Latency hiding of global reductions in pipelined Krylov methods

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What are we working on?

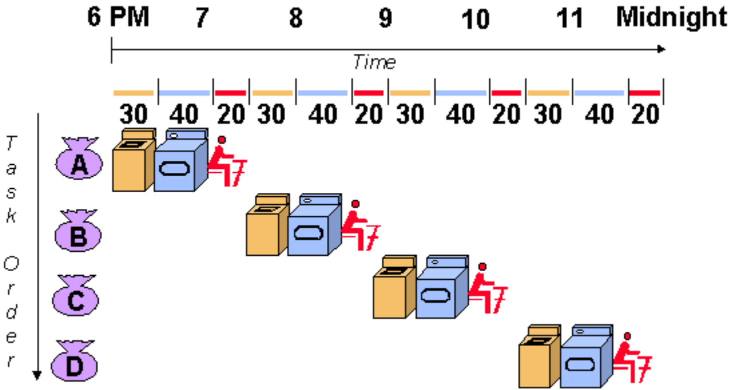

Figure: Latency hiding of global *drying* in pipelined *Laundry* methods

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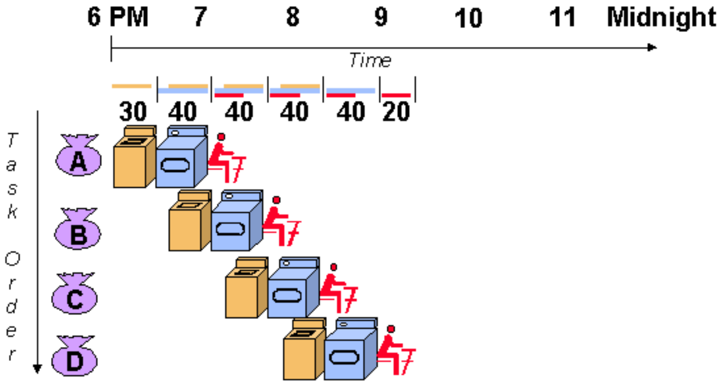
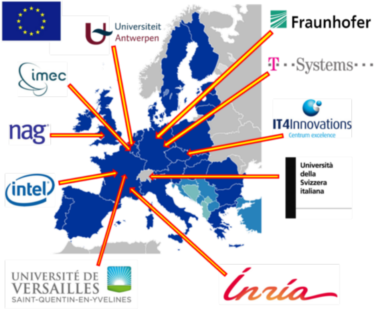


Figure: Latency hiding of global *drying* in pipelined *Laundry* methods

What EXA2CT-ly are we working on?



Increasing gap between computation and communication costs

- Floating point performance steadily increases
- Network latencies only go down marginally
- Memory latencies decline slowly
- Avoid communication by trading communication for computation
- Hide latency of communications

EXascale Algorithms and Advanced Computational Techniques

`https://projects.imec.be/exa2ct/`

Outline of the talk

Krylov subspace methods
(cf. Laundry methods)

Hiding global reductions
(cf. hiding drying time)

Increasing arithmetic intensity
(cf. piling up laundry)

Conclusions & future work
(cf. washing instructions and ecological detergents)

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General idea

Iteratively improve an approximate solution of linear system $Ax = b$,

$$x_i \in x_0 + \mathcal{K}_i(A, r_0) = x_0 + \mathrm{span}\{r_0, Ar_0, A^2 r_0, \dots, A^{i-1} r_0\}$$

- minimize an error measure over expanding Krylov subspace $\mathcal{K}_i(A, r_0)$
- usually in combination with sparse linear algebra
- three building blocks
  - i. axpy
  - ii. SpMVM
  - iii. dot-product

E.g.: Conjugate Gradients

$r^{(0)} \leftarrow b - Ax^{(0)}$
$p^{(0)} \leftarrow r^{(0)}$
for $i = 0, \dots$ **do**
  $w \leftarrow Ap^{(i)}$
  $\alpha_i \leftarrow (r^{(i)}, r^{(i)})/(w, p^{(i)})$
  $x^{(i+1)} \leftarrow x^{(i)} + \alpha_i p^{(i)}$
  $r^{(i+1)} \leftarrow r^{(i)} - \alpha_i w$
  $\beta_i \leftarrow (r^{(i+1)}, r^{(i+1)})/(r^{(i)}, r^{(i)})$
  $p^{(i+1)} \leftarrow r^{(i+1)} + \beta_i p^{(i)}$
end for

General idea

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end for

Communication patterns in the building blocks

i. axpy
  - no dependencies on other vector elements (no communication)
  - scales well

ii. SpMVM
  - dependencies given by matrix/vector partition (one-to-one communication)
  - bandwidth limited
  - scales

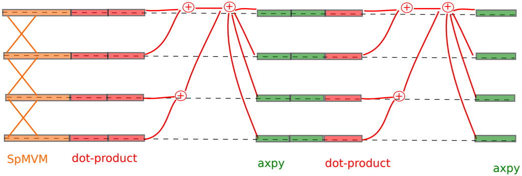
iii. dot-product
  - dependency on all vector elements (global reduction)
  - latency dominated
  - scales as $log_2(\#partitions)$

E.g.: Conjugate Gradients

1: $r^{(0)} \leftarrow b - Ax^{(0)}$
2: $p^{(0)} \leftarrow r^{(0)}$
3: **for** $i = 0, \ldots$ **do**
4: $\quad w \leftarrow Ap^{(i)}$
5: $\quad \alpha_i \leftarrow (r^{(i)}, r^{(i)})/(w, p^{(i)})$
6: $\quad x^{(i+1)} \leftarrow x^{(i)} + \alpha_i p^{(i)}$
7: $\quad r^{(i+1)} \leftarrow r^{(i)} - \alpha_i w$
8: $\quad \beta_i \leftarrow (r^{(i+1)}, r^{(i+1)})/(r^{(i)}, r^{(i)})$
9: $\quad p^{(i+1)} \leftarrow r^{(i+1)} + \beta_i p^{(i)}$
10: **end for**

Case study: Conjugate Gradients

Hestenes and Stiefel (1952)



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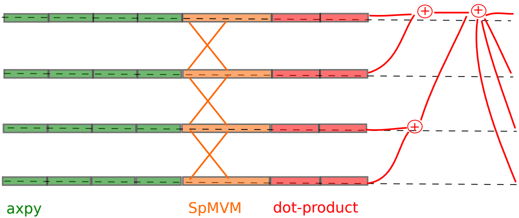
  $x^{(i+1)} \leftarrow x^{(i)} + \alpha_i p^{(i)}$
  $r^{(i+1)} \leftarrow r^{(i)} - \alpha_i w$
  $\beta_i \leftarrow (r^{(i+1)}, r^{(i+1)})/(r^{(i)}, r^{(i)})$
  $p^{(i+1)} \leftarrow r^{(i+1)} + \beta_i p^{(i)}$
end for

Case study: Conjugate Gradients

Chronopoulos and Gear (1989)



$r_{(0)} \leftarrow b - Ax^{(0)}$

... (loop-unrolling)

for $i = 1, \ldots$ **do**

$\quad p^{(i)} \leftarrow r^{(i)} + \beta_i p^{(i-1)}$

$\quad s^{(i)} \leftarrow w^{(i)} + \beta_i s^{(i-1)}$

$\quad x^{(i+1)} \leftarrow x^{(i)} + \alpha_i p^{(i)}$

$\quad r^{(i+1)} \leftarrow r^{(i)} - \alpha_i s^{(i)}$

$\quad w^{(i+1)} \leftarrow Ar^{(i+1)}$

$\quad \gamma_{i+1} \leftarrow (r^{(i+1)}, r^{(i+1)})$

$\quad \delta \leftarrow (w^{(i+1)}, r^{(i+1)})$

$\quad \beta_{i+1} \leftarrow \gamma_{i+1}/\gamma_i$

$\quad \alpha_{i+1} \leftarrow \gamma_{i+1}/(\delta - \beta_{i+1}\gamma_{i+1}/\alpha_i)$

end for

Krylov subspace methods

Case study: Conjugate Gradients

Chronopoulos and Gear (1989)

- Equivalent to CG (in infinite precision)
- Extra recurrence relation for $s^{(i)} = Ap^{(i)}$
- Two dot-products are grouped in one global reduction
- Communication avoiding

$r_{(0)} \leftarrow b - Ax^{(0)}$
. . . (loop-unrolling)
for $i = 1, \ldots$ **do**
    $p^{(i)} \leftarrow r^{(i)} + \beta_i p^{(i-1)}$
    $s^{(i)} \leftarrow w^{(i)} + \beta_i s^{(i-1)}$
    $x^{(i+1)} \leftarrow x^{(i)} + \alpha_i p^{(i)}$
    $r^{(i+1)} \leftarrow r^{(i)} - \alpha_i s^{(i)}$
    $w^{(i+1)} \leftarrow Ar^{(i+1)}$
    $\gamma_{i+1} \leftarrow (r^{(i+1)}, r^{(i+1)})$
    $\delta \leftarrow (w^{(i+1)}, r^{(i+1)})$
    $\beta_{i+1} \leftarrow \gamma_{i+1}/\gamma_i$
    $\alpha_{i+1} \leftarrow \gamma_{i+1}/(\delta - \beta_{i+1}\gamma_{i+1}/\alpha_i)$
end for

Outline of the talk

Krylov subspace methods
(cf. Laundry methods)

Hiding global reductions
(cf. hiding drying time)

Increasing arithmetic intensity
(cf. piling up laundry)

Conclusions & future work
(cf. washing instructions and ecological detergents)

- Dot-products are latency dominated
- Dot-products block all other (local) work
- Other (local) operations (SpMVM/axpy) scale well

Objective

Rewrite Krylov solvers such that latency of dot-products (global reductions) can be overlapped with application of the SpMVM and/or the preconditioner.

- Use non-blocking asynchronous global communication
- MPI-3 standard introduces `MPI_Iallreduce()`
- GPI-2 introduces `gaspi_allreduce()` + uses PGAS (partitioned global address space)

Hiding global reductions
Pipelined Conjugate Gradients

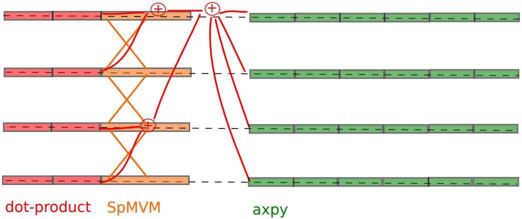
Ghysels and Vanroose (2013)

- Equivalent to CG (in infinite precision)
- Extra recurrence relations for $s^{(i)} = Ap^{(i)}$ and $z = As^{(i)}$
- Two dot-products are grouped in one global reduction
- Communication avoiding
- Overlap global communication with local computations: line 4 + 5 + 6
- Communication avoiding
  \+ communication hiding

1: $r_{(0)} \leftarrow b - Ax^{(0)}$
2: $\ldots$ (loop-unrolling)
3: **for** $i = 1, \ldots$ **do**
4: $\quad \gamma_i \leftarrow (r^{(i)}, r^{(i)})$
5: $\quad \delta \leftarrow (w^{(i)}, r^{(i)})$
6: $\quad q^{(i)} \leftarrow Aw^{(i)}$
7: $\quad \beta_i \leftarrow \gamma_i / \gamma_{i-1}$
8: $\quad \alpha_i \leftarrow \gamma_i / (\delta - \beta_i \gamma_i / \alpha_{i-1})$
9: $\quad z^{(i)} \leftarrow q^{(i)} + \beta_i z^{(i-1)}$
10: $\quad s^{(i)} \leftarrow w^{(i)} + \beta_i s^{(i-1)}$
11: $\quad p^{(i)} \leftarrow r^{(i)} + \beta_i p^{(i-1)}$
12: $\quad x^{(i+1)} \leftarrow x^{(i)} + \alpha_i p^{(i)}$
13: $\quad r^{(i+1)} \leftarrow r^{(i)} - \alpha_i s^{(i)}$
14: $\quad w^{(i+1)} \leftarrow w^{(i)} - \alpha_i z^{(i)}$
15: **end for**

Pipelined Conjugate Gradients

Ghysels and Vanroose (2013)



$r_{(0)} \leftarrow b - Ax^{(0)}$
$\ldots$ (loop-unrolling)
for $i = 1, \ldots$ **do**
$\quad \gamma_i \leftarrow (r^{(i)}, r^{(i)})$
$\quad \delta \leftarrow (w^{(i)}, r^{(i)})$
$\quad q^{(i)} \leftarrow Aw^{(i)}$
$\quad \beta_i \leftarrow \gamma_i / \gamma_{i-1}$
$\quad \alpha_i \leftarrow \gamma_i / (\delta - \beta_i \gamma_i / \alpha_{i-1})$
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$\quad r^{(i+1)} \leftarrow r^{(i)} - \alpha_i s^{(i)}$
$\quad w^{(i+1)} \leftarrow w^{(i)} - \alpha_i z^{(i)}$
end for

Preconditioned pipelined Conjugate Gradients

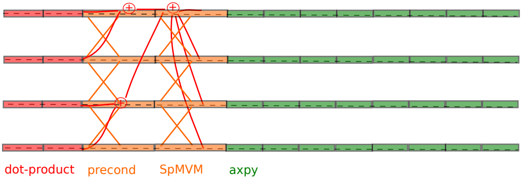
Ghysels and Vanroose (2013)

- Equivalent to CG (in infinite precision)
- Extra recurrence relations for $w^{(i)} = Au^{(i)}$, $s^{(i)} = Ap^{(i)}$ and $z = Aq^{(i)}$
- Two dot-products are grouped in one global reduction
- Overlap global communication with *extra* local computations: line 4 + 5 + 7 + 6
- Communication avoiding + communication hiding

1: $r_{(0)} \leftarrow b - Ax^{(0)}$
2: ... (loop-unrolling)
3: **for** $i = 1, \dots$ **do**
4: $\quad \gamma_i \leftarrow (r^{(i)}, u^{(i)})$
5: $\quad \delta \leftarrow (w^{(i)}, u^{(i)})$
6: $\quad m^{(i)} \leftarrow M^{-1} w^{(i)}$
7: $\quad n^{(i)} \leftarrow Am^{(i)}$
8: $\quad \beta_i \leftarrow \gamma_i / \gamma_{i-1}$
9: $\quad \alpha_i \leftarrow \gamma_i / (\delta - \beta_i \gamma_i / \alpha_{i-1})$
10: $\quad z^{(i)} \leftarrow n^{(i)} + \beta_i z^{(i-1)}$
11: $\quad q^{(i)} \leftarrow m^{(i)} + \beta_i q^{(i-1)}$
12: $\quad s^{(i)} \leftarrow w^{(i)} + \beta_i s^{(i-1)}$
13: $\quad p^{(i)} \leftarrow u^{(i)} + \beta_i p^{(i-1)}$
14: $\quad x^{(i+1)} \leftarrow x^{(i)} + \alpha_i p^{(i)}$
15: $\quad r^{(i+1)} \leftarrow r^{(i)} - \alpha_i s^{(i)}$
16: $\quad u^{(i+1)} \leftarrow u^{(i)} - \alpha_i q^{(i)}$
17: $\quad w^{(i+1)} \leftarrow w^{(i)} - \alpha_i z^{(i)}$
18: **end for**

Preconditioned pipelined Conjugate Gradients

Ghysels and Vanroose (2013)



$r_{(0)} \leftarrow b - Ax^{(0)}$
... (loop-unrolling)
for $i = 1, \ldots$ **do**
    $\gamma_i \leftarrow (r^{(i)}, u^{(i)})$
    $\delta \leftarrow (w^{(i)}, u^{(i)})$
    $m^{(i)} \leftarrow M^{-1} w^{(i)}$
    $n^{(i)} \leftarrow Am^{(i)}$
    $\beta_i \leftarrow \gamma_i / \gamma_{i-1}$
    $\alpha_i \leftarrow \gamma_i / (\delta - \beta_i \gamma_i / \alpha_{i-1})$
    $z^{(i)} \leftarrow n^{(i)} + \beta_i z^{(i-1)}$
    $q^{(i)} \leftarrow m^{(i)} + \beta_i q^{(i-1)}$
    $s^{(i)} \leftarrow w^{(i)} + \beta_i s^{(i-1)}$
    $p^{(i)} \leftarrow u^{(i)} + \beta_i p^{(i-1)}$
    $x^{(i+1)} \leftarrow x^{(i)} + \alpha_i p^{(i)}$
    $r^{(i+1)} \leftarrow r^{(i)} - \alpha_i s^{(i)}$
    $u^{(i+1)} \leftarrow u^{(i)} - \alpha_i q^{(i)}$
    $w^{(i+1)} \leftarrow w^{(i)} - \alpha_i z^{(i)}$
end for

Preconditioned pipelined Conjugate Residuals

Ghysels and Vanroose (2013)

- Equivalent to CR (in infinite precision)
- Based on $(\cdot,\cdot)_A$-inner product
- Two dot-products are grouped in one global reduction
- Overlap global communication with local computations: line 5 + 6 + 7
- No overlap with preconditioner
- Only 3 additional axpy's save memory

1: $r_{(0)} \leftarrow b - Ax^{(0)}$
2: ... (loop-unrolling)
3: **for** $i = 1, \ldots$ **do**
4: $\quad m^{(i)} \leftarrow M^{-1} w^{(i)}$
5: $\quad \gamma_i \leftarrow (w^{(i)}, u^{(i)})$
6: $\quad \delta \leftarrow (m^{(i)}, w^{(i)})$
7: $\quad n^{(i)} \leftarrow Am^{(i)}$
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14: $\quad u^{(i+1)} \leftarrow u^{(i)} - \alpha_i q^{(i)}$
15: $\quad w^{(i+1)} \leftarrow w^{(i)} - \alpha_i z^{(i)}$
16: **end for**

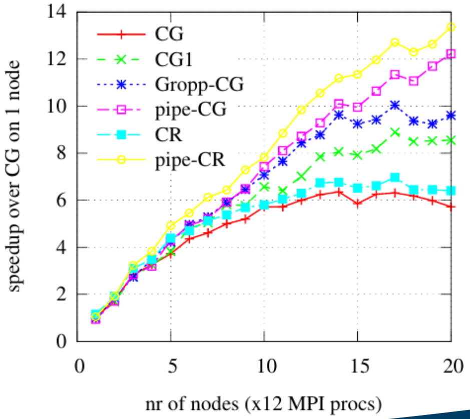
Comparison of CG variants

	flops	time (excl axpy's, dot's)	# syncs	mem
CG	10	2G + SpMVM + PC	2	4
Chron/Gear-CG	12	G + SpMVM + PC	1	5
Gropp-CG	14	max(G,SpMVM) + max(G,PC)	2	6
pipe-CG	20	max(G,SpMVM+PC)	1	9
CR	12	2G + SpMVM + PC	2	5
pipe-CR	16	max(G,SpMVM) + PC	1	7

- G: latency of global reduction
- SpMVM: sparse matrix-vector time
- PC: application of preconditioner

Strong scaling experiment

- Hydrostatic ice sheet flow, $100 \times 100 \times 50$ Q1 finite elements
- Line search Newton method (rtol$=10^{-8}$, atol$=10^{-15}$)
- CG preconditioned with block Jacobi with ICC(0) (rtol$=10^{-5}$, atol$=10^{-50}$)



- max pipe-CG/CG speedup: $2.14\times$
  max pipe-CG/CG1 speedup: $1.43\times$
- max pipe-CR/CR speedup: $2.09\times$

(CG1 = Chrono/Gear CG)

Other pipelined Krylov methods

- Preconditioned pipelined GMRES

  Ghysels, Ashby, Meerbergen and Vanroose (2012)

$$
\begin{aligned}
V_{i-\ell+1} &= [v_0, v_1, \ldots, v_{i-\ell}] \\
Z_{i+1} &= [z_0, z_1, \ldots, z_{i-\ell}, \underbrace{z_{i-\ell+1}, \ldots, z_i}_{\ell}]
\end{aligned}
$$

  - Compute ℓ new basis vectors for Krylov subspace (SpMVMs) during global communication (dot-products).
  - Orthogonalization step when previous global reduction has finished
  - More technical, but deeper and variable pipelining possible p(ℓ)-GMRES
- Augmented and deflated Krylov subspace methods

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(cf. Laundry methods)

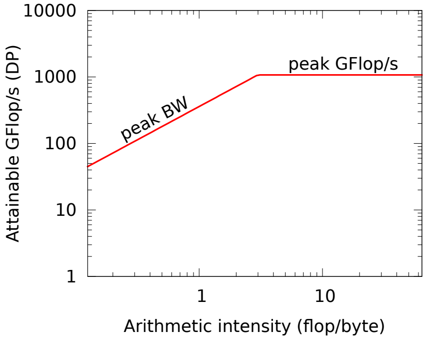
Hiding global reductions
(cf. hiding drying time)

Increasing arithmetic intensity
(cf. piling up laundry)

Conclusions & future work
(cf. washing instructions and ecological detergents)

Roofline Model

- Arithmetic intensity: $q = \dfrac{\text{floating-point operations}}{\text{byte off-chip memory traffic}}$
- High $q \rightarrow$ compute bound (dense algebra, fft, ...)
- Low $q \rightarrow$ bandwidth bound (sparse algebra, stencils, ...)
- Roofline gives upperbound for performance for given q



Williams, Waterman, Patterson (2008)

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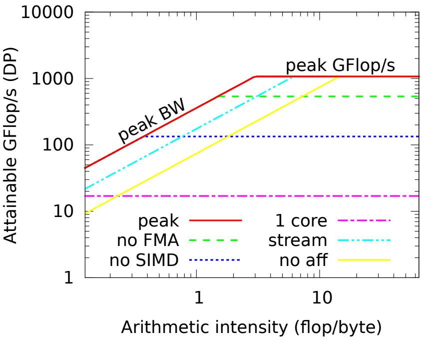

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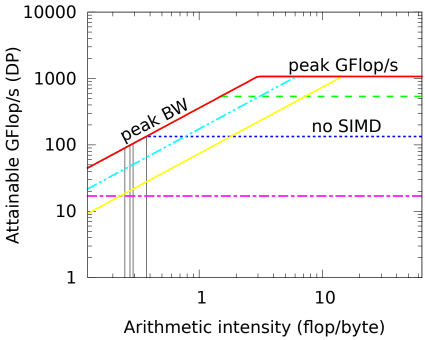


Williams, Waterman, Patterson (2008)

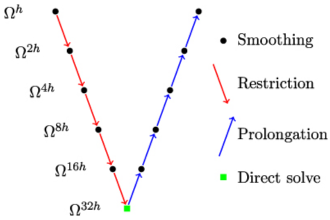
Arithmetic intensity of s dependent SpMVMs

	1 SpMVM	$s\times$ SpMVM	$s\times$ SpMVM in place
flops	$2n_{nz}$	$2s \cdot n_{nz}$	$2s \cdot n_{nz}$
words moved	$n_{nz} + 2n$	$sn_{nz} + 2sn$	$n_{nz} + 2n$
q	2	2	**2s**

See J. Demmel's course: CS 294-76 on Communication-Avoiding algorithms

V(ν_1,ν_2)-cycle multigrid

while $\|r^h\| > \texttt{tol}\|f^h\|$ **do**
  V-cycle(v^h, f^h)
end while

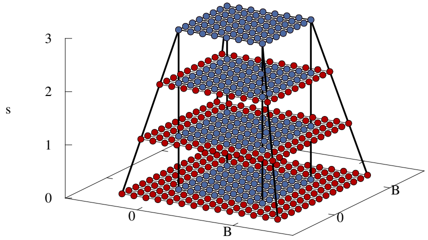


- I_h^{2h} Full weighting
- I_{2h}^h Linear interpolation

V-cycle(v^h, f^h)
  if Coarsest level **then**
    $v^h \leftarrow (A^h)^{-1} f^h$
  else
    for $k = 1, \ldots, \nu_1$ **do**
      $v^h \leftarrow (1 - \omega D^{-1} A^h) v^h + \omega D^{-1} f^h$
    end for
    $r^h \leftarrow f^h - A^h v^h$
    $r^{2h} \leftarrow I_h^{2h} r^h$
    $e^{2h} \leftarrow \text{V-cycle}^{2h}(0, r^{2h})$
    $e^h \leftarrow I_{2h}^h e^{2h}$
    $v^h \leftarrow v^h + e^h$
    for $k = 1, \ldots, \nu_2$ **do**
      $v^h \leftarrow (1 - \omega D^{-1} A^h) v^h + \omega D^{-1} f^h$
    end for
  end if

Consecutive smoothing steps

- A smoother is an SpMVM kernel with dependent vectors where only the last vector is required
  - Possibility to increase arithmetic intensity
  - Tiling over different smoother iterations
  - $q(\nu \times \omega\text{-Jac}) = \nu q_1(\omega\text{-Jac})$
- Divide the domain in tiles which fit in the cache
- Ground surface is loaded in cache and reused s $(= \nu)$ times
- Redundant work at the tile edges



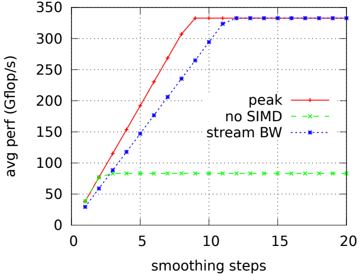
Cost of ν smoothing steps

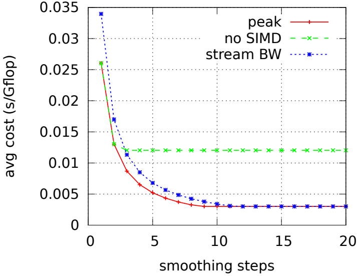
Since the arithmetic intensity increases for more smoothing steps

$$q(\nu \times \omega\text{-Jac}) = \nu q_1(\omega\text{-Jac})$$

according to the roofline:

performance increases & the average cost decreases



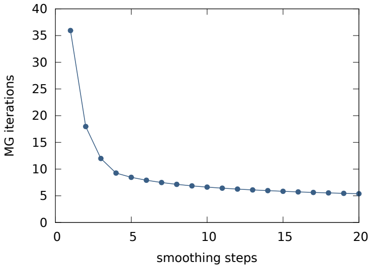


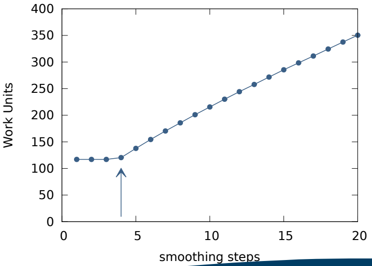
Work Unit Cost model

- Classical Work Unit cost model ignores memory bandwidth

$$1\,\mathrm{WU} = \text{smoother cost} = \mathcal{O}(n)$$

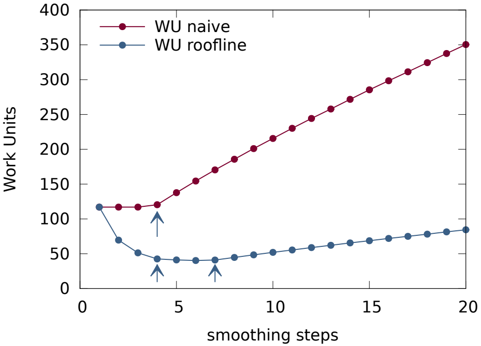
- Cost of multigrid to reach tolerance
$$= (9\nu + 19)\left(1 + \frac{1}{4} + \frac{1}{16} + \dots\right)\left\lceil \frac{\log(\texttt{tol})}{\log(\rho(\nu))} \right\rceil \mathrm{WU} \leq (9\nu + 19)\,\frac{4}{3}\left\lceil \frac{\log(\texttt{tol})}{\log(\rho(\nu))} \right\rceil \mathrm{WU}$$
- Optimum for low ν because computational cost increases with ν
- ... but communication overhead decreases!





Roofline Cost model

In contrast to naive model, the modified cost model suggests to repeat application of the smoother.

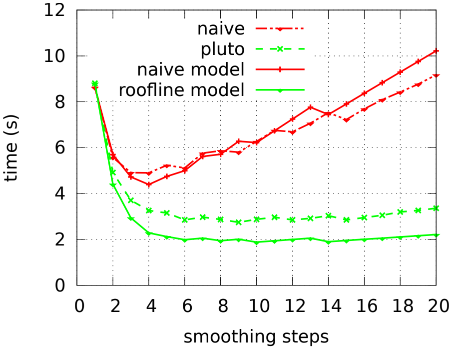


By tiling the smoother

- the optimal number of smoothing steps shifts to the right
- vectorization can be exploited

Roofline Cost model

In contrast to naive model, the modified cost model suggests to repeat application of the smoother.



By tiling the smoother

- the optimal number of smoothing steps shifts to the right
- vectorization can be exploited

Outline of the talk

Krylov subspace methods
(cf. Laundry methods)

Hiding global reductions
(cf. hiding drying time)

Increasing arithmetic intensity
(cf. piling up laundry)

Conclusions & future work
(cf. washing instructions and ecological detergents)

Summary

- **Krylov subspace methods**
  - 3 building blocks: axpy, SpMVM, dot-product
  - CG variants that group building blocks
  - Reduce global reduction steps
  - Communication avoiding
- **Hiding global reductions**
  - Pipelined CG and pipelined CR
  - Preconditioned versions
  - Overlap global reduction steps with other computational steps
  - Communication hiding (+ communication avoiding)
- **Increasing arithmetic intensity**
  - Tiling of smoother improves data locality and scalability
  - Trade-off between better convergence and increasing cost of smoother
  - Optimal number of smoothing steps increases
  - This allows exploiting of vector units
  - Still to be combined with an improved interpolation and restriction

References

- P. Ghysels, T.J. Ashby, K. Meerbergen & W. Vanroose, Hiding Global Communication Latency in the GMRES Algorithm on Massively Parallel Machines, SIAM J. Sci. Comput., 35, 2013.
- P. Ghysels, W. Vanroose, Hiding global synchronization latency in the preconditioned Conjugate Gradient algorithm, Parallel Computing, 2013.
- P. Ghysels, P. Klosiewicz, W. Vanroose, Improving the arithmetic intensity of multigrid with the help of polynomial smoothers, Num. Linear Algebra Appl., 19, 2012.

References & FAQs

- P. Ghysels, T.J. Ashby, K. Meerbergen & W. Vanroose, Hiding Global Communication Latency in the GMRES Algorithm on Massively Parallel Machines, SIAM J. Sci. Comput., 35, 2013.
- P. Ghysels, W. Vanroose, Hiding global synchronization latency in the preconditioned Conjugate Gradient algorithm, Parallel Computing, 2013.
- P. Ghysels, P. Klosiewicz, W. Vanroose, Improving the arithmetic intensity of multigrid with the help of polynomial smoothers, Num. Linear Algebra Appl., 19, 2012.

Q: *What's the difference between pipelined and s-step Krylov methods?*

- A: Global communication is hidden vs avoided
- A: Off-the-shelf preconditioning possible vs specialized preconditioning

Q: *Is the code available online?*

- A: Yes, pipe-CG, Gropp-CG, pipe-CR and p(ℓ)-GMRES are in the PETSc library