Predict-and-recompute conjugate gradient variants

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Acknowledgements

We are gathered on the unceded land of the Coast Salish people, and in particular of the Duwamish Tribe.

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- Kelly Liu

Introduction

- Conjugate gradient (CG) is used to solve a linear system $\mathbf{Ax} = \mathbf{b}$ when $\mathbf{A} \in \mathbb{R}^{n \times n}$ is symmetric positive definite
- CG has low storage and floating point operation costs
  - one matrix vector product, two inner products, and a few vector updates each iteration
- Modern supercomputers have reached exascale (10^{18} flops)
  - Krylov subspace methods can only reach a fraction of this rate because of communication costs
- Convergence of CG in finite precision is not very well understood in general
- **Need to address communication costs, while considering numerical properties!**

The conjugate gradient algorithm

Algorithm 1 Hestenes and Stiefel Conjugate Gradient (preconditioned)

procedure HS-CG($\mathbf{A}$, $\mathbf{M}$, $\mathbf{b}$, $\mathbf{x}_0$)
  initialize()
  for $k = 1, 2, \ldots$ **do**
    $\mathbf{x}_k = \mathbf{x}_{k-1} + \alpha_{k-1}\mathbf{p}_{k-1}$
    $\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_{k-1}\mathbf{s}_{k-1},\ \tilde{\mathbf{r}}_k = \mathbf{M}^{-1}\mathbf{r}_k$
    $\nu_k = \langle \tilde{\mathbf{r}}_k, \mathbf{r}_k \rangle$
    $\beta_k = \nu_k / \nu_{k-1}$
    $\mathbf{p}_k = \tilde{\mathbf{r}}_k + \beta_k \mathbf{p}_{k-1}$
    $\mathbf{s}_k = \mathbf{A}\mathbf{p}_k$
    $\mu_k = \langle \mathbf{p}_k, \mathbf{s}_k \rangle$
    $\alpha_k = \nu_k / \mu_k$
  end for
end procedure

Communication costs

- on large machines the cost of reading and moving data dominates the cost of floating point operations
- inner products and dense matrix vector products require global communication
- sparse matrix vector products require local communication
- vector updates require no communication

Hiding communication

- In each iteration we would like to hide communication by computing all inner products and matrix vector products simultaneously
- Do this by finding mathematically equivalent expressions for an inner product using recurrences
  - the new expressions are not equivalent in finite precision; i.e. the order of things has changed
- various ways of doing this have been studied before; see for instance[1]
  - typically maintain two inner products and one matrix vector product per iteration

[1] Saad 1985; Meurant 1987; Saad 1989; Chronopoulos and Gear 1989; Ghysels and Vanroose 2014; Cornelis, Cools, and Vanroose 2019.

Hiding communication

- CG is particularly sensitive to any rounding errors
- changing the order in which computations are performed can have an impact
- some of the communication hiding variants have very different behavior[2]
  - various approaches to deal with this; e.g. residual replacement[3], basis vector shifts[4], etc.

[2] Carson, Rozložník, Strakoš, Tichý, and Tůma 2018.

[3] Cools, Fatih Yetkin, Agullo, Giraud, and Vanroose 2018.

[4] Cornelis, Cools, and Vanroose 2019.

Hiding communication

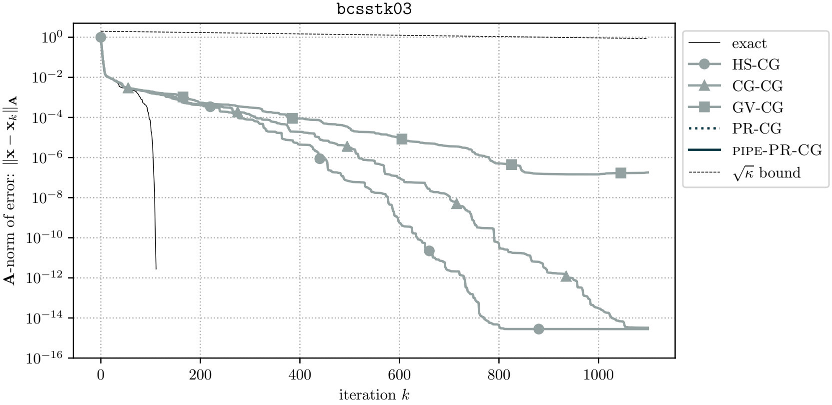
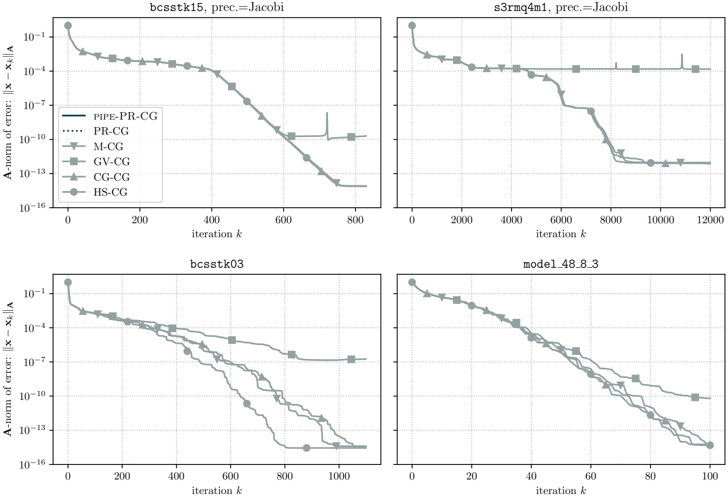


Figure: Convergence of finite precision conjugate gradient

Hiding communication



Finite precision conjugate gradient

- In finite precision orthogonality is lost, so induction based arguments for optimality of iterates no longer hold
- The primary effects are:
  - Delay of convergence
  - Loss of ultimately attainable accuracy
- There is numerical analysis theory for both effects:
  - Delay of convergence: perturbed Lanczos recurrence[5]
    - $\mathbf{A}\mathbf{Q}_k = \mathbf{Q}_k\mathbf{T}_k + \gamma_k \mathbf{q}_{k+1}\mathbf{e}_k^\top + \mathbf{F}_k$
  - Loss of accuracy: residual gap[6]
    - $\Delta_{\mathbf{r}_k} := (\mathbf{b} - \mathbf{A}\mathbf{x}_k) - \mathbf{r}_k$

[5] Paige 1976; Paige 1980; Greenbaum 1989.

[6] Greenbaum 1997.

Finite precision conjugate gradient

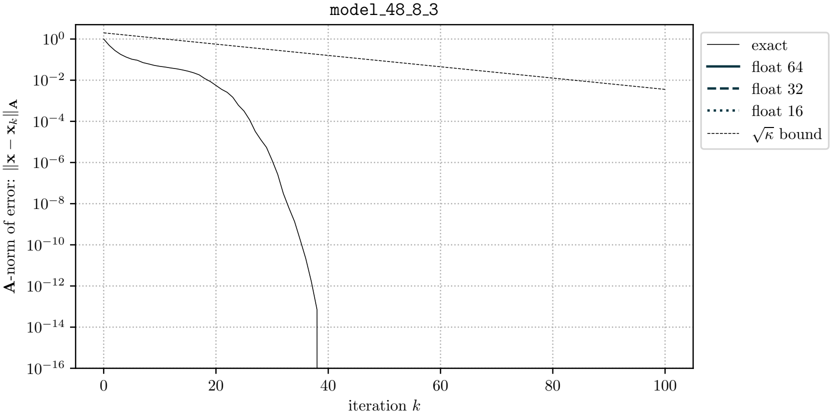


Figure: Convergence of finite precision conjugate gradient

Finite precision conjugate gradient

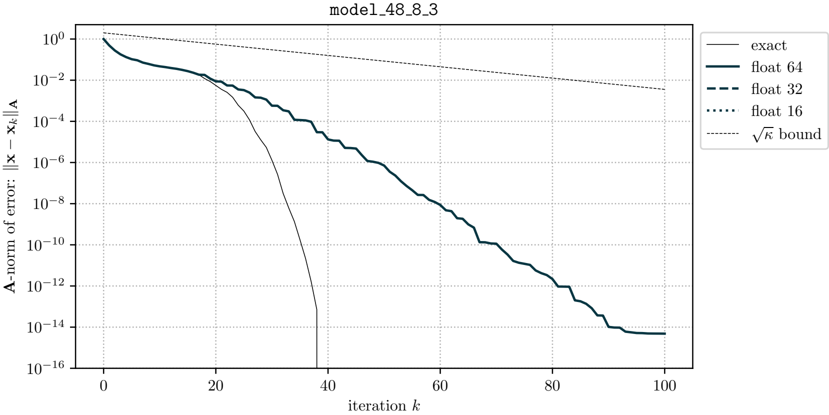


Figure: Convergence of finite precision conjugate gradient

Finite precision conjugate gradient

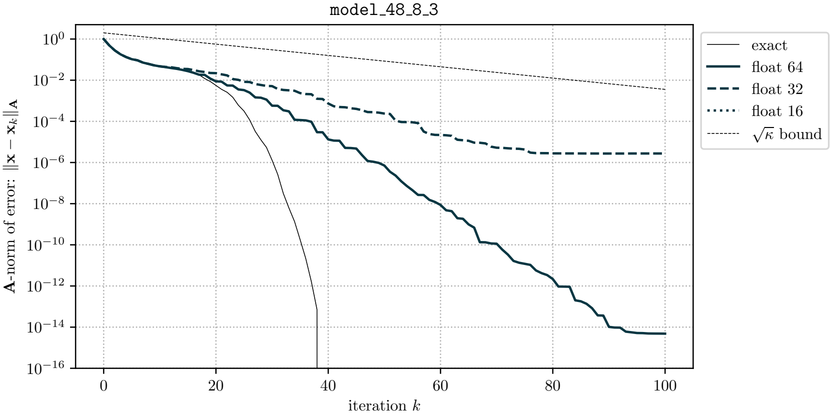


Figure: Convergence of finite precision conjugate gradient

Finite precision conjugate gradient

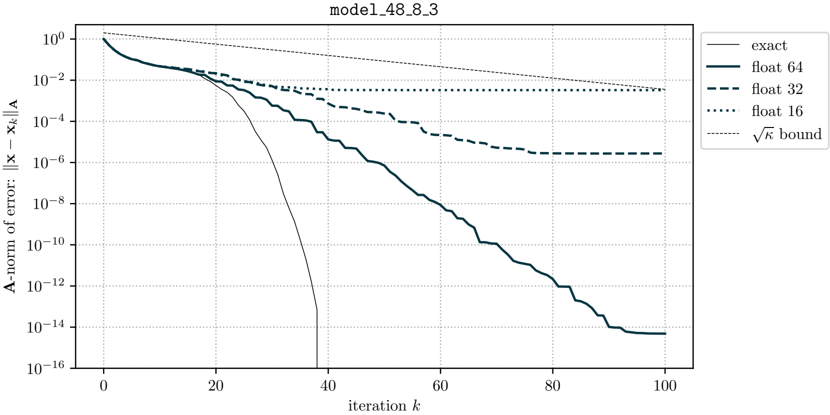


Figure: Convergence of finite precision conjugate gradient

Predict-and-recompute variants

- **idea**: use recursively updated quantities as a predictor for their true values to allow iteration to continue, then recompute them directly at a later point in the iteration
- if this is done in a smart way, it won't affect the communication structure of the algorithm

Predict-and-recompute variants

Algorithm 2 Hestenes and Stiefel Conjugate Gradient (preconditioned)

procedure HS-CG($\mathbf{A}$, $\mathbf{M}$, $\mathbf{b}$, $\mathbf{x}_0$)
  initialize()
  for $k = 1, 2, \ldots$ **do**
    $\mathbf{x}_k = \mathbf{x}_{k-1} + \alpha_{k-1}\mathbf{p}_{k-1}$
    $\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_{k-1}\mathbf{s}_{k-1}, \;\; \tilde{\mathbf{r}}_k = \mathbf{M}^{-1}\mathbf{r}_k$
    $\nu_k = \langle \tilde{\mathbf{r}}_k, \mathbf{r}_k \rangle$
    $\beta_k = \nu_k / \nu_{k-1}$
    $\mathbf{p}_k = \tilde{\mathbf{r}}_k + \beta_k \mathbf{p}_{k-1}$
    $\mathbf{s}_k = \mathbf{A}\mathbf{p}_k$
    $\mu_k = \langle \mathbf{p}_k, \mathbf{s}_k \rangle$
    $\alpha_k = \nu_k / \mu_k$
  end for
end procedure

Predict-and-recompute variants

Algorithm 3 Predict-and-recompute conjugate gradient

procedure PR-CG($\mathbf{A}$, $\mathbf{M}$, $\mathbf{b}$, $\mathbf{x}_0$)
    initialize()
    for $k = 1, 2, \ldots$ **do**
        $\mathbf{x}_k = \mathbf{x}_{k-1} + \alpha_{k-1}\mathbf{p}_{k-1}$
        $\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_{k-1}\mathbf{s}_{k-1},\ \tilde{\mathbf{r}}_k = \tilde{\mathbf{r}}_{k-1} - \alpha_{k-1}\tilde{\mathbf{s}}_{k-1}$
        $\nu'_k = \nu_{k-1} - 2\alpha_{k-1}\delta_{k-1} + \alpha_{k-1}^2\gamma_{k-1}$
        $\beta_k = \nu'_k/\nu_{k-1}$
        $\mathbf{p}_k = \tilde{\mathbf{r}}_k + \beta_k\mathbf{p}_{k-1}$
        $\mathbf{s}_k = \mathbf{A}\mathbf{p}_k,\ \tilde{\mathbf{s}}_k = \mathbf{M}^{-1}\mathbf{s}_k$
        $\mu_k = \langle \mathbf{p}_k, \mathbf{s}_k\rangle,\ \delta_k = \langle \tilde{\mathbf{r}}_k, \mathbf{s}_k\rangle,\ \gamma_k = \langle \tilde{\mathbf{s}}_k, \mathbf{s}_k\rangle,\ \nu_k = \langle \tilde{\mathbf{r}}_k, \mathbf{r}_k\rangle$
        $\alpha_k = \nu_k/\mu_k$
    end for
end procedure

Predict-and-recompute variants

Algorithm 4 Pipelined predict-and-recompute conjugate gradient

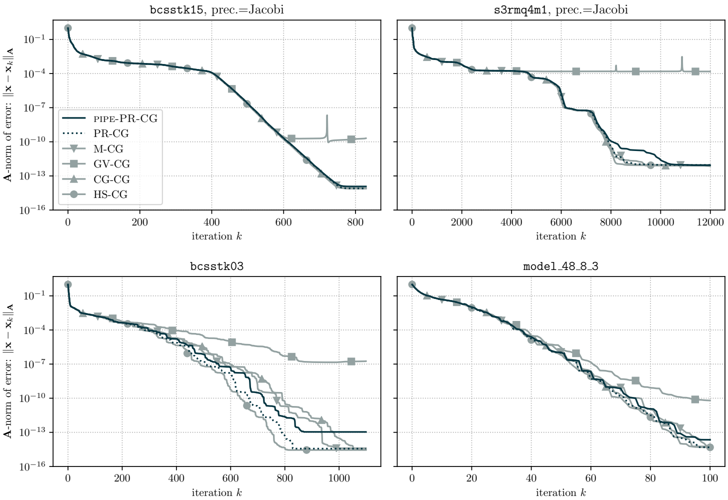
procedure pipe-PR-CG($\mathbf{A}$, $\mathbf{M}$, $\mathbf{b}$, $\mathbf{x}_0$)
  initialize()
  for $k = 1, 2, \ldots$ **do**
    $\mathbf{x}_k = \mathbf{x}_{k-1} + \alpha_{k-1}\mathbf{p}_{k-1}$
    $\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_{k-1}\mathbf{s}_{k-1}$, $\tilde{\mathbf{r}}_k = \tilde{\mathbf{r}}_{k-1} - \alpha_{k-1}\tilde{\mathbf{s}}_{k-1}$
    $\mathbf{w}'_k = \mathbf{w}_{k-1} - \alpha_{k-1}\mathbf{u}_{k-1},\ \tilde{\mathbf{w}}'_k = \tilde{\mathbf{w}}_{k-1} - \alpha_{k-1}\tilde{\mathbf{u}}_{k-1}$
    $\nu'_k = \nu_{k-1} - 2\alpha_{k-1}\delta_{k-1} + \alpha_{k-1}^2\gamma_{k-1}$
    $\beta_k = \nu'_k/\nu_{k-1}$
    $\mathbf{p}_k = \tilde{\mathbf{r}}_k + \beta_k\mathbf{p}_{k-1}$
    $\mathbf{s}_k = \mathbf{w}'_k + \beta_k\mathbf{s}_{k-1},\ \tilde{\mathbf{s}}_k = \tilde{\mathbf{w}}'_k + \beta_k\tilde{\mathbf{s}}_{k-1}$
    $\mathbf{u}_k = \mathbf{A}\tilde{\mathbf{s}}_k,\ \tilde{\mathbf{u}}_k = \mathbf{M}^{-1}\mathbf{u}_k$
    $\mathbf{w}_k = \mathbf{A}\tilde{\mathbf{r}}_k,\ \tilde{\mathbf{w}}_k = \mathbf{M}^{-1}\mathbf{w}_k$
    $\mu_k = \langle \mathbf{p}_k, \mathbf{s}_k\rangle,\ \delta_k = \langle \tilde{\mathbf{r}}_k, \mathbf{s}_k\rangle,\ \gamma_k = \langle \tilde{\mathbf{s}}_k, \mathbf{s}_k\rangle,\ \nu_k = \langle \tilde{\mathbf{r}}_k, \mathbf{r}_k\rangle$
    $\alpha_k = \nu_k/\mu_k$
  end for
end procedure

Predict-and-recompute variants

variant	mem.	vec.	scal.	time
HS-CG	4 (+1)	3 (+0)	2	$2\,\mathrm{C}_{\mathsf{gr}} + \mathrm{T}_{\mathsf{mv}} + \mathrm{C}_{\mathsf{mv}}$
CG-CG	5 (+1)	4 (+0)	2	$\mathrm{C}_{\mathsf{gr}} + \mathrm{T}_{\mathsf{mv}} + \mathrm{C}_{\mathsf{mv}}$
M-CG	4 (+2)	3 (+1)	3	$\mathrm{C}_{\mathsf{gr}} + \mathrm{T}_{\mathsf{mv}} + \mathrm{C}_{\mathsf{mv}}$
PR-CG	4 (+2)	3 (+1)	4	$\mathrm{C}_{\mathsf{gr}} + \mathrm{T}_{\mathsf{mv}} + \mathrm{C}_{\mathsf{mv}}$
GV-CG	7 (+3)	6 (+2)	2	$\max(\mathrm{C}_{\mathsf{gr}}, \mathrm{T}_{\mathsf{mv}} + \mathrm{C}_{\mathsf{mv}})$
pipe-PR-M-CG	6 (+4)	5 (+3)	3	$\max(\mathrm{C}_{\mathsf{gr}}, \mathrm{T}_{2\mathsf{mv}} + \mathrm{C}_{\mathsf{mv}})$
pipe-PR-CG	6 (+4)	5 (+3)	4	$\max(\mathrm{C}_{\mathsf{gr}}, \mathrm{T}_{2\mathsf{mv}} + \mathrm{C}_{\mathsf{mv}})$

Table: Summary of costs for various conjugate gradient variants. Values in parenthesis are the additional costs for the preconditioned variants.

Predict-and-recompute variants



Predict-and-recompute variants

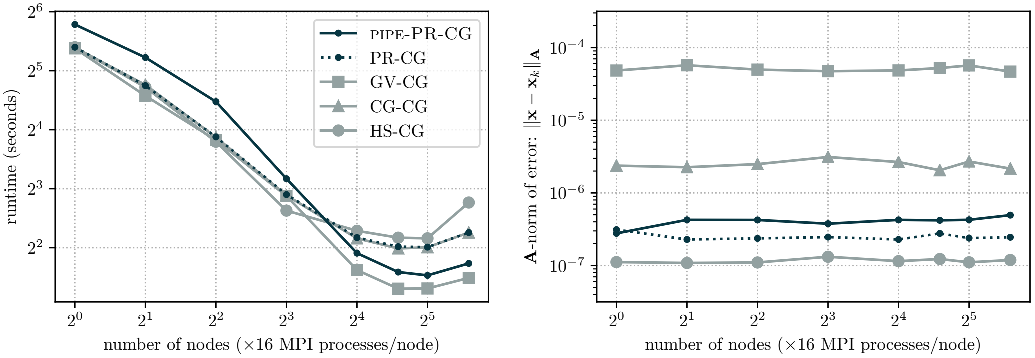


Figure: Convergence of conjugate gradient variants

Predict-and-recompute variants

- expressions for residual gap, and three term Lanczos recurrence, and ν'_k gap for PR-CG and pipe-PR-CG provides insight into improved convergence[7]
- practical use remains to be determined
- but, will be included in PETSc v3.13: `-ksp_type pipeprcg`
  - in this code the two matrix products are not overlapped with one another: is there an easy way to do this in PETSc?

[7] Chen and Carson 2020.

Predict-and-recompute variants

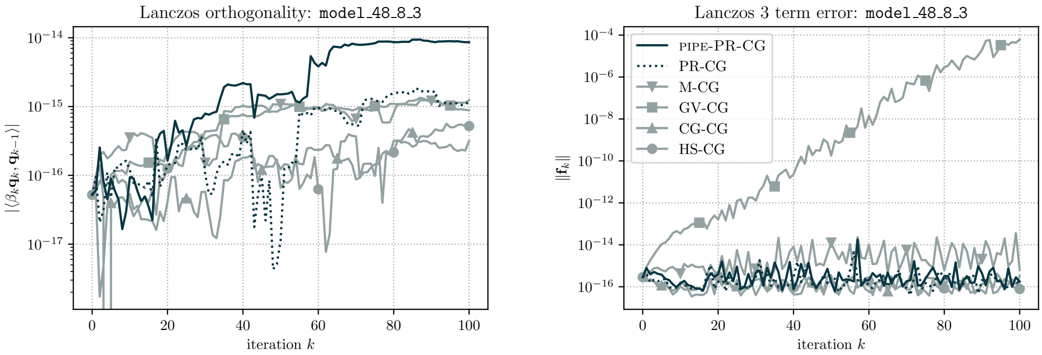


Figure: Perturbed Lanczos recurrence measures

Future work

- Try to incorporate predict-and-recompute idea into s-step methods
- Selective re-orthogonalization in low precision or high performance contexts
- Further numerical analysis of CG
  - when does $\mathbf{r}_k \to 0$?
  - when is $\langle \mathbf{r}_k, \mathbf{r}_{k-1} \rangle \approx 0$?
  - can we determine which problems will be "hard" ahead of time?

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