



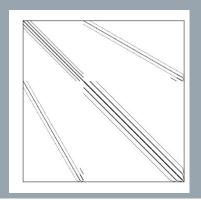
Advanced Matrix-Vector Multiplication – improving Code **Balance** → **RACE**

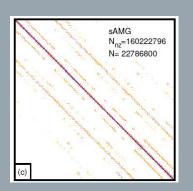
$$y = A x ; A^t = A$$

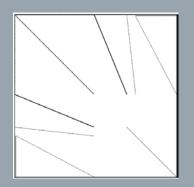
y = A x; A^t=A \rightarrow symmetric SpMV

$$y = A^p x$$

→ Matrix Power Kernel









Starting Ground

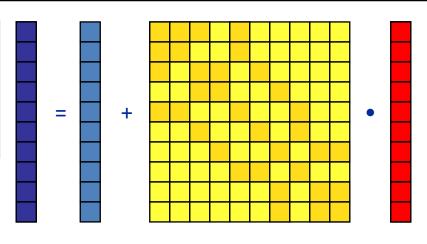
do i = 1,
$$N_r$$

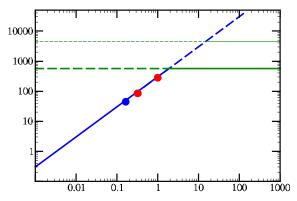
do j = $row_ptr(i)$, $row_ptr(i+1)$ - 1
 $C(i)$ = $C(i)$ + $val(j)$ * $B(col_idx(j))$
enddo
enddo

$$B_{C,min} = \frac{12 + 20/N_{nzr} + 8/N_{nzc}}{2} \frac{B}{F}$$

$$B_C(\alpha) = \frac{12 + 20/N_{nzr} + 8 \alpha}{2} \frac{B}{F}$$

Move upwards in the RLM Reduce data traffic (B_C) / increase I!



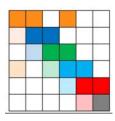


Agenda

Basic ideas to improve Code Balance for SpMV based algorithms

RACE: A different approach to Sparse Matrix-Vector Multiplication (SpMV)

Parallelization of Symmetric SpMV



Cache blocking for Matrix Power Kernels

$$y = A^p x$$

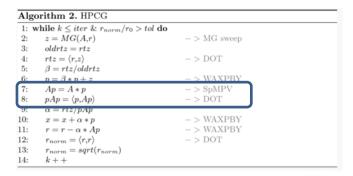
Conclusion

!WARNING! This talk considers single multicore processors only: Cascade Lake, Ice Lake, Rome (20c – 64c)

Motivation – Sparse Matrix Vector Multiplication

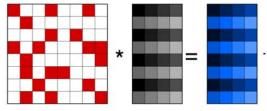
Improve code balance of SpMV-algorithms

Kernel fusion, e.g. HPCG:



Sparse Matrix Multiple Vector Multiplication

Gropp et al.: Towards Realistic Performance Bounds for Implicit CFD Codes ParCFD 1999. https://wgropp.cs.illinois.edu/bib/papers/pdata/1999/pcfd99/gkks.ps



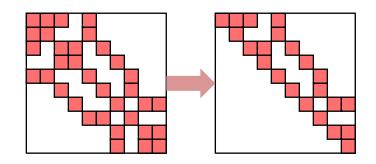
Both, e.g. Chebyshev Filter Computation for eigenvalue computations:

Kreutzer et al.: Chebyshev Filter Diagonalization on Modern Manycore Processors and GPGPUs. ISC 2018. DOI: https://dx.doi.org/10.1007/978-3-319-92040-5 17

Motivation – Sparse Matrix Vector Multiplication

Further opportunities to improve code balance of SpMV-kernels:

- Exploit symmetry (SymmSpMV): $A = A^t$
 - Naive speed-up: max. 2



- Cache blocking for Sparse Matrix Power Kernels (MPK): $y = A^p x$
 - Data locality in "sparse matrix-matrix multiply" ←→ Irregular sparsity pattern
 - Naive speed up: max. p

PE for SpMV

Symmetric SpMV – serial execution

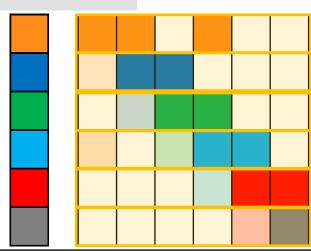
Store only upper (lower) triangular part of symmetric sparse matrix

Improve code balance by up to 2x

$$B_C = \frac{12 + 20/N_{nzr} + 8 \alpha}{2} \frac{B}{F}$$

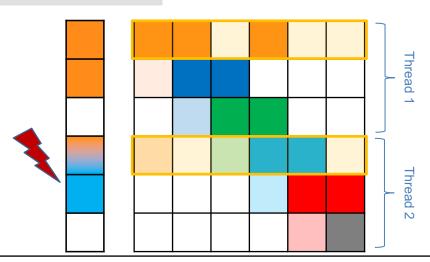


$$B_C^{sym} = \frac{12 + 4/N_{nzr}^{sym} + 24 \alpha^{sym}}{4} \frac{B}{F}$$



Symmetric SpMV – parallelisation: write conflicts





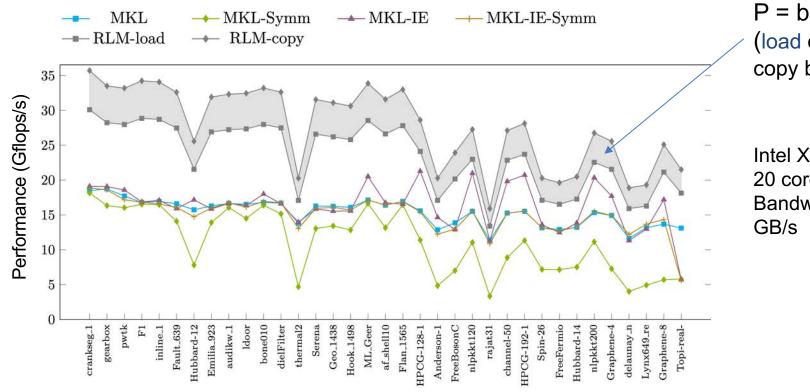
SymmetricSpMV – Intel MKL options

Intel math kernel library (MKL) supports SpMV and SymmSpMV:

- Plain SpMV calls using CRS
 - SpMV-call → MKL
 - SymmSpMV-call → MKL-Symm
- Inspector-Executor takes (1) CRS as input, (2) analyses matrix structure and (3) may optimize (e.g. data structure) and then (4) run the kernel
 - No additional hints → MKL-IE
 - HINT=symmetric → MKL-IE-Symm

Intel MKL Symmetric SpMV performance

Performance of SymmSpMV on 1 socket of Intel Cascade Lake

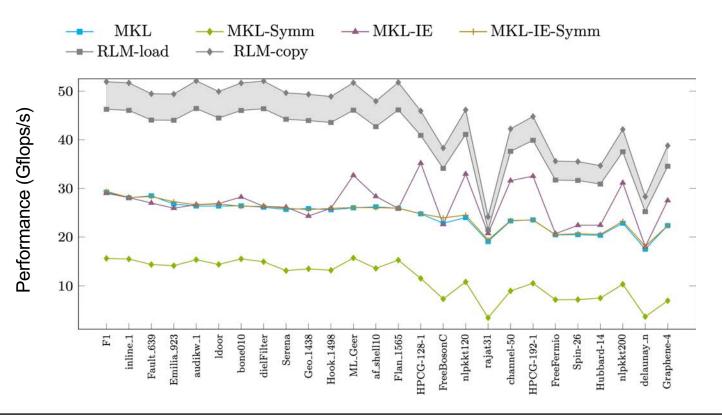


 $P = b_S / B_{C,min}$ (load only and copy bandwidth)

Intel Xeon 6248 20 cores Bandwidth 115 GB/s

Intel MKL Symmetric SpMV performance

Performance of SymmSpMV on 1 socket of Intel Ice Lake

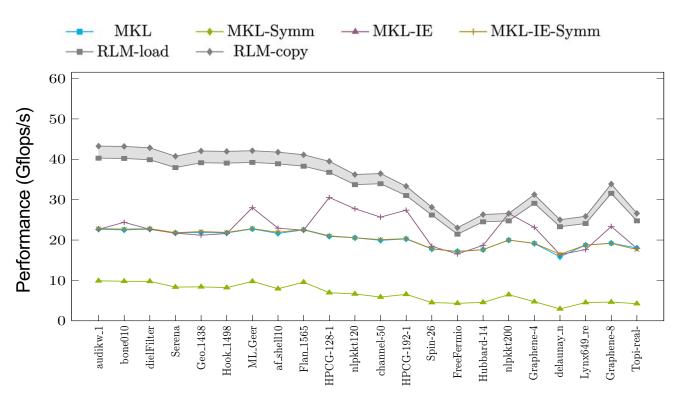


Intel Xeon 8368 38 cores Bandwidth 170 GB/s

10

Intel MKL Symmetric SpMV performance

Performance of SymmSpMV on 1 socket of AMD ROME



AMD EPYC 7662 64 cores Bandwidth 146 GB/s

How to parallelize SymmSpMV efficiently????

11





SpMV – graph traversal – RACE



Alappat et al., A Recursive Algebraic Coloring Technique for Hardware-efficient Symmetric Sparse Matrix-vector Multiplication. ACM Trans. Parallel Comput., 2020, DOI:10.1145/3399732

Consider SpMV as "graph traversal"

Standard view: Run over all rows i=1,..., nr and calculate

$$y_i = \sum_{j \in COL(i)} A_{i,j} x_j$$

where COL(i) contains the column indices of the non-zeros in i-th row

■ RACE – graph-based view: row ← → vertex & non-zero entry ← → edge

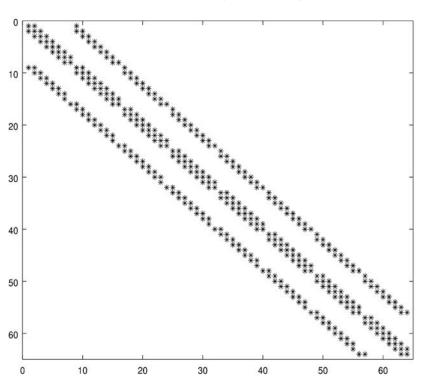
In the graph terminology a SpMV operation (y = Ax) can be formulated as follows: If G = (V, E) is the graph representation of the sparse matrix A then for every vertex $u \in V(G)$ calculate

$$y_u = \sum_{v \in N(u)} A_{u,v} x_v . \tag{2}$$

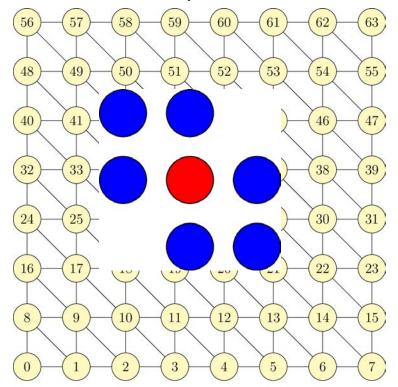
PE for SpMV

Sample Stencil Matrix and its graph representation

Symmetric Matrix (Stencil)

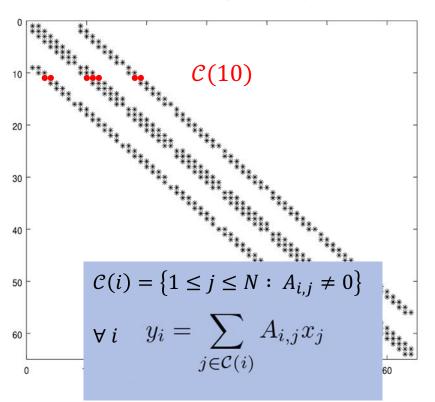


Undirected Graph

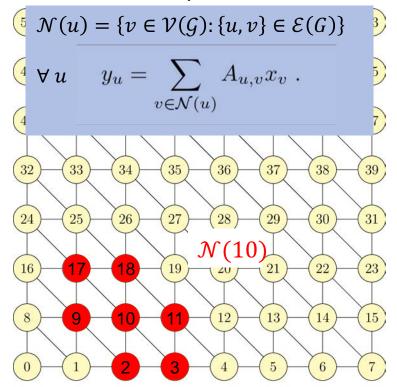


Sample Stencil Matrix and its graph representation

Symmetric Matrix (Stencil)

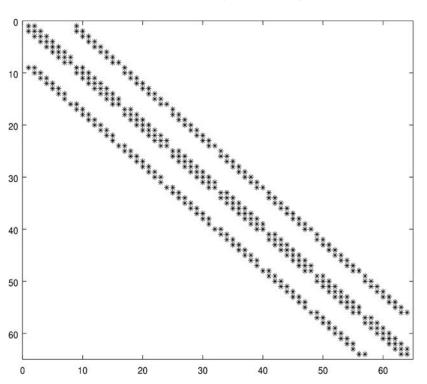


Undirected Graph

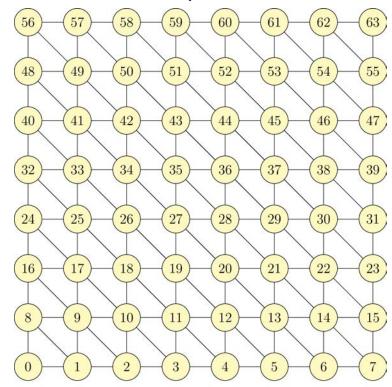


Sample Stencil Matrix and its graph representation

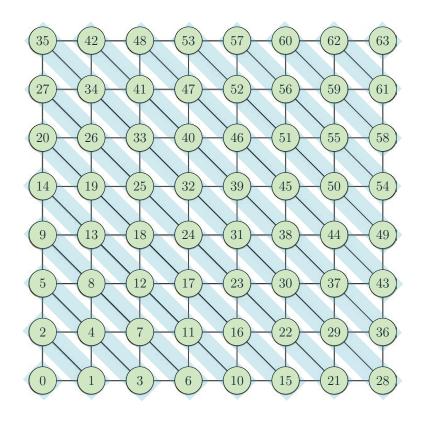
Symmetric Matrix (Stencil)



Undirected Graph



RACE: Get BFS-levels



- Get levels of a Breadth-First-Search (BFS)
- Reorder vertices → consecutive witin level

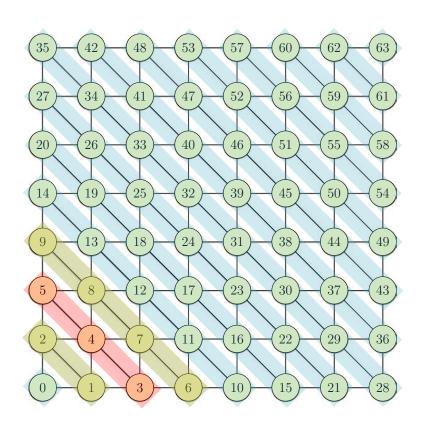


levels

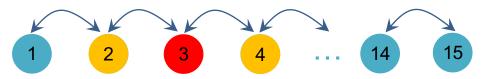
Dependencies only between neighboring levels!

PE for SpMV

RACE: SpMV - Dependencies and Implementation



Update $3 \rightarrow$ indirect access to 3, 2 and 4

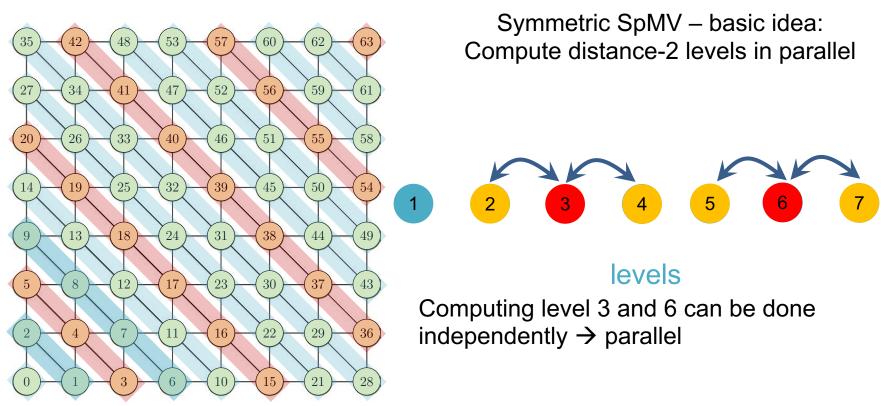


levels

```
do i = 1,L //loop over Levels
   SpMV_CRS(level_ptr[i], level_ptr[i+1])
enddo
```

```
function SpMV_CRS(start, end)
do i = start, end
do j = row_ptr(i), row_ptr(i+1) - 1
   y(i) = y(i) + val(j) * x(col_idx(j))
enddo
enddo
```

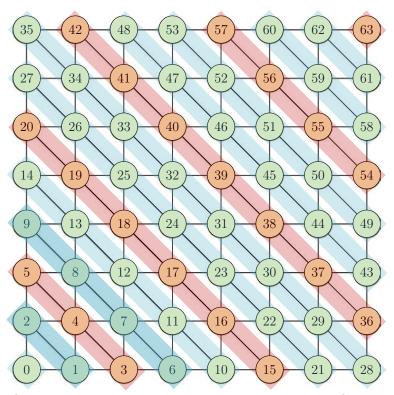
RACE: SymmSpMV - Parallelization



C. Alappat, A. Basermann, A. R. Bishop, H. Fehske, G. Hager, O. Schenk, J. Thies, and G. Wellein: *A Recursive Algebraic Coloring Technique for Hardware-efficient Symmetric Sparse Matrix-vector Multiplication.* ACM Trans. Parallel Comput. (2020). DOI: 10.1145/3399732

PE for SpMV

RACE: SymmSpMV - Parallelization



In general:

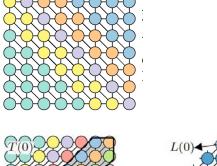
- "Distance-2" levels can be updated in parallel (same color)
- Assign levels to threads
- But: Load imbalance!!!!
- #levels >> #threads

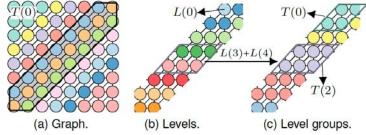
C. Alappat, A. Basermann, A. R. Bishop, H. Fehske, G. Hager, O. Schenk, J. Thies, and G. Wellein: *A Recursive Algebraic Coloring Technique for Hardware-efficient Symmetric Sparse Matrix-vector Multiplication*. ACM Trans. Parallel Comput. (2020). DOI: 10.1145/3399732

RACE: SymmSpMV - Parallelization

- Further optimization strategies (for details see MPK)
 - Replace levels by level groups
 → better load balancing

Recursive level refinement
 → Cache locality / parallelism

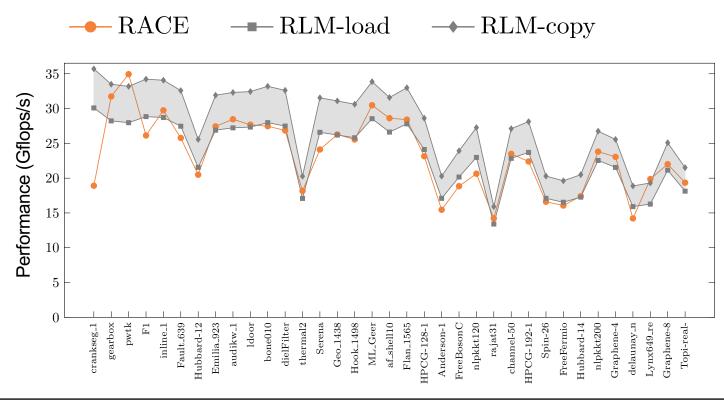




Avoid global thread sync → Pair-wise if required

MKL Symmetric SpMV performance

Performance of SymmSpMV on 1 socket of Intel Cascade Lake



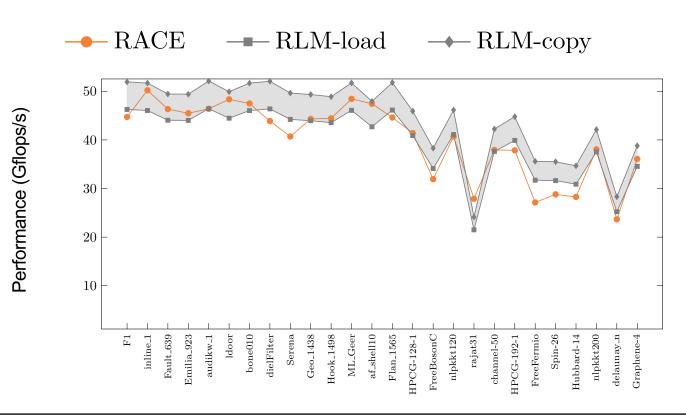
Intel Xeon 6248 20 cores Bandwidth 115 GB/s

Looks good ©

23

MKL Symmetric SpMV performance

Performance of SymmSpMV on 1 socket of Intel Ice Lake



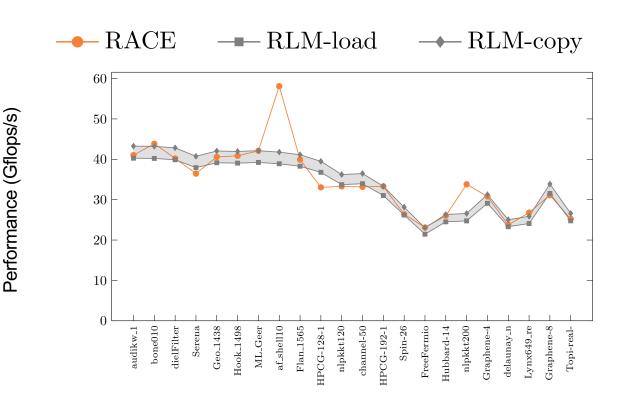
Intel Xeon 8368 38 cores Bandwidth 170 GB/s

Looks good ©

24

MKL Symmetric SpMV performance

Performance of SymmSpMV on 1 socket of AMD ROME



AMD EPYC 7662 64 cores Bandwidth 146 GB/s

Looks good ©

25





RACE & Cache Blocking for MPK

IEEE TRANSACTIONS ON PARALLEL AND DISTRIBUTED SYSTEMS, VOL. 34, NO. 2, FEBRUARY 2023

Level-Based Blocking for Sparse Matrices: Sparse Matrix-Power-Vector Multiplication

Christie Alappat[®], Georg Hager[®], Olaf Schenk[®], Senior Member, IEEE, and Gerhard Wellein[®]

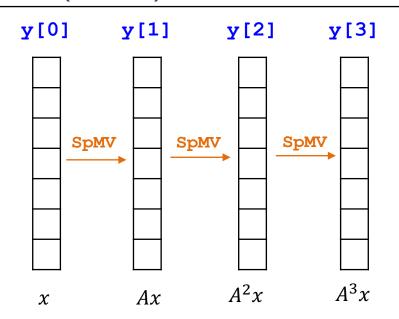
C. Alappat, et al, doi: 10.1109/TPDS.2022.3223512



Motivation – Matrix power kernel (MPK)

- Calculate: $y = A^p x$
- Repeatedly perform back to back SpMVs

```
for k=1:p; do
  y[k] = SpMV(A, y[k-1])
done
```



Same matrix *A* loaded *p* times from main memory!!!

How to cache the matrix *A* across the matrix power calculation?

MPK – existing caching approaches

- Huber et al.: Graph-based higher-order time integration of PDEs¹
 - "Geometrical approach" based on matrix bandwidth
 - Works for 2D stencil matrices → Runs into problem for 3D and/or unstructured matrices
- Mohiyuddin et al.: Minimizing communication in sparse matrix solvers²
 - "Domain decomposition" of underlying graph
 - Requires "ghosting" → Indirect accesses or redundant copies of the matrix entries → Scalability!!
- → Exploit level structure in RACE for cache blocking!

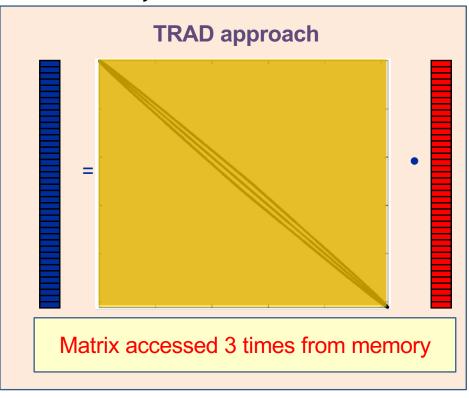


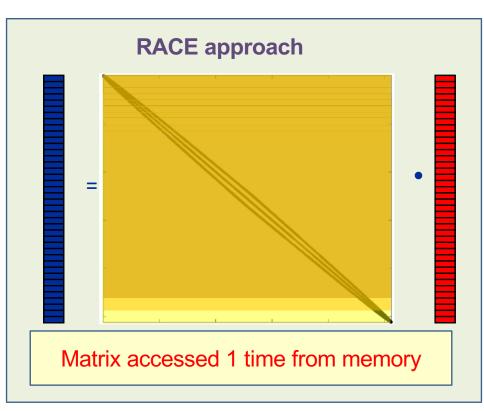
¹Huber et al., 2021. Graph-based multi-core higher-order time integration of linear autonomous partial differential equations. J. Comput. Sci. <u>DOI:10.1016/j.jocs.2021.101349</u>
²Mohiyuddin et al., 2009. Minimizing communication in sparse matrix solvers. In Proceedings of the SC'09. <u>DOI:10.1145/1654059.1654096</u>

PE for SpMV 21.03.2023 28

Matrix power - Traditional approach vs. Cache Blocking

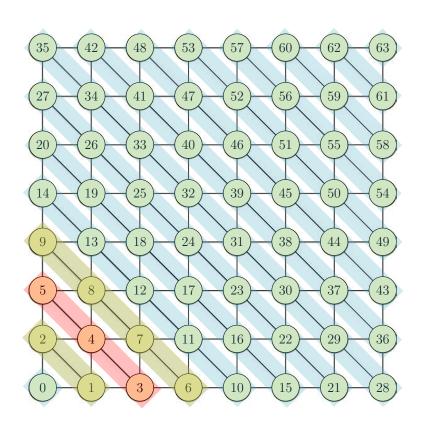
Calculate $y = A^3x$

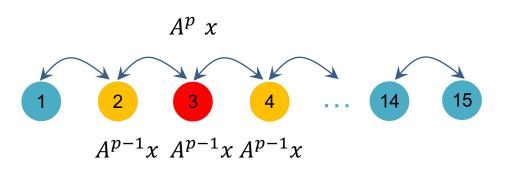




How to do that in general for sparse matrices?

RACE





PE for SpMV 21.03.2023 30

do k = 1, py(:, k) = SpMV(A, y(:,k-1))enddo

No cache blocking!

Levels

Ax

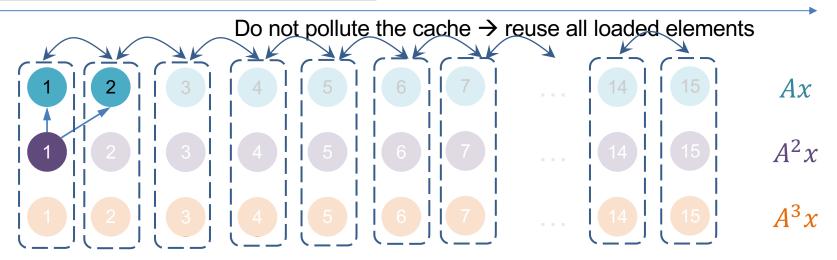
 A^2x

Matrix Powers

RACE – Level traversal and matrix powers

```
do k = 1, p
  y(:, k) = SpMV(A, y(:,k-1))
enddo
```

Levels

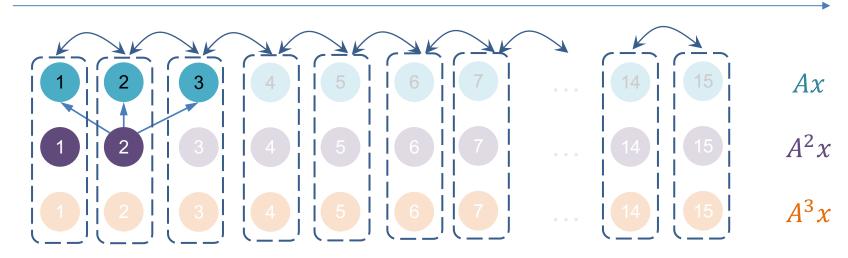


When updating level 1, indirect reads also go to level 2

PE for SpMV 21.03.2023 32

do k = 1, p y(:, k) = SpMV(A, y(:,k-1))enddo

Levels



When updating level 2, indirect reads also go to levels 1 and 3

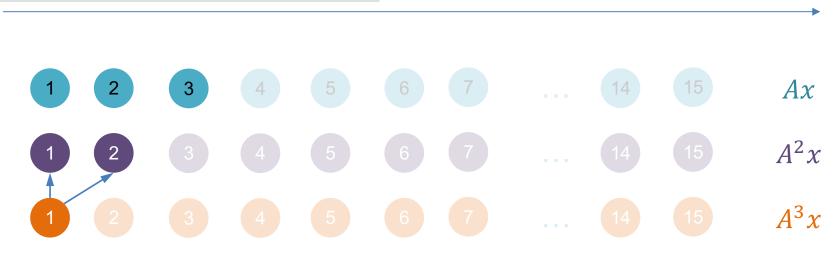
PE for SpMV

Matrix Powers

```
Matrix Powers
```

do k = 1, p
 y(:, k) = SpMV(A, y(:,k-1))
enddo

Levels



PE for SpMV 21.03.2023

```
Matrix Powers
```

```
do k = 1, p
y(:, k) = SpMV(A, y(:,k-1))
enddo
```

Levels

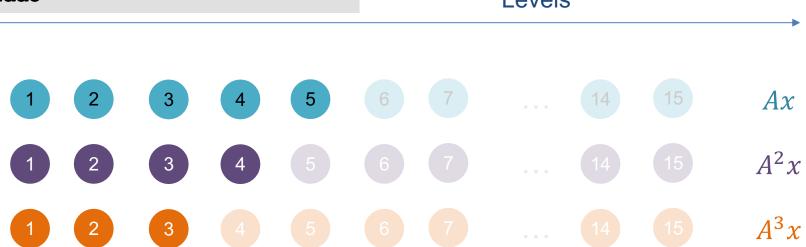
Ax A^2x

PE for SpMV 21.03.2023

```
Matrix Powers
```

```
do k = 1, p
  y(:, k) = SpMV(A, y(:,k-1))
enddo
```

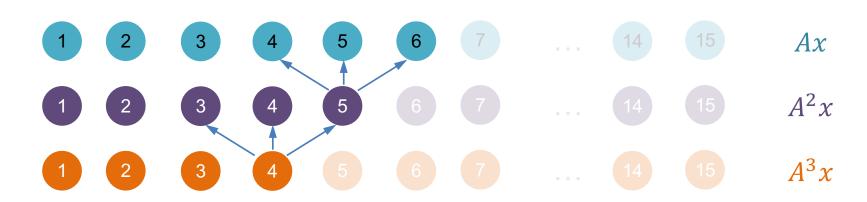
Levels



PE for SpMV

do
$$k = 1$$
, p
 $y(:, k) = SpMV(A, y(:,k-1))$
enddo

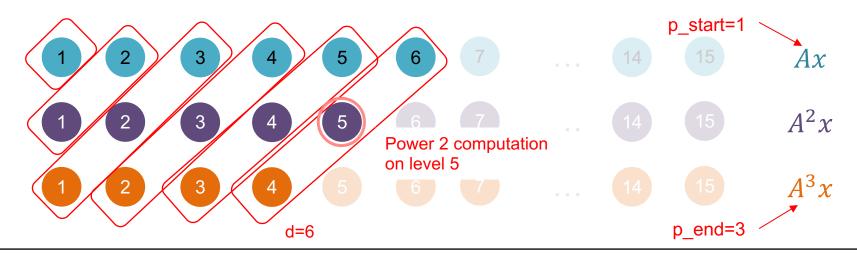
Levels



A is loaded only once if $(p+1) \times N_{nz}(L) \times 12$ bytes < C

 $N_{nz}(L)$ — avg. non-zeros in a level C — cache size

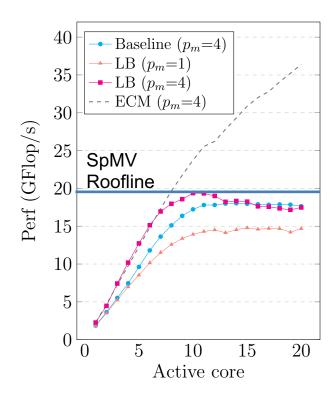
RACE: MPK Pseudocode

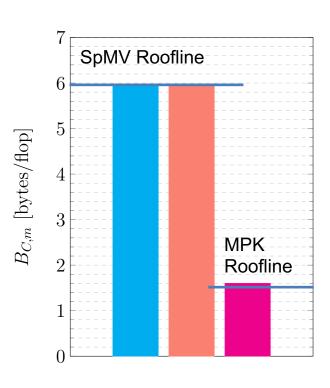


PE for SpMV 21.03.2023

38

RACE MPK – First Implementation





Intel Xeon Gold 6248

• 1 Socket (20c)

pwtk matrix

- $N_r = 217,918$
- $N_{nz} = 11,634,424$

Performance

Memory traffic

RACE MPK – Performance Problem Identified

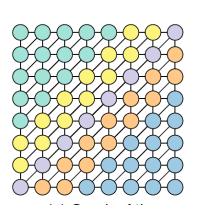
- Scheme seems to work (reduces data traffic) at least for pwtk
- But: Performance ⊗ !!!!

- Analysis of hardware performance counters (LIKWID) for pwtk matrix: INSTR_RETIRED_ANY up 2x for level based SpMV!
 - → Frequent thread syncronisations!

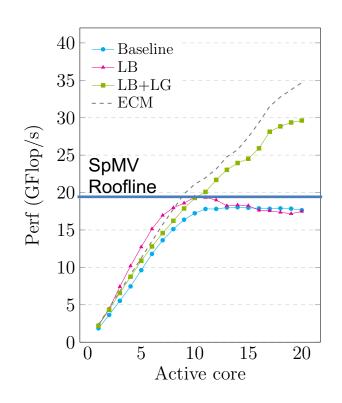
Reason: After each level threads sync!

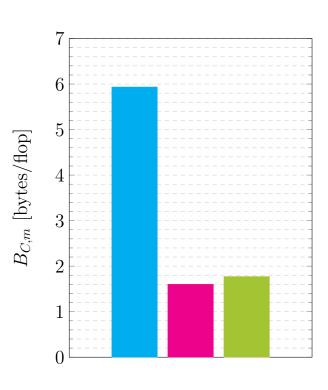
Measures:

- → Reduce #levels by level aggregation ("LG")
- → Global sync. replaced by point-to-point sync. ("p2p")



RACE MPK – LG optimization





Intel Xeon Gold 6248

• 1 Socket (20c)

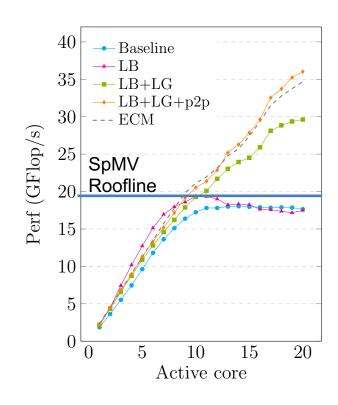
pwtk matrix

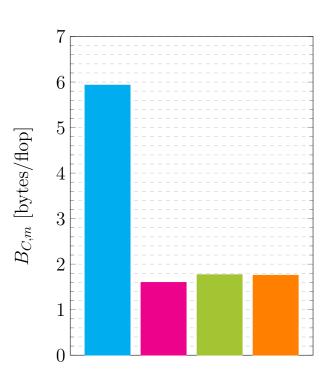
- $N_r = 217,918$
- $N_{nz} = 11,634,424$

Performance

Memory traffic

RACE MPK – LG+p2p optimization





Intel Xeon Gold 6248

• 1 Socket (20c)

pwtk matrix

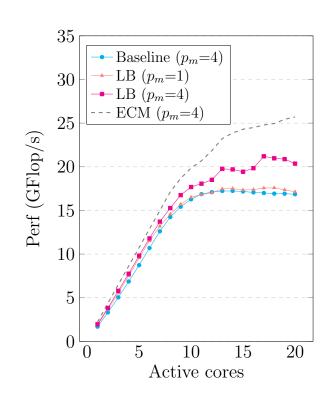
- $N_r = 217,918$
- $N_{nz} = 11,634,424$



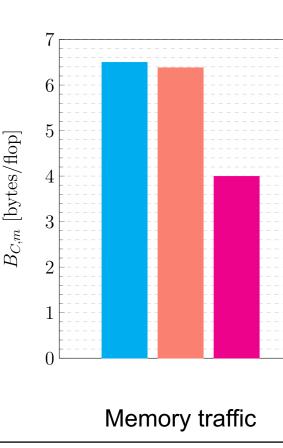
Performance

Memory traffic

RACE MPK – Yet another problem



Performance



Intel Xeon Gold 6248

• 1 Socket (20c)

Flan 1565 matrix

- $N_r = 1,564,794$
- $N_{nz} = 117,406,044$

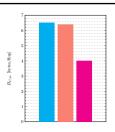
Data traffic not reduced by factor of 4

Representative for large matrices!

PE for SpMV

RACE MPK – Performance Problem Identified (II)

- Flan_1565 matrix no significant adequate in data volume
- Analysis of level distribution for Flan_1565 matrix:



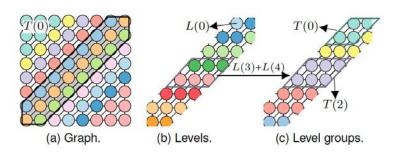
Few large levels → do not fit in cache!

$$(p+1) \times N_{nz}(L) \times 12 \text{ bytes} < C$$

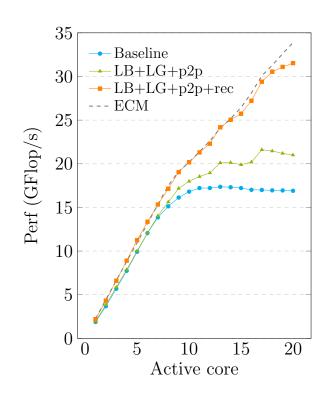
Counter - Measure:

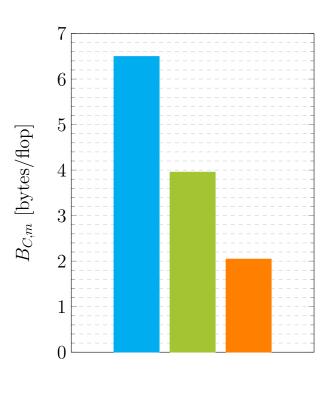
Too big!!!

→ Apply RACE to a single / few levels recursively ("rec")!



RACE MPK - rec





Intel Xeon Gold 6248

• 1 Socket (20c)

Flan 1565 matrix

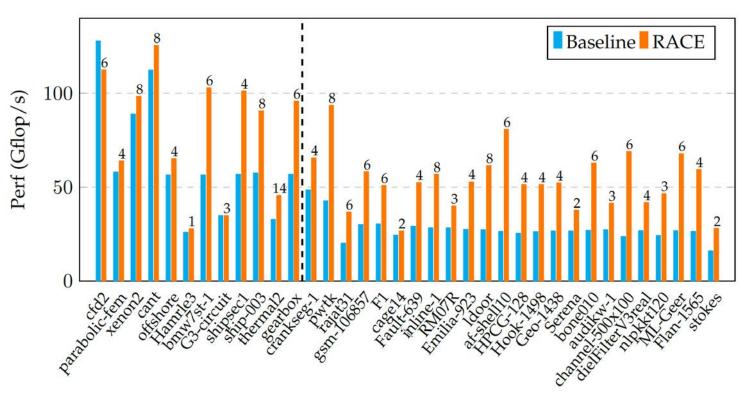
- $N_r = 1,564,794$
- $N_{nz} = 117,406,044$



Performance

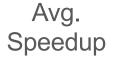
Memory traffic

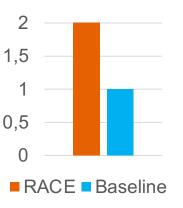
Matrix power kernel: Performance – Intel Ice Lake



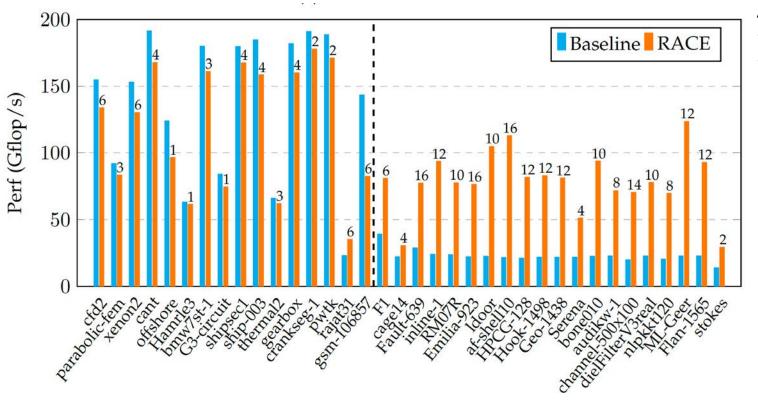
Intel Xeon Platinum 8368

- 38 cores
- 104 MB cache (L2+L3)



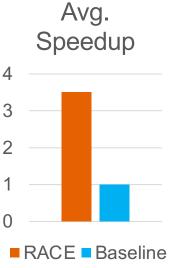


Matrix power kernel: Performance – AMD Rome



AMD EPYC 7662

- 64 cores
- 288 MB cache (L2+L3)



RACE - summary

- Inner kernel: OpenMP parallel standard SpMV routine
- Overhead: BFS & Set up of data structures (approx. ≤ 50 SpMVs)
- Parameters: Power (p_m), Available Cache Size, Max. recursion depth
- Cache size $\leftarrow \rightarrow$ max. polynomial degree (p_m)
 - Larger caches → larger p_m → better performance
 - Polynomial degree higher than p_m→ Computation in chunks of p_m
- No loss of accuracy!

RACE – MPK applications

- Exponential Integrators → Polynomial approximations
- s-step Krylov methods (CA-GMRES)
- Polynomial preconditionung
- Algebraic Multigrid smoothers
- Trilinos interface available

Summary

- MPK kernel's performance → substantial boost by level-based cache blocking using RACE.
- MPK + RACE is attractive for s-step Krylov solvers. For example CA-GMRES solver
- Very promising results if combined with polynomial preconditioners
- Chebyshev smoothers for multigrid
 - → Large Scale Sparse Solvers
- Exponential integrators, e.g. Chebyshev time propagation

. . .





Thank you

Questions





https://github.com/RRZE-HPC/RACE





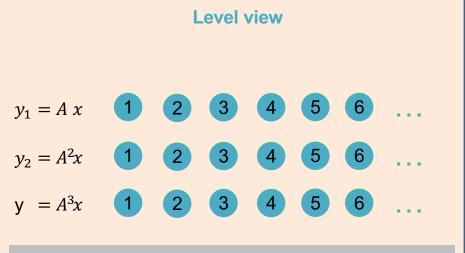




Matrix power

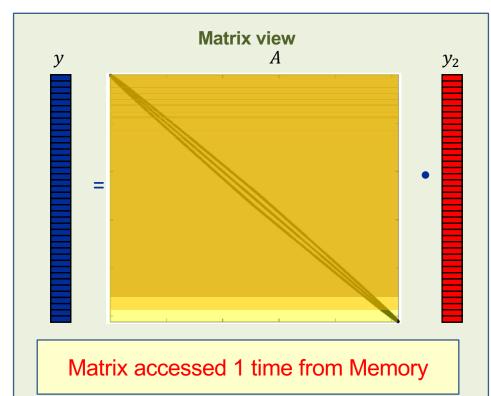
Calculate
$$y = A^3x$$

RACE approach



For more details on RACE MPK:

C. Alappat, G. Hager, O. Schenk, G. Wellein, 2022, Level-based Blocking for Sparse Matrices: Sparse Matrix-Power-Vector Multiplication, Submitted, Preprint: https://arxiv.org/abs/2205.01598



Matrix power kernel (MPK)

- Calculate: $y = A^p x$
- Repeatedly perform back to back SpMVs

```
do k = 1, p
  y(:, k) = SpMV(A, y(:,k-1))
enddo
```

Applications

s-step Krylov solvers

- s-step GMRES
- s-step CG

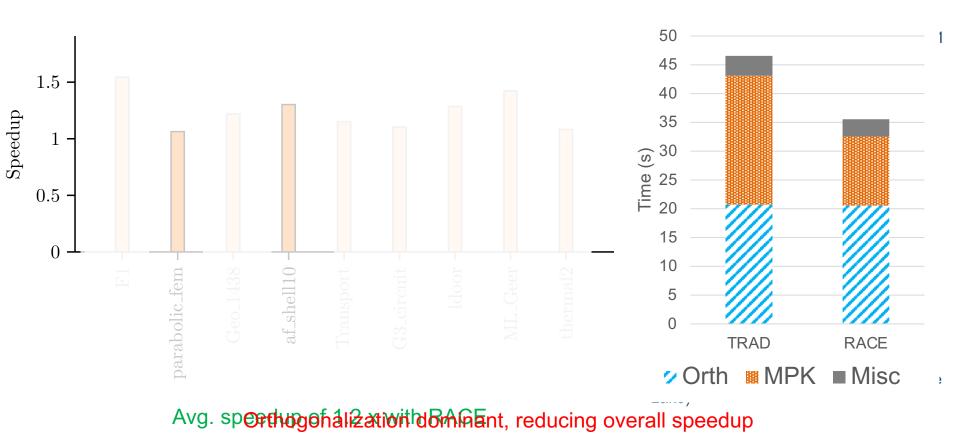
Matrix polynomials

- Chebyshev time propagation
- Exponential integrators
- Polynomial preconditioning

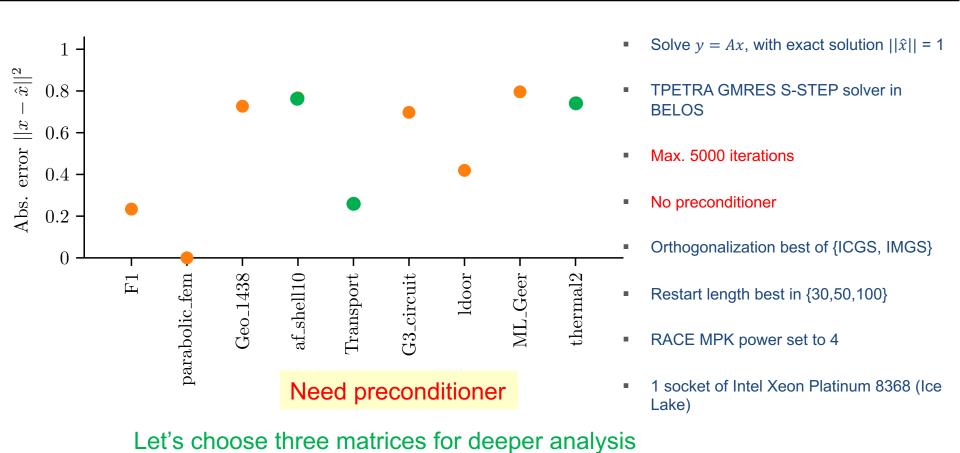
Power iterations

- Eigenvalue computations
- Power iteration clustering

Application: Communication avoiding GMRES



Application: Communication avoiding GMRES



Polynomial preconditioners (AMy = b, x = My)

The idea

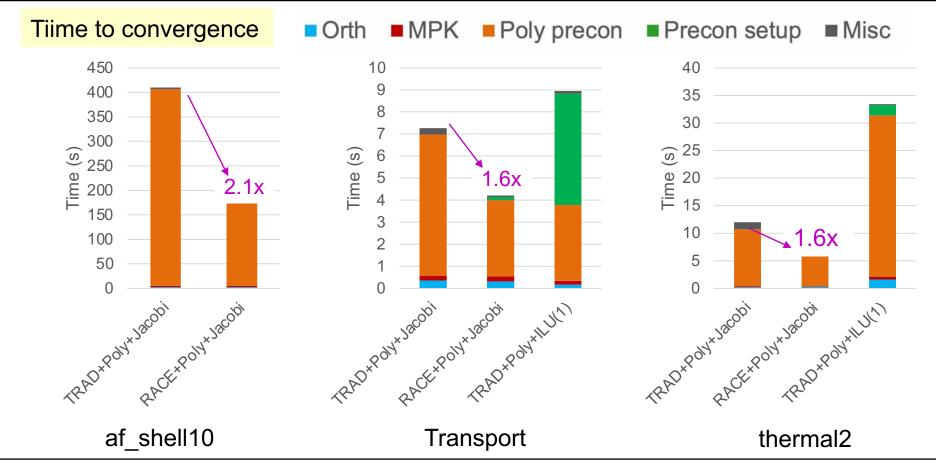
- Find roots of (I Ap(A)), i.e., solve: (I Ap(A)) = 0
- The resulting p(A) is an approximation for A^{-1}
- Degree of the polynomial is determined by the number of roots sought after

How to find roots of (I - Ap(A))?

- Higher the degree → more accuracy (in infinite precision)
- But becomes more costly to evaluate
- Run d steps of GMRES with a starting vector (random) b
- Then the solution x in $K(A, b) = span\{b, Ab, A^2b, ...\}$
- This implies x = p(A)b
- ||r|| = ||b Ax|| = ||(I Ap(A))b|| \rightarrow This residual is what GMRES minimizes

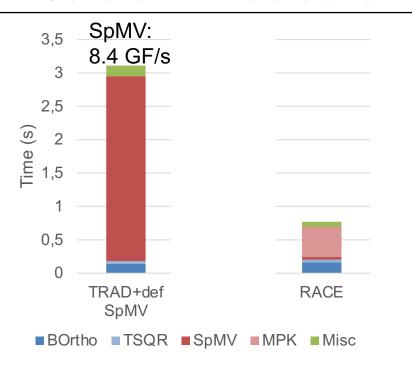
Best thing here is after creating the polynomial p(A), applying it is just MPK, since $p(A)x = \alpha_0 + \alpha_1 Ax + \alpha_2 A^2 x + \dots$

Application: Polynomial preconditioning



PE for SpMV

Careful with defaults



 $SpMV_RLM = 170/6 = 28.3 GF/s$

Matrix size = 140 MB

L3+L2 = 104MB

In Kokkos, if Nnz > 1e7 dynamic scheduling

```
if(((A.nnz()>10000000) || use_dynamic_schedule) && !use_static_schedule)
```

Kokkos::parallel_for("KokkosSparse::spmv<NoTranspose,Dynamic>",Kokkos::RangePolicy<execution_space, Kokkos::Schedule<Kokkos::Dynamic>>(0, A.numRows()),func);

else

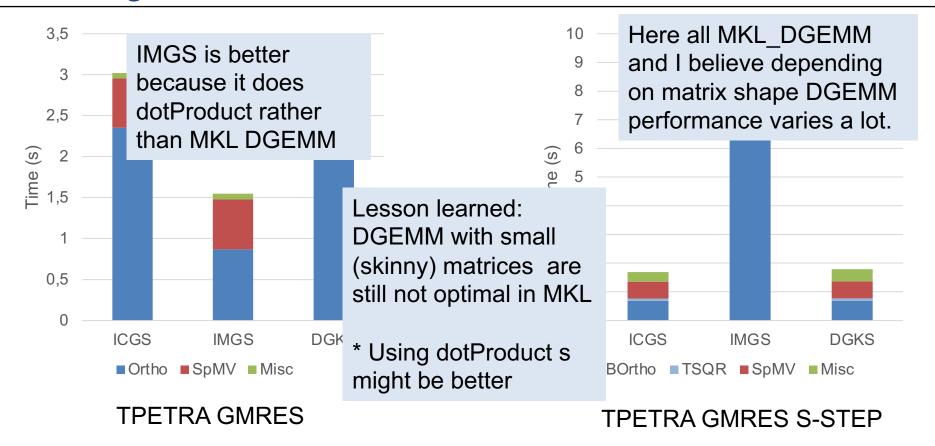
Kokkos::parallel_for("KokkosSparse::spmv<NoTranspose,Static>",Kokkos::RangePolicy<execution_space, Kokkos::Schedule<Kokkos::Static>>(0, A.numRows()),func);

Careful with defaults



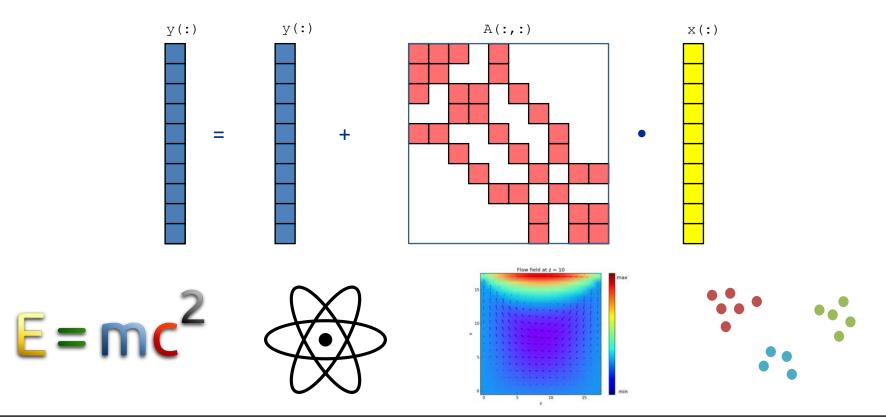
PE for SpMV 21.03.2023 72

Orthogonalization with MKL is not the best



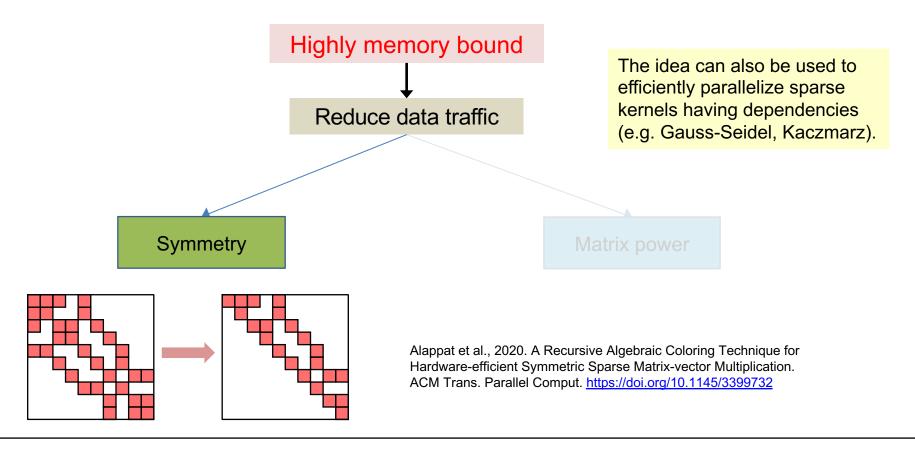
SpMV

SpMV: Multiplication of a sparse matrix (A) with a dense vector (x)



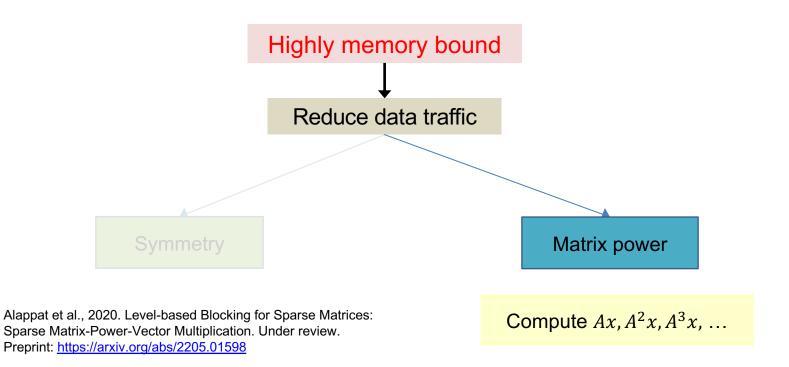
PE for SpMV

SpMV: optimizations using RACE



PE for SpMV 21.03.2023 75

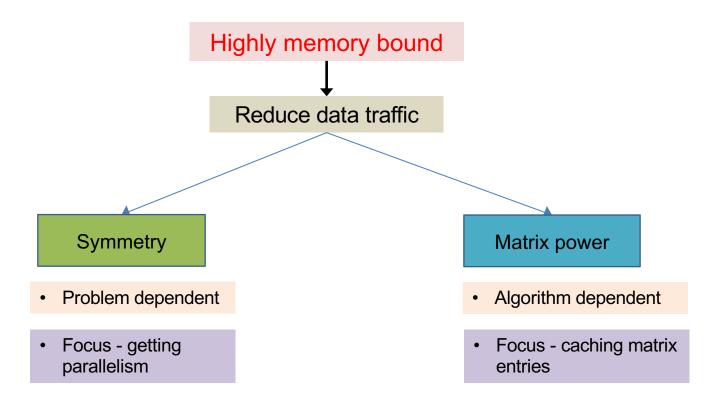
SpMV: optimizations using RACE



Focus of today's talk: Node-level (CPU) implementation of Matrix power kernels for "large" matrices

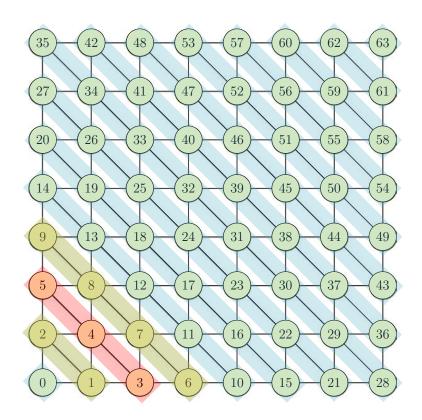
PE for SpMV 21.03.2023 76

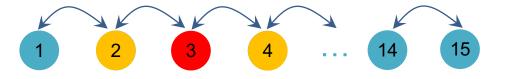
SpMV: optimizations using RACE



PE for SpMV

RACE



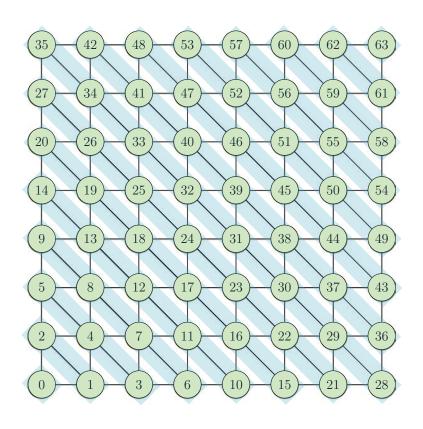


levels

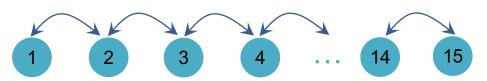
When updating level 3, indirect accesses on levels 3, 2 and 4

PE for SpMV 21.03.2023 79

RACE



Use Breadth First Search (BFS) Levels



levels

```
do i = 1,L //loop over Levels
   SpMV_CRS(level_ptr[i], level_ptr[i+1])
enddo
```

```
function SpMV_CRS(start, end)
do i = start, end
do j = row_ptr(i), row_ptr(i+1) - 1
  y(i) = y(i) + val(j) * y(col_idx(j))
  enddo
enddo
```

PE for SpMV 21.03.2023 81