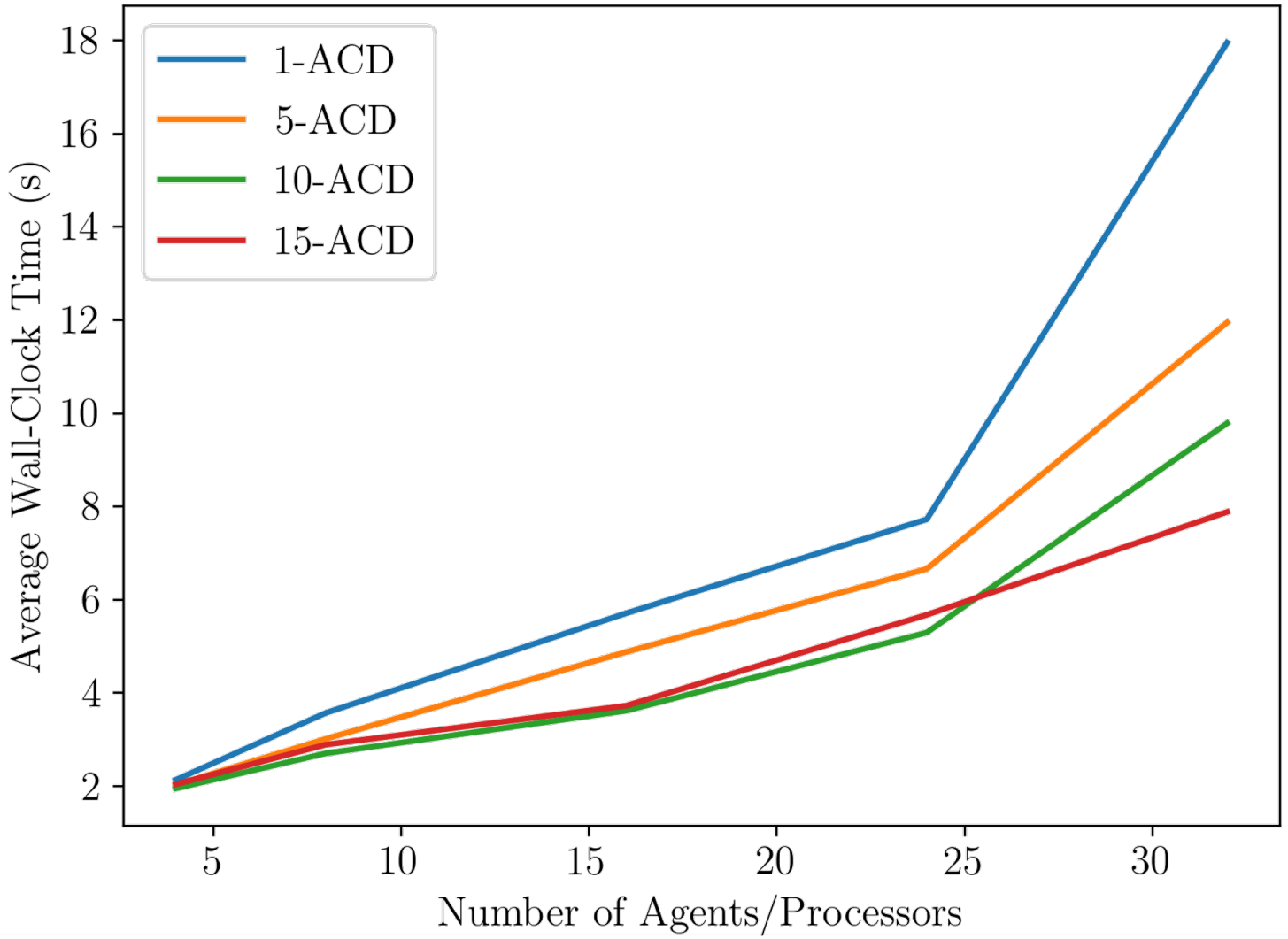
$$A\mathbf{x} = \mathbf{b}$$

Numerical Results
Test Problem

- Matrix $A \in \mathbb{R}^{400\times400}$ is given by the 2D discrete Laplacian on a 20×20 grid
- Right-hand side vector b is discretization of
$$f(x,y) = \pi^2 \sin \pi x \sin \pi y$$
- Note that with this f, the 2D Poisson problem yields the exact solution
$$u(x,y) = \sin \pi x \sin \pi y$$
- We perform strong scaling tests of s-ACD with different values of s
- Additionally, we compare results with a low tolerance against a high tolerance

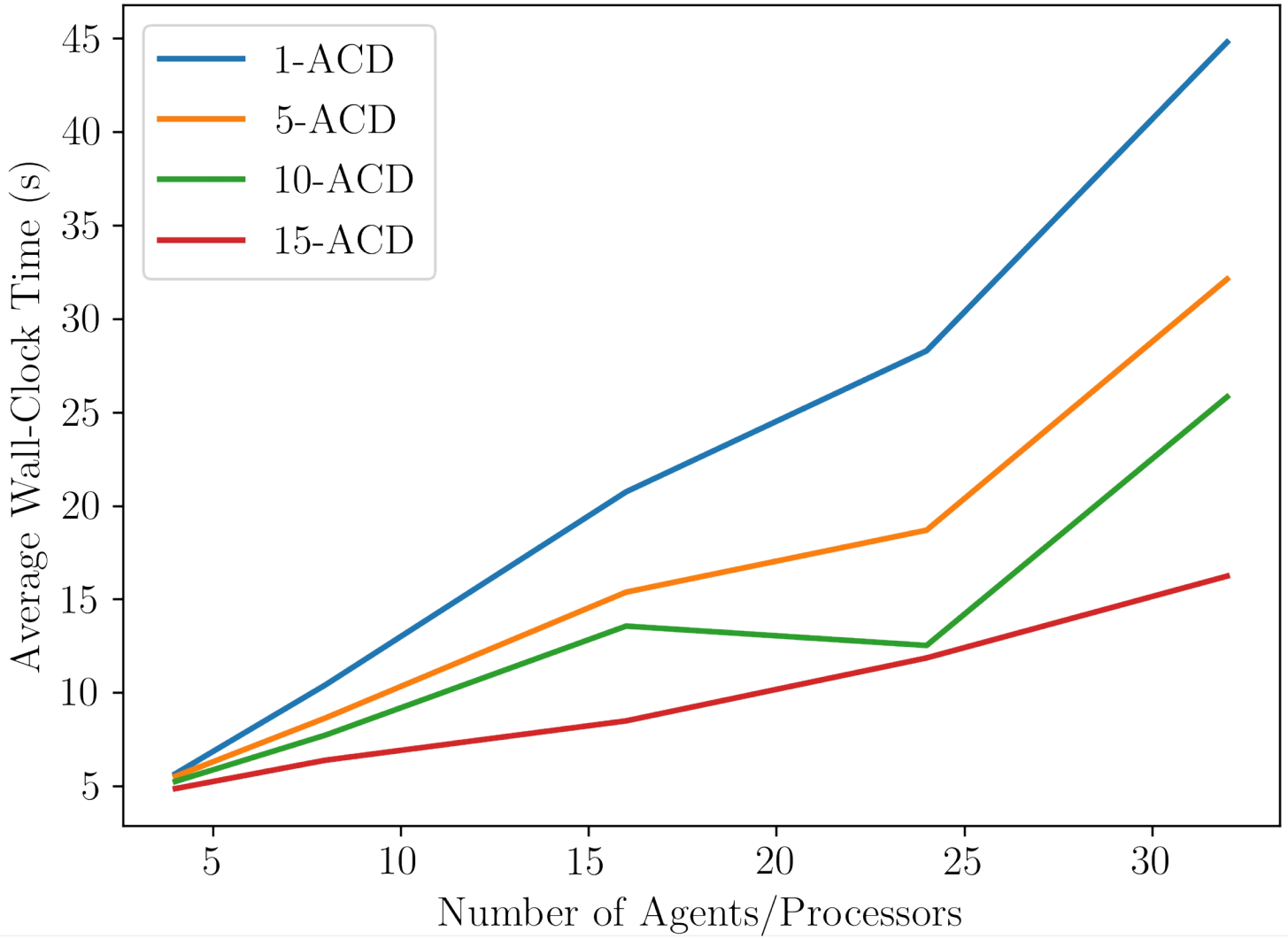
Numerical Results

Convergence Time for Different s Values (tolerance 1e-3)



Numerical Results

Convergence Time for Different s Values (tolerance 1e-8)



Numerical Results

Comparison with CG of Condition Number vs Iterations Necessary for Convergence

- CG iteration bound is given as

$$\tau_{CG}(A) = \log_{c(A)} {}^{\epsilon}/_{2}$$

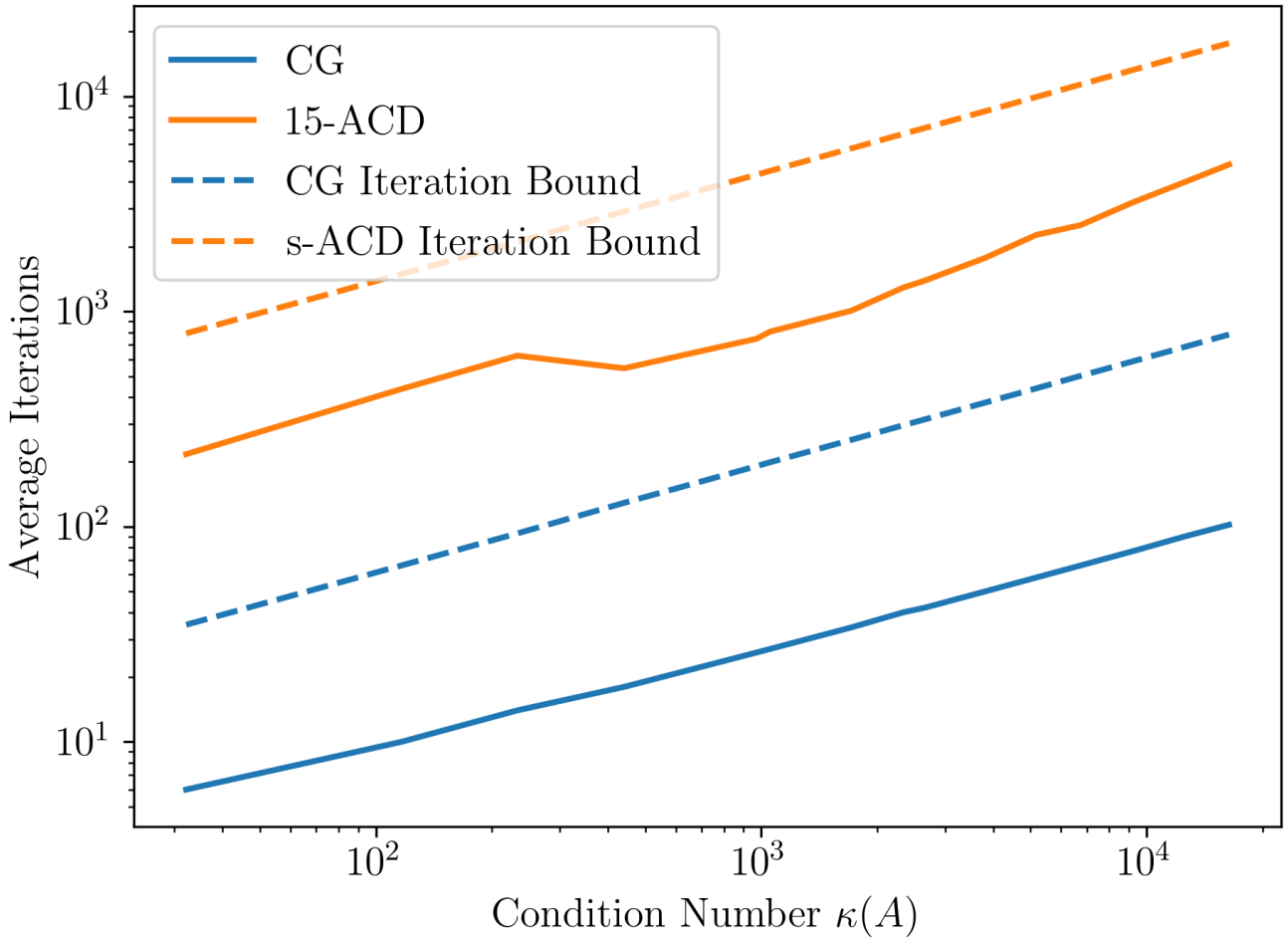
where $\epsilon = 10^{-3}$ and

$$c(A) = \frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1}$$

- ACD iteration bound is given as

$$\tau_{ACD}(A) = 22.7\tau_{CG}(A)$$

  - Constant is derived from the slope of the strong scaling experiments



Future Work

- Theoretical convergence results
- Improve orthogonality of residuals
- Other methods for restarting
  - Robust averaging on solution vector and residual
  - Could be run in a concurrent Skynet job
- Add resiliency measures
  - Communication delay
  - Data corruption
  - Agent failure/restart

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Questions?

Implementation Details

Collaborative Autonomy with Skynet

- Skynet is an LLNL-developed framework for decentralized computing
  - Existing frameworks (e.g. MPI) only provide communication primitives
- In contrast, Skynet provides
  - Subscription-based communication of most C++ built-in types and std::vector
  - Flexible high-level iterative templates, which allow for more sophisticated communication patterns
  - Built-in implementations of algorithms such as the Jacobi method and robust push-sum averaging
- Uses TCP for flexible communication
  - Same program can run on an HPC cluster, across a collection of microcontrollers, etc.
  - Only configuration necessary is neighbor IP addresses and listening ports
- See Colin Ponce's talk at Session 11A on Friday morning

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