High-Performance Variants of Krylov Subspace Methods: I/II

Erin C. Carson
Katedra numerické matematiky, Matematicko-fyzikální fakulta, Univerzita Karlova

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Lecture Outline

• Parallel computers and performance modeling
  • Architecture trends

• Krylov subspace methods
  • Properties
  • Performance bottlenecks at scale

• High-performance variants of Krylov subspace methods
  • Early approaches
  • Pipelined methods
  • s-step methods

• Practical implementation issues and challenges
Why are we interested in solving larger and larger problems?

- Enables new frontiers in computational science and engineering
  - Finer-grained simulation, over longer time scales, processing huge amounts of available data
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• Atmosphere, Earth, Environment
• Physics - applied, nuclear, particle, fusion, photonics
• Bioscience, Biotechnology, Genetics
• Chemistry, Molecular Sciences
• Geology, Seismology
• Electrical Engineering, Circuit Design, Microelectronics
• Mechanical Engineering - from prosthetics to spacecraft
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Also industrial and commercial interests

- "Big Data", databases, data mining
- Artificial Intelligence (AI)
- Medical imaging and diagnosis
- Pharmaceutical design
- Financial and economic modeling
- Advanced graphics and virtual reality
- Oil exploration
Technology Trends: Microprocessor Capacity

2X transistors/Chip Every 1.5 years
“Moore's Law”

Microprocessors have become smaller, denser, and more powerful.

Gordon Moore (co-founder of Intel) predicted in 1965 that the transistor density of semiconductor chips would double roughly every 18 months.

Slide source: Jack Dongarra

Slide source: Kathy Yelick
Historical Impact of Device Shrinkage

• What happens when the feature size (transistor size) shrinks by a factor of $x$?
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- Transistors per unit area goes up by $x^2$
- Die size has also increased
  - typically another factor of $\sim x$
- Raw computing power of the chip goes up by $\sim x^4$!
  - typically $x^3$ is devoted to either on-chip
    - **parallelism**: hidden parallelism such as ILP
    - **locality**: caches
- So most programs $x^3$ times faster, without changing them
Power Density Limits Serial Performance

Scaling clock speed (business as usual) will not work

Source: Patrick Gelsinger, Shenkar Bokar, Intel®

Slide source: Kathy Yelick
Power Density Limits Serial Performance

- Concurrent systems are more power efficient
  - Dynamic power is proportional to $V^2 f C$
  - Increasing frequency ($f$) also increases supply voltage ($V$) $\Rightarrow$ cubic effect
  - Increasing cores increases capacitance ($C$) but only linearly
  - Save power by lowering clock speed

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- High performance serial processors waste power
  - Speculation, dynamic dependence checking, etc. burn power
  - Implicit parallelism discovery
- More transistors, but not faster serial processors

Slide source: Kathy Yelick
• Chip density is continuing increase ~2x every 2 years
• Clock speed is not
• Number of processor cores may double instead
• Power is under control, no longer growing
Parallel Computer Architectures

• Takeaway: *all* programs that need to run faster will have to become parallel programs

• Since mid 2000s - not only are fastest computers parallel, but nearly *all* computers are parallel
Evolution of HPC Nodes

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1995
Single CPU per node with main memory

2000–2010
Multiple CPUs per node sharing main memory

New programming models

2000–2010
Accelerators usher in era of heterogeneity

Evolution of HPC Nodes

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Central processing unit (CPU)
Multicore CPU
Memory (MEM)
Cache
Graphic processing unit (GPU)

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Single CPU per node with main memory

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Multiple CPUs per node sharing main memory

New programming models

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Accelerators usher in era of heterogeneity

2014
Accelerators share common view of memory with CPU

2015
Simple low-power cores and non-uniform memory access

Evolution of HPC Nodes

HPC Architectures Today

Summit (Oak Ridge National Lab, Tennessee)
• current #1 on the TOP500
One Processor: 22 SIMD processing cores, on-chip accelerators
- Each core supports 4 hardware threads
- Each core has separate L1 cache; pairs of cores share L2 and L3 cache

HPC Architectures Today

One GPU (NVIDIA V100): 80 streaming multiprocessors (SMs), 16 GB of high-bandwidth memory (HBM2), 6 MB L2 cache shared by SMs

https://www.olcf.ornl.gov/for-users/system-user-guides/summit/summit-user-guide/#nvidia-v100-gpus
HPC Architectures Today

One SM:
32 FP64 (double-precision) cores,
64 FP32 (single-precision) cores,
64 INT32 cores,
8 tensor cores,
128-KB shared memory/L1 cache

https://www.olcf.ornl.gov/for-users/system-user-guides/summit/summit-user-guide/#nvidia-v100-gpus
HPC Architectures Today

One Socket: 1 CPU, 3 GPUs

https://www.olcf.ornl.gov/for-users/system-user-guides/summit/summit-user-guide
HPC Architectures Today

One Node: 2 sockets

https://www.olcf.ornl.gov/for-users/system-user-guides/summit/summit-user-guide
One Rack: 18 nodes
- Dual-rail EDR InfiniBand network with non-blocking fat-tree topology
- Node bandwidth of 23 GB/s
HPC Architectures Today

https://en.wikichip.org/wiki/supercomputers/summit
To design an efficient parallel algorithm, must first model physical costs --- runtime or energy consumption --- of executing a program on a machine.

Tradeoff:

- More detailed model: more accurate results for a particular machine, but results may not apply to other machines.
- Less detailed model: results applicable to a variety of machines, but may not be accurate for any.
  - but abstracting machine details can still give us a general sense of an efficient implementation.
A simplified runtime model:

- Time to perform a floating point operation: $\gamma$
- Time to move a message of $n$ words: $\alpha + \beta n$
  - $\alpha = \text{latency (seconds)}$, $\beta = \frac{1}{\text{bandwidth (seconds/word)}}$

$$\text{Runtime} = \gamma \text{ (# flops)} + \beta \text{ (# words)} + \alpha \text{ (# msgs)}$$

#flops,words,msgs are counted along a critical path in the schedule:
\( \gamma \) is per-flop:

- To improve: more parallelism (no longer increase clock frequency)
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\( \beta \) is per-word:

- Models bandwidth: maximum amount of data that can be in-flight simultaneously
- To improve: add more ports/wires/etc.
Performance Modeling: Latency-Bandwidth Model

\( \gamma \) is per-flop:
- To improve: more parallelism (no longer increase clock frequency)

\( \beta \) is per-word:
- Models bandwidth: maximum amount of data that can be in-flight simultaneously
- To improve: add more ports/wires/etc.

\( \alpha \) is per-message and independent of message size
- Models latency: time for data to travel across machine
- Difficult to improve, due to fundamental limits (speed of light, atomic radius,...)

“Bandwidth is money, but latency is physics”
## Exascale System Projections

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- Movement of data (communication) is much more expensive than floating point operations (computation), in terms of both time and energy.
- Gaps will only grow larger.
- Reducing time spent moving data/waiting for data will be essential for applications at exascale!
Exascale Computing: The Modern Space Race

• "Exascale": $10^{18}$ floating point operations per second
  • with maximum energy consumption around 20-40 MWatts

• Advancing knowledge, addressing social challenges, improving quality of life, influencing policy, economic competitiveness

Nothing tends so much to the advancement of knowledge as the application of a new instrument.
- Sir Humphry Davy

• Large investment in HPC worldwide

USA – Aurora at Argonne 2021
Europe 2022
China 2019-2020
Japan – Post-K computer 2021
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• Technical challenges at all levels
  - hardware to algorithms to applications
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  hardware to algorithms to applications
An Exaflop of what?

- When will victory be declared?
  - When a supercomputer reaches exaflop performance on the LINPACK benchmark (TOP500)
    - Solving dense $Ax = b$ using Gaussian elimination with partial pivoting
An Exaflop of what?

• When will victory be declared?
  • When a supercomputer reaches exaflop performance on the LINPACK benchmark (TOP500)
    • Solving dense $Ax = b$ using Gaussian elimination with partial pivoting
  • Summit supercomputer has already exceeded exaflop performance for a certain genomics code (https://www.olcf.ornl.gov/2018/06/08/genomics-code-exceeds-exaops-on-summit-supercomputer/)
An Exaflop of what?

• When will victory be declared?
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• Does that mean we are done?
An Exaflop of what?

• When will victory be declared?
  • When a supercomputer reaches exaflop performance on the LINPACK benchmark (TOP500)
    • Solving dense $Ax = b$ using Gaussian elimination with partial pivoting

• Does that mean we are done?
  • LINPACK benchmark is typically a compute-bound problem ("BLAS-3")
  • Not a good indication of performance for a large number of scientific applications!
    • Lots of remaining work even after exascale performance is achieved
    • Has led to incorporation of other benchmarks into the TOP500 ranking
      • e.g., HPCG: Solving sparse $Ax = b$ iteratively using the conjugate gradient method
Krylov subspace methods

- **Linear systems** $Ax = b$, eigenvalue problems, singular value problems, least squares, etc.
- Best for: $A$ large & very sparse, stored implicitly, or only approximation needed

- **Krylov Subspace Method** is a projection process onto the Krylov subspace
  \[ \mathcal{K}_i(A, r_0) = \text{span}\{r_0, Ar_0, A^2r_0, \ldots, A^{i-1}r_0\} \]
  where $A$ is an $N \times N$ matrix and $r_0 = b - Ax_0$ is a length-$N$ vector

- In each iteration,
  - Add a dimension to the Krylov subspace
    - Forms nested sequence of Krylov subspaces
      \[ \mathcal{K}_1(A, r_0) \subset \mathcal{K}_2(A, r_0) \subset \cdots \subset \mathcal{K}_i(A, r_0) \]
  - Orthogonalize (with respect to some $\mathcal{C}_i$)
  - Select approximate solution $x_i \in x_0 + \mathcal{K}_i(A, r_0)$ using $r_i = b - Ax_i \perp \mathcal{C}_i$

- Ex: Lanczos/Conjugate Gradient (CG), Arnoldi/Generalized Minimum Residual (GMRES), Biconjugate Gradient (BICG), BICGSTAB, GKL, LSQR, etc.
Krylov Subspace Methods in the Wild

Climate Modeling

Computer Vision

Medical Treatment

Chemical Engineering

Power Grid Modeling

Computational Cosmology

Financial Portfolio Optimization

Latent Semantic Analysis
The conjugate gradient method

$A$ is symmetric positive definite, $C_i = \mathcal{K}_i(A, r_0)$
The conjugate gradient method

\( A \) is symmetric positive definite, \( C_i = \mathcal{K}_i(A, r_0) \)

\[ r_i \perp \mathcal{K}_i(A, r_0) \iff \|x - x_i\|_A = \min_{z \in x_0 + \mathcal{K}_i(A, r_0)} \|x - z\|_A \]
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\[ \Rightarrow r_{N+1} = 0 \]
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    \leq 0
\]

Connection with Lanczos

- With \( v_1 = r_0/\|r_0\| \), \( i \) iterations of Lanczos produces \( N \times i \) matrix \( V_i = [v_1, \ldots, v_i] \), and \( i \times i \) tridiagonal matrix \( T_i \) such that
  \[
  AV_i = V_i T_i + \delta_{i+1} v_{i+1} e_i^T, \quad T_i = V_i^* A V_i
  \]

- CG approximation \( x_i \) is obtained by solving the reduced model
  \[
  T_i y_i = \|r_0\| e_1, \quad x_i = x_0 + V_i y_i
  \]
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- Connections with orthogonal polynomials, Stieltjes problem of moments, Gauss-Cristoffel quadrature, others (see 2013 book of Liesen and Strakoš)
The conjugate gradient method

$A$ is symmetric positive definite, $C_i = \mathcal{K}_i(A, r_0)$

$$r_i \perp \mathcal{K}_i(A, r_0) \iff \|x - x_i\|_A = \min_{z \in x_0 + \mathcal{K}_i(A, r_0)} \|x - z\|_A$$

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Connection with Lanczos

• With $v_1 = r_0/\|r_0\|$, $i$ iterations of Lanczos produces $N \times i$ matrix $V_i = [v_1, \ldots, v_i]$, and $i \times i$ tridiagonal matrix $T_i$ such that

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$\Rightarrow$ CG (and other Krylov subspace methods) are highly nonlinear

• Good for convergence, bad for ease of finite precision analysis
Implementation of CG

- Standard implementation due to Hestenes and Stiefel (1952) (HSCG)
- Uses three 2-term recurrences for updating \( x_i, r_i, p_i \)

\[
\begin{align*}
r_0 &= b - Ax_0, \quad p_0 = r_0 \\
\text{for } i &= 1:nmax \\
\alpha_{i-1} &= \frac{r_{i-1}^T r_{i-1}}{p_{i-1}^T Ap_{i-1}} \\
x_i &= x_{i-1} + \alpha_{i-1} p_{i-1} \\
r_i &= r_{i-1} - \alpha_{i-1} A p_{i-1} \\
\beta_i &= \frac{r_i^T r_i}{r_{i-1}^T r_{i-1}} \\
p_i &= r_i + \beta_i p_{i-1}
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  p_i &= r_i + \beta_i p_{i-1} \\
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minimizes $\|x - x_i\|_A$ along line $z(\alpha) = x_{i-1} + \alpha p_{i-1}$
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for $i = 1:n_{\text{max}}$

\[ \alpha_{i-1} = \frac{r_{i-1}^T r_{i-1}}{p_{i-1}^T A p_{i-1}} \]

\[ x_i = x_{i-1} + \alpha_{i-1} p_{i-1} \]

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\[ p_i = r_i + \beta_i p_{i-1} \]

end

minimizes $||x - x_i||_A$ along line

\[ z(\alpha) = x_{i-1} + \alpha p_{i-1} \]

If

\[ p_i \perp_A p_j \text{ for } i \neq j, \]

1-dimensional minimizations in each iteration give $i$-dimensional minimization over the whole subspace

\[ x_0 + \mathcal{K}_i(A, r_0) = x_0 + \text{span}\{p_0, \ldots, p_{i-1}\} \]
**Summit - IBM Power System AC922**

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<tr>
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<tr>
<td>Memory:</td>
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**Performance**

| Theoretical peak: | 187,659 TFlops/s |
| LINPACK benchmark: | 122,300 Tflops/s |
| HPCG benchmark:   | 2,926 Tflops/s   |
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Conjugate Gradient on the World's Fastest Computer

Summit - IBM Power System AC922

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**Performance**

- Theoretical peak: 187,659 TFlops/s
- LINPACK benchmark: 122,300 Tflops/s
- HPCG benchmark: 2,926 Tflops/s

LINPACK benchmark (dense $Ax = b$, direct) 65% efficiency

Current #1 on top500
### Summit - IBM Power System AC922

<table>
<thead>
<tr>
<th>Site:</th>
<th>Oak Ridge National Laboratory</th>
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</thead>
<tbody>
<tr>
<td>Manufacturer:</td>
<td>IBM</td>
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<tr>
<td>Cores:</td>
<td>2,282,544</td>
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- **LINPACK benchmark** (dense $Ax = b$, direct) 65% efficiency
- **HPCG benchmark** (sparse $Ax = b$, iterative) 1.5% efficiency

*Summit* is currently #1 on the top500 list.
The Conjugate Gradient (CG) Method

\[ r_0 = b - Ax_0, \quad p_0 = r_0 \]
for \( i = 1:n_{\text{max}} \)

\[ \alpha_{i-1} = \frac{r_{i-1}^T r_{i-1}}{p_{i-1}^T Ap_{i-1}} \]

\[ x_i = x_{i-1} + \alpha_{i-1} p_{i-1} \]

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\[ \text{Cost Per Iteration} \]

→ Sparse matrix-vector multiplication (SpMV)
  - $O(\text{nnz})$ flops
  - Must communicate vector entries w/neighbor processors (nearest neighbor MPI collective)
  - Must read A/vector from slow memory
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→ Inner products
  • $O(N)$ flops
  • **global synchronization** (MPI_Allreduce)
    • all processors must exchange data and wait for all communication to finish before proceeding
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Low computation/communication ratio
⇒ Performance is communication-bound
**Arithmetic Intensity**

- **0.1-1.0** flops per byte
  - SpMV
  - BLAS1,2
  - Stencils (PDEs)
  - Lattice Boltzmann Methods
  - \(O(1)\)

- **Typically < 2** flops per byte
  - FFTs, Spectral Methods
  - \(O(\log(N))\)

- **O(10)** flops per byte
  - Dense Linear Algebra (BLAS3)
  - Particle Methods
  - \(O(N)\)
Roofline Model (Williams, Waterman, Patterson, 2009)

- Provides estimates of performance for various applications (based on arithmetic intensity) for given machine
- attainable flop/s = min(peak flop/s, peak bandwidth × arithmetic intensity)
- "ceilings" give peak bandwidth or peak flops in absence of possible optimizations

Image source: Sam Williams
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Generally three approaches to improving performance:
- Maximize in-core performance (e.g. get compiler to vectorize)
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Generally three approaches to improving performance:
- Maximize in-core performance (e.g. get compiler to vectorize)
- Maximize memory bandwidth (e.g. NUMA-aware allocation)
- Minimize data movement (increase AI)
Synchronization-reducing variants

Motivated many approaches to reducing synchronization (increasing ratio of computation to communication) in CG:
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- Early work: CG with a single synchronization point per iteration
  - 3-term recurrence CG
  - Using modified computation of recurrence coefficients
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- **Pipelined Krylov subspace methods**
  - Uses modified coefficients and auxiliary vectors to reduce synchronization points to 1 per iteration
  - Modifications also allow decoupling of SpMV and inner products - enables overlapping (MPI non-blocking collectives)
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• s-step Krylov subspace methods
  • Compute iterations in blocks of s using a different Krylov subspace basis
  • Enables one synchronization per s iterations
To improve performance of Krylov subspace methods, we must reduce the cost of data movement.

Communication "hiding" approaches:
- Use non-blocking MPI communication
- Do useful computation while waiting for communication (overlapping)
- "Pipelined" Krylov subspace methods
  - Historical background, derivation
  - Performance results
  - Recent work on "deep pipelined" methods

Communication "avoiding" approaches:
- Mathematically unroll iteration loop, allows all communication for multiple iterations to be done in one step
- "s-step" Krylov subspace methods
  - Historical background, derivation
  - Implementation details (matrix powers kernel, TSQR)
  - Performance results

Other approaches: enlarged KSMs, combination of pipelined and s-step approaches
Early approaches to reducing synchronization

- Goal: Reduce the 2 synchronization points per iteration in (HS)CG to 1 synchronization point per iteration
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• Compute $\beta_i$ from $\alpha_{i-1}$ and $Ap_{i-1}$ using relation

$$\|r_i\|^2 = \alpha_{i-1}^2 \|Ap_{i-1}\|^2 - \|r_{i-1}\|^2$$

• Can then also merge the updates of $x_i$, $r_i$, and $p_i$


• Many other similar approaches
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- Can then also merge the updates of $x_i$, $r_i$, and $p_i$
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- Could also compute $\alpha_{i-1}$ from $\beta_{i-1}$:

$$\alpha_{i-1} = \left( \frac{r_{i-1}^T Ar_{i-1}}{r_{i-1}^T r_{i-1}} - \frac{\beta_{i-1}}{\alpha_{i-2}} \right)^{-1}$$
• HSCG recurrences can be written as

\[ AP_i = R_{i+1}L_i, \quad R_i = P_iU_i \]

we can combine these to obtain a 3-term recurrence for the residuals (STCG):

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- First developed by Stiefel (1952/53), also Rutishauser (1959) and Hageman and Young (1981)
- Motivated by relation to three-term recurrences for orthogonal polynomials

\[
\begin{align*}
  r_0 &= b - Ax_0, \quad p_0 = r_0, \quad x_{-1} = x_0, \quad r_{-1} = r_0, \quad e_{-1} = 0 \\
  \text{for } i &= 1:\text{nmax} \\
  q_{i-1} &= \frac{(r_{i-1} Ar_{i-1})}{(r_{i-1} r_{i-1})} - e_{i-2} \\
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Can be accomplished with a single synchronization point on parallel computers (Strakoš 1985, 1987)
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- Similar approach (computing \( \alpha_i \) using \( \beta_{i-1} \)) used by D'Azevedo, Eijkhout, Romaine (1992, 1993)
Chronopoulos and Gear's CG (ChG CG)

• Chronopoulos and Gear (1989)

• Looks like HSCG, but very similar to 3-term recurrence CG (STCG)

• Reduces synchronizations/iteration to 1 by changing computation of $\alpha_i$ and using an auxiliary recurrence for $Ap_i$

\[r_0 = b - Ax_0, \quad p_0 = r_0,\]
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\end{align*}
$$

end
Pipelined CG (GVC CG)

- Pipelined CG of Ghysels and Vanroose (2014)

- Similar to Chronopoulos and Gear approach
  - Uses auxiliary vector $s_i \equiv A p_i$ and same formula for $\alpha_i$
• Pipelined CG of Ghysels and Vanroose (2014)

• Similar to Chronopoulos and Gear approach
  • Uses auxiliary vector $s_i \equiv Ap_i$ and same formula for $\alpha_i$

• Also uses auxiliary vectors for $Ar_i$ and $A^2r_i$ to remove sequential dependency between SpMV and inner products
Pipelined CG (GVCG)

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  - Uses auxiliary vector $s_i \equiv Ap_i$ and same formula for $\alpha_i$

- Also uses auxiliary vectors for $Ar_i$ and $A^2r_i$ to remove sequential dependency between SpMV and inner products
  - Allows the use of nonblocking (asynchronous) MPI communication to overlap SpMV and inner products
  - Hides the latency of global communications
\[ r_0 = b - Ax_0, \quad p_0 = r_0 \]
\[ s_0 = Ap_0, w_0 = Ar_0, z_0 = Aw_0, \]
\[ \alpha_0 = r_0^T r_0 / p_0^T s_0 \]
for \( i = 1 : \text{nmax} \)

\[ x_i = x_{i-1} + \alpha_{i-1} p_{i-1} \]
\[ r_i = r_{i-1} - \alpha_{i-1} s_{i-1} \]
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\[ p_i = r_i + \beta_i p_{i-1} \]
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for \( i = 1: n_{\text{max}} \)

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for \( i = 1 : n_{\text{max}} \)

\[
\begin{aligned}
x_i &= x_{i-1} + \alpha_{i-1} p_{i-1} \\
r_i &= r_{i-1} - \alpha_{i-1} s_{i-1} \\
w_i &= w_{i-1} - \alpha_{i-1} z_{i-1} \\
q_i &= Aw_i \end{aligned}
\]

\[
\begin{aligned}
\beta_i &= \frac{r_i^T r_i}{r_{i-1}^T r_{i-1}} \\
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p_i &= r_i + \beta_i p_{i-1} \\
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\end{aligned}
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\[\alpha_i = \frac{r_i^T r_i}{w_i^T (r_i (\beta_i / \alpha_{i-1}) r_i^T r_i)}\]
\[p_i = r_i + \beta_i p_{i-1}\]
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\[ s_i = w_i + \beta_i s_{i-1} \]

\[ z_i = q_i + \beta_i z_{i-1} \]

end
**MPI Non-Blocking Communication**

- "Non-blocking" or "asynchronous" collectives available since MPI 3

```c
MPI_Iallreduce(...,MPI_Request,...)
// ...other work (SpMV, precond., etc)
MPI_Wait(...,MPI_Request)
```

PETSc provides a construct for asynchronous dot-products:

```c
VecDotBegin (...,&dot);
PetscCommSplitReductionBegin (comm);
// ...other work
VecDotEnd (...,&dot);
```

**Classical GMRES**

**Pipelined GMRES**

Deep Pipelining

- Motivation: want to have perfect overlap of computation of inner products and SpMVs/preconditioner application
- But this depends on the machine, matrix, etc.
- If inner products take much longer than 1 SpMV, do $\ell$ SpMVs instead
  - $\Rightarrow$ "deep" pipelined method with pipeline length $\ell$
  - $\ell$ should be chosen to be the number of SpMV/precond. operations that can be done in the time it takes for one Allreduce

Available Software

- Implementations in PETSc:
  - KSPPGMRES: pipelined GMRES
  - KSPPPIPECG: pipelined CG
  - KSPPPIPECR: pipelined CR
  - KSPGROPPCG: Gropp asynchronous variant
  - KSPPPIPEBCGS: pipelined BiCGSTAB
  - KSPPPIPEELCG: deep pipelined CG
Performance of (Deep) Pipelined CG

Fig. 5. Strong scaling experiment on up to 20 nodes (240 processes) for a 5-point stencil 2D Poisson problem with 1,000,000 unknowns. Speedup over single-node classic CG for various pipeline lengths. All methods converged to $\|r_i\|_2/\|b\|_2 = 1.0e^{-5}$ in 1342 iterations.

Fig. 6. Strong scaling experiment on up to 48 nodes (672 processes) for a 5-point stencil 2D Poisson problem with 3,062,500 unknowns. Speedup over single-node classic CG for various pipeline lengths. All methods performed 1500 iterations with $\|r_i\|_2/\|b\|_2 = 6.3e^{-4}$.

Fig. 7. Strong scaling experiment on up to 32 nodes (448 processes) for a block Jacobi preconditioned 2D Poisson problem with 3,062,500 unknowns. All methods performed 600 iterations with $\|r_i\|_2/\|b\|_2 = 1.8e^{-4}$ (on 1 node) and $\|r_i\|_2/\|b\|_2 \leq 9.3e^{-4}$ (on 32 nodes).

20 compute nodes, each with two 6-core Intel Xeon X5660 Nehalem 2:80 GHz processors each (12 cores per node); 4QDR InfiniBand

48 compute nodes, each with two 14-core Intel E5-2680v4, Broadwell generation CPUs; EDR InfiniBand

(Cornelis, Cools, Vanroose, arXiv: 1801.04728, 2018)
s-step Krylov subspace methods

• Idea: Compute blocks of $s$ iterations at once
  • Compute updates in a different basis
  • Communicate every $s$ iterations instead of every iteration
  • Reduces number of synchronizations per iteration by a factor of $s$
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• Resurgence of interest in recent years due to growing problem sizes; growing relative cost of communication
History of $s$-step Krylov Subspace Methods

- Bai, Hu, and Reichel: GMRES
- de Sturler: GMRES
- Joubert and Carey: GMRES
- Kim and Chronopoulos: Arndoli, Symm. Lanczos
- Chronopoulos and Kim: Orthomin, Nonsymm. Lanczos
- Chronopoulos: MINRES, GCR, Orthomin
- Leland: CG
- Walker: GMRES
- Chronopoulos and Gear: CG
- Van Rosendale: CG
- Chronopoulos and Kim: Orthomin, GMRES
- Toledo: CG
- Erhel: GMRES
- de Sturler and van der Vorst: GMRES
- Chronopoulos and Kinkaid: Orthodir

First termed “$s$-step methods”
Key observation: After iteration $i$, for $j \in \{0, \ldots, s\}$,

$$x_{i+j} - x_i, \ r_{i+j}, \ p_{i+j} \in \mathcal{K}_{s+1}(A, p_i) + \mathcal{K}_s(A, r_i)$$
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s steps of s-step CG:
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\[
x_{i+j} - x_i, \quad r_{i+j}, \quad p_{i+j} \in \mathcal{K}_{s+1}(A, p_i) + \mathcal{K}_s(A, r_i)
\]

**s steps of s-step CG:**

Expand solution space $s$ dimensions at once
Compute “basis” matrix $Y$ such that $\text{span}(Y) = \mathcal{K}_{s+1}(A, p_i) + \mathcal{K}_s(A, r_i)$ according to the recurrence $AY = YB$
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**s steps of s-step CG:**

- **Expand solution space $s$ dimensions at once**
  - Compute “basis” matrix $Y$ such that $\text{span}(Y) = \mathcal{K}_{s+1}(A, p_i) + \mathcal{K}_s(A, r_i)$ according to the recurrence $AY = YB$

- **Compute inner products between basis vectors in one synchronization**
  - $G = Y^T Y$
Key observation: After iteration $i$, for $j \in \{0, \ldots, s\}$,

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$s$ steps of $s$-step CG:

Expand solution space $s$ dimensions at once
Compute “basis” matrix $Y$ such that $\text{span}(Y) = \mathcal{K}_{s+1}(A, p_i) + \mathcal{K}_s(A, r_i)$ according to the recurrence $AY = YB$

Compute inner products between basis vectors in one synchronization
$$G = Y^T Y$$

Compute $s$ iterations of vector updates
Perform $s$ iterations of vector updates by updating coordinates in basis $Y$:
$$x_{i+j} - x_i = Yx'_j, \quad r_{i+j} = Yr'_j, \quad p_{i+j} = Yp'_j$$
s-step CG

For $s$ iterations of updates, inner products and SpMVs (in basis $\mathcal{Y}$) can be computed by independently by each processor without communication:
s-step CG

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\[ Ap_{i+j} \]
s-step CG

For s iterations of updates, inner products and SpMVs (in basis $\mathcal{Y}$) can be computed by independently by each processor without communication:

$$A p_{i+j} = A \mathcal{Y} p'_j$$
s-step CG

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For s iterations of updates, inner products and SpMVs (in basis $\mathcal{Y}$) can be computed by independently by each processor without communication:

$$Ap_{i+j} = A\mathcal{Y}p'_j = \mathcal{Y}(Bp'_j)$$

$$\langle r_{i+j}, r_{i+j} \rangle = r_{j'}^T \mathcal{Y}^T \mathcal{Y} r_{j'}$$
s-step CG

For s iterations of updates, inner products and SpMVs (in basis $\mathcal{Y}$) can be computed by independently by each processor without communication:
s-step CG

\[ r_0 = b - Ax_0, p_0 = r_0 \]

for \( k = 0 : \text{nmax}/s \)

Compute \( y_k \) and \( B_k \) such that \( A y_k = y_k B_k \) and

\[ \text{span}(y_k) = \mathcal{K}_{s+1}(A,p_{sk}) + \mathcal{K}_s(A,r_{sk}) \]

\[ G_k = y_k^T y_k \]

\[ x_0' = 0, r_0' = e_{s+2}, p_0' = e_1 \]

for \( j = 1 : s \)

\[ \alpha_{sk+j-1} = \frac{r_{j-1}'^T G_k r_{j-1}'}{p_{j-1}'^T G_k B_k p_{j-1}'} \]

\[ x_j' = x_{j-1}' + \alpha_{sk+j-1} p_{j-1}' \]

\[ r_j' = r_{j-1}' - \alpha_{sk+j-1} B_k p_{j-1}' \]

\[ \beta_{sk+j} = \frac{r_j'^T G_k r_j'}{r_{j-1}'^T G_k r_{j-1}'} \]

\[ p_j' = r_j' + \beta_{sk+j} p_{j-1}' \]

end

\[ [x_{s(k+1)} - x_{sk}, r_{s(k+1)}, p_{s(k+1)}] = y_k [x_s', r_s', p_s'] \]

end
s-step CG

\[ r_0 = b - Ax_0, p_0 = r_0 \]

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\[ [x_{s(k+1)} - x_{sk}, r_{s(k+1)}, p_{s(k+1)}] = Y_k [x_s', r_s', p_s'] \]

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s-step CG

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Compute \( y_k \) and \( B_k \) such that \( A y_k = y_k B_k \) and

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\[ \alpha_{sk+j-1} = \frac{r_{j-1}'^T G_k r_{j-1}'}{p_{j-1}'^T G_k B_k p_{j-1}'} \]

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\[ p_j' = r_j' + \beta_{sk+j} p_{j-1}' \]

end

\[ [x_{s(k+1)} - x_{sk}, r_{s(k+1)}, p_{s(k+1)}] = y_k [x_s', r_s', p_s'] \]

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s-step CG

\[ r_0 = b - Ax_0, p_0 = r_0 \]

for \( k = 0:\text{nmax/s} \)

- Compute \( y_k \) and \( B_k \) such that \( A y_k = y_k B_k \) and \( \text{span}(y_k) = K_{s+1}(A, p_{sk}) + K_s(A, r_{sk}) \)

\[ G_k = y_k^T y_k \]

\[ x'_0 = 0, r'_0 = e_{s+2}, p'_0 = e_1 \]

for \( j = 1:s \)

\[ \alpha_{sk+j-1} = \frac{r_{j-1}' G_k r_{j-1}'}{p_{j-1}' G_k B_k p_{j-1}'} \]

\[ x'_j = x'_{j-1} + \alpha_{sk+j-1} p'_{j-1} \]

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\[ p'_j = r'_j + \beta_{sk+j} p'_{j-1} \]

end

\[ [x_s(k+1)-x_{sk}, r_s(k+1), p_s(k+1)] = y_k [x'_s, r'_s, p'_s] \]

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for \( j = 1 : s \)
\[
\alpha_{sk+j-1} = \frac{r'_{j-1}^T \mathcal{G}_k r'_{j-1}}{p'_{j-1}^T \mathcal{G}_k B_k p'_{j-1}}
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end

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end
Sparse Matrix Computations

• Sparse Matrix $\times$ Vector (SpMV) ($y = Ax$)
  • Very communication-bound; no reuse
  • Lower bound depends on sparsity structure, algorithm used (1D rowwise/colwise, 2D, etc.)
  • Communication cost depends on partition
  • Hypergraph models capture communication dependencies (Catalyurek, Aykanat, 1999)
    • minimize hypergraph cut = minimize words moved

Example: matrix of general linear operator on structured grid
  explicit values implicit positions

Example: general sparse matrix
  explicit values explicit positions

Example: stencil matrix
  implicit values implicit positions

Example: Laplacian matrix of a graph
  implicit values explicit positions
Sparse Matrix Computations

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- **Repeated SpMVs \((Y = [Ax, A^2x, ..., A^kx])\)**
  - Naive approach: \(k\) repeated SpMVs
  - Communication-avoiding approach: "matrix powers kernel"
    - see, e.g., (Demmel, Hoemmen, Mohiyuddin, Yelick, 2008)
$G = (V, E)$ where $V = \{y_0, ..., y_{n-1}\} \cup \{x_0, ..., x_{n-1}\}$ and $(y_i, x_j) \in E$ if $A_{ij} \neq 0$

Example: Tridiagonal matrix
SpMV Dependency Graph

\[ G = (V, E) \text{ where } V = \{y_0, \ldots, y_{n-1}\} \cup \{x_0, \ldots, x_{n-1}\} \text{ and } (y_i, x_j) \in E \text{ if } A_{ij} \neq 0 \]

Example: Tridiagonal matrix

\[
\begin{bmatrix}
  y_0 \\
  y_1 \\
  y_2 \\
  y_3 \\
  y_4 \\
  y
\end{bmatrix}
= \begin{bmatrix}
  x & x \\
  x & x & x \\
  x & x & x & x \\
  x & x & x & x \\
  x & x \\
  A
\end{bmatrix}
\begin{bmatrix}
  x_0 \\
  x_1 \\
  x_2 \\
  x_3 \\
  x_4 \\
  x
\end{bmatrix}
\Rightarrow A^2x
\]

\[ A^2x \]

\[
x_1 \quad x_2 \quad x_3
\]
Avoids communication:

- In serial, by exploiting temporal locality:
  - Reading $A$, reading vectors
- In parallel, by doing only 1 ‘expand’ phase (instead of $s$).
- Requires sufficiently low ‘surface-to-volume’ ratio

Tridiagonal Example:
Avoids communication:

• In serial, by exploiting temporal locality:
  • Reading $A$, reading vectors
• In parallel, by doing only 1 ‘expand’ phase (instead of $s$).
• Requires sufficiently low ‘surface-to-volume’ ratio

Tridiagonal Example:

Also works for general graphs!
Example: tridiagonal matrix, \( s = 3, n = 40, p = 4 \)
Parallel Matrix Powers Kernel

Example: tridiagonal matrix, \( s = 3, \ n = 40, \ p = 4 \)
Parallel Matrix Powers Kernel

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Naïve algorithm:
$s$ messages per neighbor
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**Naïve algorithm:**
$s$ messages per neighbor

**Matrix powers optimization:**
1 message per neighbor
Example of parallel (per processor) complexity for $s$ iterations of CG vs. $s$-step CG for a 2D 9-point stencil:

(Assuming each of $p$ processors owns $N/p$ rows of the matrix and $s \leq \sqrt{N/p}$)

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All values in the table meant in the Big-O sense (i.e., lower order terms and constants not included)
Complexity comparison

Example of parallel (per processor) complexity for $s$ iterations of CG vs. s-step CG for a 2D 9-point stencil:
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Classical GMRES

\[ r_0 = b - Ax_0, \quad v_0 = r_0 / \|r_0\| \]

for \( i = 1: k \)

\[ w = Av_{i-1} \]

Orthogonalize \( w \) against \([v_0, ..., v_{i-1}]\)

Update vector \( v_i \), matrix \( H \)

end

Use \( H, [v_0, ..., v_k] \) to construct the solution

e.g., Modified Gram-Schmidt
s-step GMRES

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s-step GMRES

\[ r_0 = b - Ax_0, v_0 = r_0 / \|r_0\| \]
for \( i = 0: s: k - s \)
\[ \text{Compute } W \text{ such that span}([v_i, W]) = \mathcal{K}_{s+1}(A, v_i) \]
Make \( W \) orthogonal against \([v_0, ..., v_i]\)
Make \( W \) orthogonal
Update \([v_{i+1}, ..., v_{i+s}]\), matrix \( H \)
end
Use \( H, [v_0, ..., v_k] \) to construct the solution

- "matrix powers kernel"
- Block Gram-Schmidt
- "Tall-Skinny QR"
Tall-Skinny QR (TSQR)

- TSQR: QR factorization of a tall skinny matrix using Householder transformations
- QR decomposition of $m \times b$ matrix $W$, $m \gg b$
  - $P$ processors, block row layout
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  • Compute Householder vector for each column
  • Number of messages $\propto b \log P$
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$$W = \begin{bmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{bmatrix}$$

- **Parallel**
  - $W = \begin{bmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{bmatrix}$
  - Reduction operation with QR as operator
  - Number of messages $\propto \log P$
  - Dual Core

- **Sequential**
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Parallel

$$W = \begin{bmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{bmatrix} \rightarrow R_{00} \rightarrow R_{01} \rightarrow R_{02}$$

Sequential

$$W = \begin{bmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{bmatrix} \rightarrow R_{00} \rightarrow R_{01} \rightarrow R_{02} \rightarrow R_{03}$$

Dual Core

$$W = \begin{bmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{bmatrix} \rightarrow R_{00} \rightarrow R_{01} \rightarrow R_{02} \rightarrow R_{03}$$

TSQR implementations in Intel MKL library, GNU Scientific Library, ScaLAPACK, Spark
Performance Results

Intel Clovertown ($r = k \cdot t = 60$)

(Mohiyuddin et al, 2009)
Performance and Applications

- Performance studies
  - s-step GMRES on hybrid CPU/GPU arch. (Yamazaki et al., 2014)
  - comparison of s-step and pipelined GMRES (Yamazaki et al., 2017)

Fig. 6. Parallel Strong Scaling of CA-GMRES and GMRES on 120 distributed GPUs (over GMRES on one GPU), for the G3 Circuit matrix.
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Fig. 6. Parallel Strong Scaling of CA-GMRES and GMRES on 120 distributed GPUs (over GMRES on one GPU), for the G3 Circuit matrix.

up to 4.2x on 24K cores on Cray XE6
Alternative Approaches

• Enlarged Krylov subspace methods (Grigori, Moufawad, Nataf, 2016)
  • Split vector into t parts based on domain decomposition of A; enlarge Krylov subspace by t dimensions each iteration
    • Faster convergence, more parallelizable

• Combined s-step pipelined methods
  • $(\ell, s)$-GMRES (Yamazaki, Hoemmen, Luszczek, Dongarra, 2017)
  • Hybrid approach which combines ideas of s-step and pipelined methods; reduces number of global synchronizations and also overlaps them with other work
Practical Implementation Challenges

• How to pick parameters? (pipeline depth in pipelined method; s in s-step method)
  • Choice must take into account matrix structure, machine, partition, as well as numerical properties (more on this next time!)

• Preconditioning
  • Must consider overlap in pipelined methods (if enough to overlap with)
  • For s-step, can diminish potential gain from matrix powers kernel if preconditioner is dense (but still win from savings in Allreduce)
Choosing s

• How do we expect communication costs to change as s increases?
  • Initially decrease, but at some point, start increasing
    • Point depends on sparsity structure of matrix, partition of matrix, and latency/bandwidth parameters of the machine
  • Bandwidth cost can start to dominate
  • For s large enough, the extra entries we need go past our neighbors boundaries
    • more messages required → increased latency cost

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Choosing s

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  • more messages required $\rightarrow$ increased latency cost

• For GMRES, best $s$ for matrix powers may not be best $s$ for TSQR kernel
  • Choice of $s$ requires co-tuning

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• Solomonik, C., Knight, Demmel (2014): Lower bounds on tradeoffs between three basic costs of a parallel algorithm: synchronization, data movement, and computational cost.

• By considering critical path, tradeoffs give lower bounds on the execution time which are dependent on the problem size but independent of the number of processors (assuming homogeneity)
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• Theorem: Any parallel execution of an $s$-dimensional Krylov basis computation for a $(2m + 1)^d$-point stencil on a $d$-dimensional regular mesh requires

$$\Omega(m^d b^d s) \text{ flops,}$$
$$\Omega(m^d b^{d-1} s) \text{ words,}$$
$$\Omega(s/b) \text{ messages,}$$

for some $b \in \{1, \ldots, s\}$
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for some $b \in \{1, \ldots, s\}$

• Matrix powers kernel attains this lower bound when $n^d / p \geq m^d b^d$

where $n^d$ is # mesh points
• Goal: estimate best blocking factor $b$ for matrix powers computation
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• Cost model:

\[
\text{Time} = \gamma \times \text{flops} + \beta \times \text{words moved} + \alpha \times \# \text{ messages}
\]
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• Choose $b$ to minimize

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Performance Modeling to Estimate Parameters

- Goal: estimate best blocking factor $b$ for matrix powers computation

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  \]

- Latency/BW tradeoff point: $b \sim \frac{\alpha^{1/d}}{m\beta^{1/d}}$
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• Starting place for parameter selection – to get close to optimal answer, would need more accurate model of time, costs including constants
Matrix Partitioning

• For computing matrix powers (i.e., constructing the basis matrix in s-step methods, we really want to partition the structure of $A^s$ rather than $A$
  • Analogous to single SpMV, can construct a hypergraph model such that the minimum cut gives a partition with minimum communication volume

• Load balancing
  • The parallel matrix powers kernel involves redundantly computing entries of the vectors on different processors
  • Entries which need to be redundantly computed determined by partition
Hypergraph Partitioning for Matrix Powers

Parallel communication for
\[ V = [x, Ax, A^2x, \ldots, A^s x], \]
given a sparse tiling of \( A \)

Parallel communication for
\[ y = A^s x, \]
given 1D rowwise layout of \( A^s \)

- “s-level” row- and column-nets encode the structure of \( A^s \)

\[ x \quad processor 1 \quad 10 \quad processor 2 \quad 20 \quad processor 3 \quad 30 \quad processor 4 \]

row-nets represent domain of dependence

column-nets represent domain of influence

(assuming no cancellation and nonzero diagonal)
Hypergraph Partitioning for Matrix Powers

Parallel communication for $V = [x, Ax, A^2x, ..., A^s x]$, given a sparse tiling of $A$

Parallel communication for $y = A^s x$, given 1D rowwise layout of $A^s$

- “s-level” row- and column-nets encode the structure of $A^s$
- But expensive to compute ($s \times$ Boolean sparse matrix-matrix multiplies)
  - Only worth it if $A$ has particularly irregular sparsity structure (e.g., number of nonzeros per column in $A^i$ grows at various rates) and same matrix will be reused
  - Potential use of randomized algorithms to estimate nnz/column in $A^i$
Preconditioning for s-step variants

• Preconditioners improve spectrum of system to improve convergence rate
  • E.g., instead of $Ax = b$, solve $M^{-1}Ax = M^{-1}b$, where $M^{-1} \approx A^{-1}$
  • Essential in practice
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    - Still potential gain from blocking inner products/avoiding global synchronization
  - If possible to avoid communication at all, usually necessitates significant modifications to the algorithm
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- Tradeoff: speed up convergence, but increase time per iteration due to communication!
  - For each specific app, must evaluate tradeoff between preconditioner quality and sparsity of the system
Preconditioning for s-step KSMs

• Much recent/ongoing work in developing communication-avoiding preconditioned methods

• Many approaches shown to be compatible
  • **Diagonal**
  • **Sparse Approx. Inverse (SPAI)** – for s-step BICGSTAB by Mehri (2014)
  • **HSS preconditioning** (Hoemmen, 2010); for banded matrices (Knight, C., Demmel, 2014); same general technique for any system that can be written as sparse + low-rank
  • **Deflation** for s-step CG (C., Knight, Demmel, 2014), for s-step GMRES (Yamazaki et al., 2014)
  • **CA-ILU(0)** – Moufawad and Grigori (2013)
  • **Domain decomposition** – avoid introducing additional communication by “underlapping” subdomains (Yamazaki et al., 2014)
"Underlapping" Domain Decomposition

(Yamazaki et al., 2014)

- Variant of an additive Schwarz preconditioner, modified to ensure consistent interfaces between the subdomains without additional communication beyond what is required by sparsity structure of $A$

In order to "localize" effects of preconditioner,
- form "interior" by removing s-level "underlap"
- apply "local" preconditioner on "interior"
  - ILU(k), SAI(k), Jacobi, GaussSeidel, etc. on "interior"
- apply diagonal Jacobi on "underlap"
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- apply diagonal Jacobi on "underlap"

Fig. 8. Matrix Partitioning for the CA Preconditioner for two subdomains. The underlap and the overlap relative to subdomain 1 are shown.

Fig. 11. Solution Convergence, using Different Domain Decomposition Preconditioners with Local ILU(0)'s on 6 GPUs.
The effects of finite precision

Well-known that roundoff error has two effects:

1. **Delay of convergence**
   - No longer have exact Krylov subspace
   - Can lose numerical rank deficiency
   - Residuals no longer orthogonal - Minimization of \( \| x - x_i \|_A \) no longer exact

2. **Loss of attainable accuracy**
   - Rounding errors cause true residual \( b - Ax_i \) and updated residual \( r_i \) deviate!

Much work on these results for CG; See Meurant and Strakoš (2006) for a thorough summary of early developments in finite precision analysis of Lanczos and CG
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   • Can lose numerical rank deficiency
   • Residuals no longer orthogonal - Minimization of \( \|x - x_i\|_A \) no longer exact

2. Loss of attainable accuracy
   • Rounding errors cause true residual \( b - Ax_i \) and updated residual \( r_i \) deviate!

Much work on these results for CG; See Meurant and Strakoš (2006) for a thorough summary of early developments in finite precision analysis of Lanczos and CG
Conjugate Gradient method for solving $Ax = b$

double precision ($\varepsilon = 2^{-53}$)

$$\|x_i - x\|_A = \sqrt{(x_i - x)^T A (x_i - x)}$$

\begin{align*}
x_i &= x_{i-1} + \alpha_i p_i \\
r_i &= r_{i-1} - \alpha_i A p_i \\
p_i &= r_i + \beta_i p_i
\end{align*}
Conjugate Gradient method for solving $Ax = b$

double precision ($\varepsilon = 2^{-53}$)

$$\|x_i - x\|_A = \sqrt{(x_i - x)^T A (x_i - x)}$$

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