CSC367 Parallel computing

Lecture 3: Single Processor Machines-Performance Model

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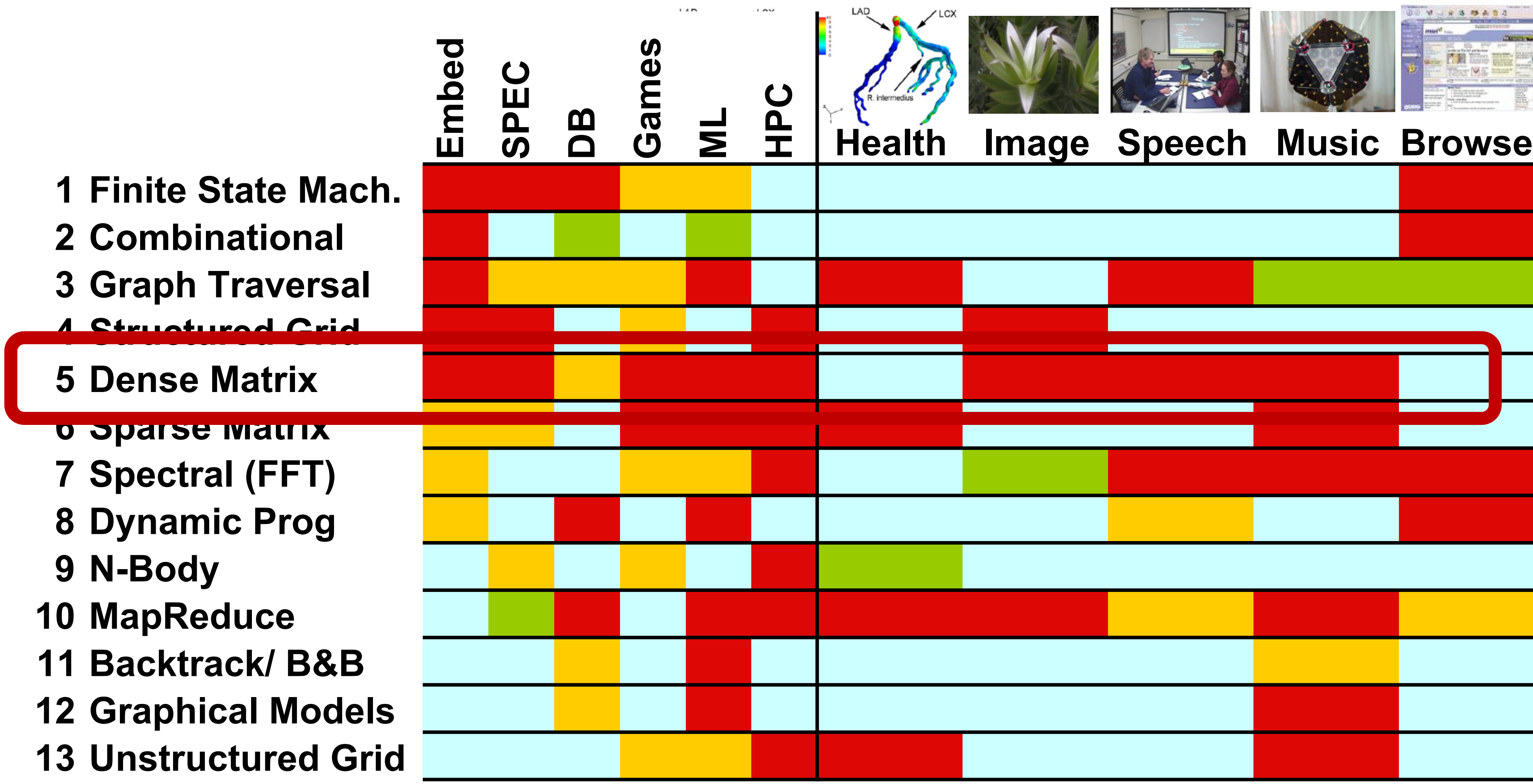
Outline

A performance model for Matrix Multiplication

- Use of performance models to understand performance
- Attainable lower bounds on communication
- Simple cache model
- Warm-up: Matrix-vector multiplication
- Naïve vs optimized Matrix-Matrix Multiply
  - Minimizing data movement
  - Beating $O(n^3)$ operations
- BLAS routines

What do commercial and CSE applications have in common?

Motif/Dwarf: Common Computational Methods
(Red Hot → Blue Cool)



Note on Matrix Storage

- A matrix is a 2-D array of elements, but memory addresses are "1-D"
- Conventions for matrix layout
  - by column, or "column major" (Fortran default); A(i,j) at A+i+j*n
  - by row, or "row major" (C default) A(i,j) at A+i*n+j
  - Recursive

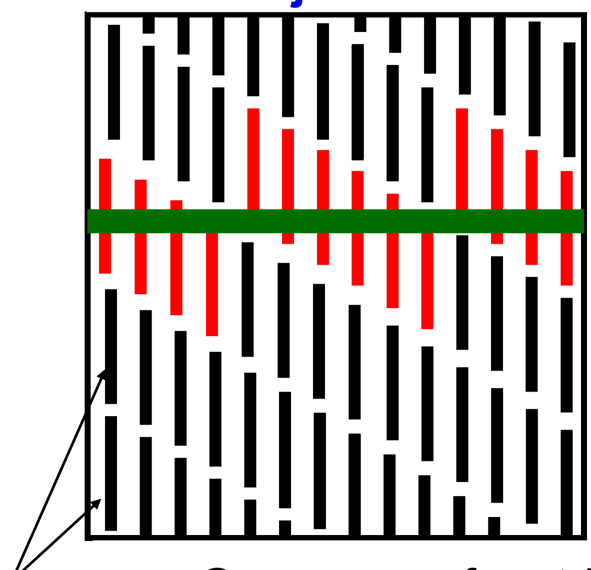
Column major

0	5	10	15
1	6	11	16
2	7	12	17
3	8	13	18
4	9	14	19

Row major

0	1	2	3
4	5	6	7
8	9	10	11
12	13	14	15
16	17	18	19

Column major matrix in memory



cachelines

Green row of matrix is stored in red cachelines

Figure source: Larry Carter, UCSD

- Column major (for now)

Using a Simple Model of Memory to Optimize

- Assume just 2 levels in the hierarchy, fast and slow
- All data initially in slow memory
  - m = number of memory elements (words) moved between fast and slow memory
  - t_m = time per slow memory operation
  - f = number of arithmetic operations
  - t_f = time per arithmetic operation $<< t_m$
  - $q = f / m$ average number of flops per slow memory access
- Minimum possible time = $f * t_f$ when all data in fast memory
- Actual time
  - $f * t_f + m * t_m = f * t_f * (1 + \boxed{t_m/t_f} * 1/q)$
- Larger q means time closer to minimum $f * t_f$
  - $q \geq t_m/t_f$ needed to get at least half of peak speed
  - Speed is inverse of time so peak speed is $1/(f * t_f)$

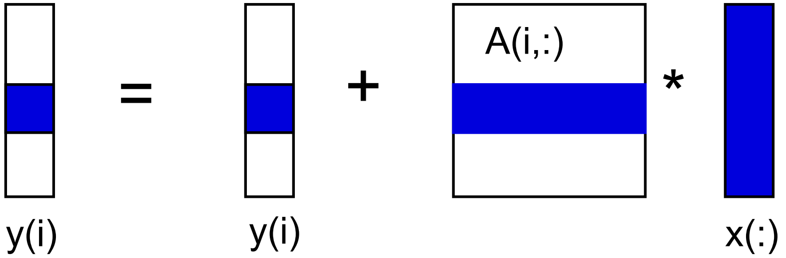
***Computational Intensity:* Key to algorithm efficiency**

***Machine Balance:* Key to machine efficiency**

Assume an element is a float and is equal to word!

Warm up: Matrix-Vector Multiplication

```
{implements y = y + A*x}
for i = 1:n
        for j = 1:n
                y(i) = y(i) + A(i,j)*x(j)
```



- m = ?
- f = ?
- q = ?

Warm up: Matrix-Vector Multiplication

{read x(1:n) into fast memory} **This line needs n memory references**

{read y(1:n) into fast memory} **This line needs n memory references**

for i = 1:n

    {read row i of A into fast memory} **This line needs n memory references but note that there is loop around this line so we do n^2 references in total from this line**

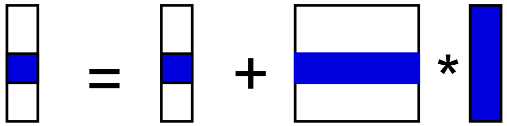
    for j = 1:n

        y(i) = y(i) + A(i,j)*x(j)

{write y(1:n) back to slow memory} **This line needs n memory references**

More explanation: m is computed as follows: n + n + n (n) + n

- m = number of slow memory refs = $3n + n^2$
- f = number of arithmetic operations = $2n^2$
- q = $f / m \approx 2$



- Matrix-vector multiplication limited by slow memory speed

Assume for simplicity vectors x and y, and one row of A, all fit in fast memory

Modeling Matrix-Vector Multiplication

- Examples of some architectures and their machine balance
- So the computational intensity of 2 in matrix-vector multiply means that we can not get close to half peak of these machines: Matrix-Vector Multiplication is a ***memory bound operation!***

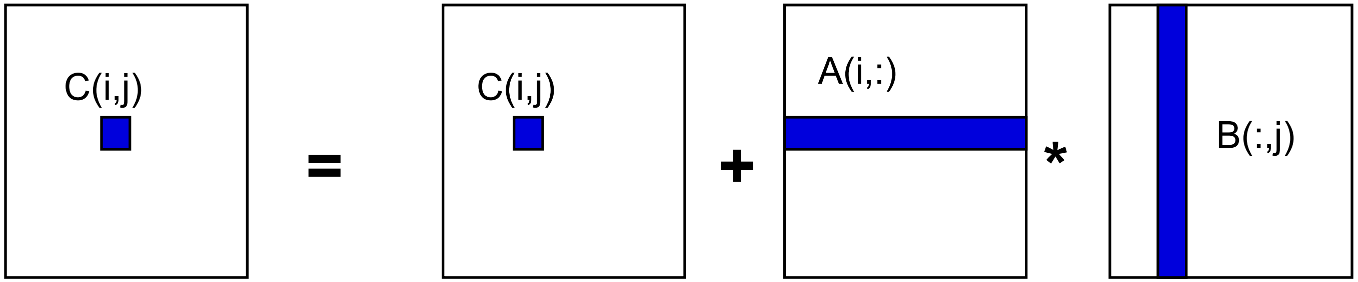
	Clock	Peak	Mem Lat (Min,Max)		Linesize	t_m/t_f
	MHz	Mflop/s	cycles		Bytes	
Ultra 2i	333	667	38	66	16	24.8
Ultra 3	900	1800	28	200	32	14.0
Pentium 3	500	500	25	60	32	6.3
Pentium3M	800	800	40	60	32	10.0
Power3	375	1500	35	139	128	8.8
Power4	1300	5200	60	10000	128	15.0
Itanium1	800	3200	36	85	32	36.0
Itanium2	900	3600	11	60	64	5.5

machine balance **(q must be at least this for ½ peak speed)**

Naïve Matrix Multiply

```
{implements C = C + A*B}
for i = 1 to n
    for j = 1 to n
        for k = 1 to n
            C(i,j) = C(i,j) + A(i,k) * B(k,j)
```

- Algorithm has $2*n^3 = O(n^3)$ Flops.
- If all the data would fit in fast memory (ideal case!) we would only make $3*n^2$ memory references because you only need to read each matrix once form slow memory and then it sticks around in fast memory!
- q potentially as large as* $2*n^3 / 3*n^2 = O(n)$

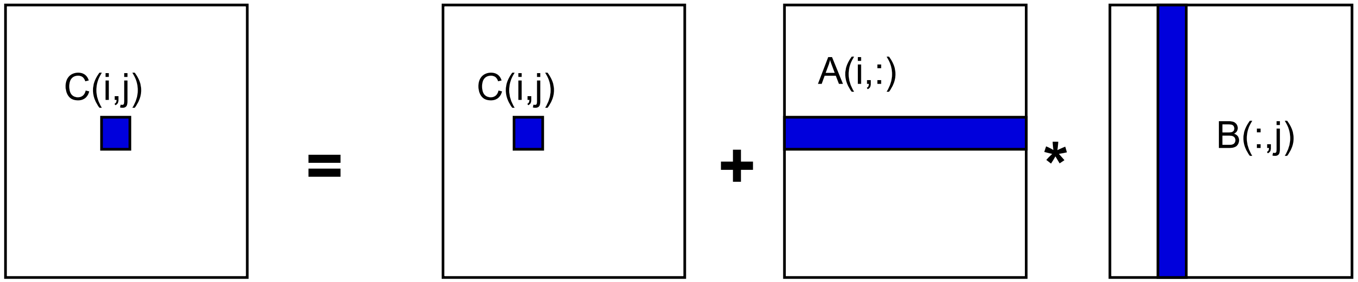


Assume for simplicity that data is layed out in slow memory in the order it is being accessed. For example, here A is stored in row-major and B is stored in column-major.

* Replace 3 with a 4 if you need to write C back to slow memory.

Naïve Matrix Multiply

```
{implements C = C + A*B}
for i = 1 to n
 {read row i of A into fast memory}
  for j = 1 to n
     {read C(i,j) into fast memory}
     {read column j of B into fast memory}
     for k = 1 to n
        C(i,j) = C(i,j) + A(i,k) * B(k,j)
     {write C(i,j) back to slow memory}
```



m = ?

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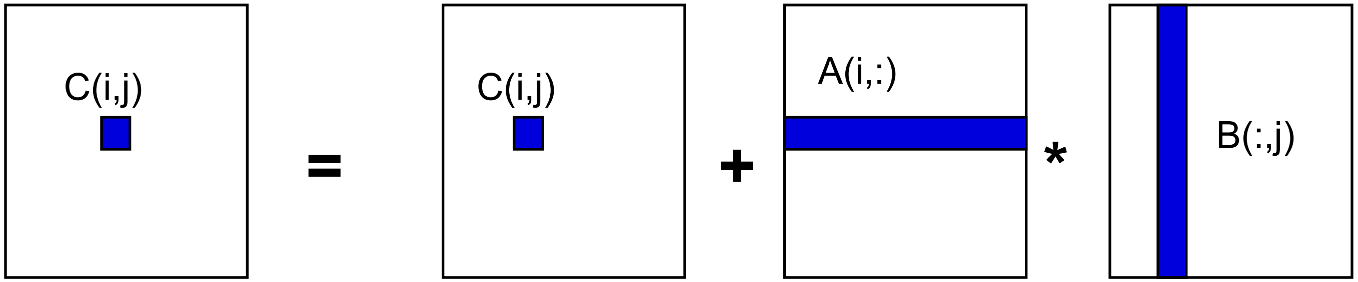
This line needs n memory references but note that there is a loop around this line so we do n^2 references in total for this line.

This line needs n memory reference but note that there are two loops around this line so we do n^3 references in total for this line

This line needs 1 memory reference but note that there are two loops around this line so we do n^2 references in total for this line



$$m = n * (n + n * (1 + n + 1)) = n^3 + 3n^2$$

Naïve Matrix Multiply

Number of slow memory references on unblocked matrix multiply

$m = n^3$ to read each column of B n times

$+ n^2$ to read each row of A once

$+ 2n^2$ to read and write each element of C once

$= n^3 + 3n^2$

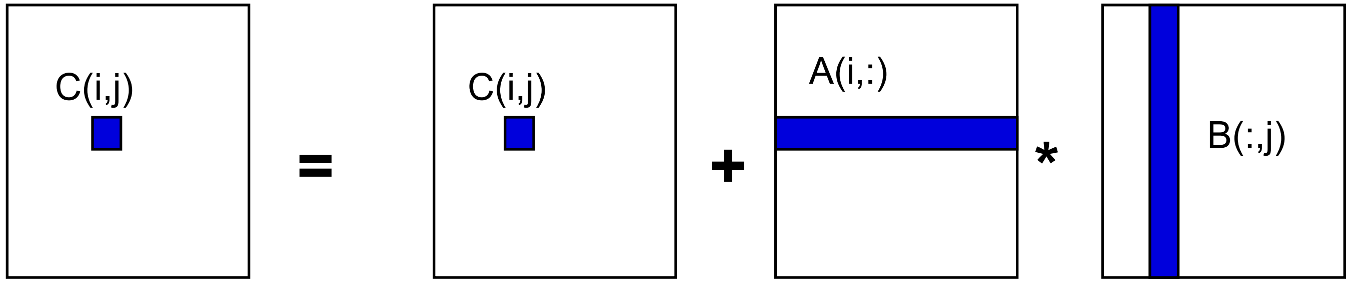
Read the green lines in the previous slide, we are adding those here to get to total m.

So $q = f / m = 2n^3 / (n^3 + 3n^2)$

≈ 2 for large n, no improvement over matrix-vector multiply

Inner two loops are just matrix-vector multiply, of row i of A times B

Similar for any other order of 3 loops



Another way: B gets read n times, A gets read once, and C is read/written 2 times so m is n (n^2)+ n^2 + 2 n^2

Blocked (Tiled) Matrix Multiply

Consider A,B,C to be N-by-N matrices of b-by-b subblocks where
b=n / N is called the block size

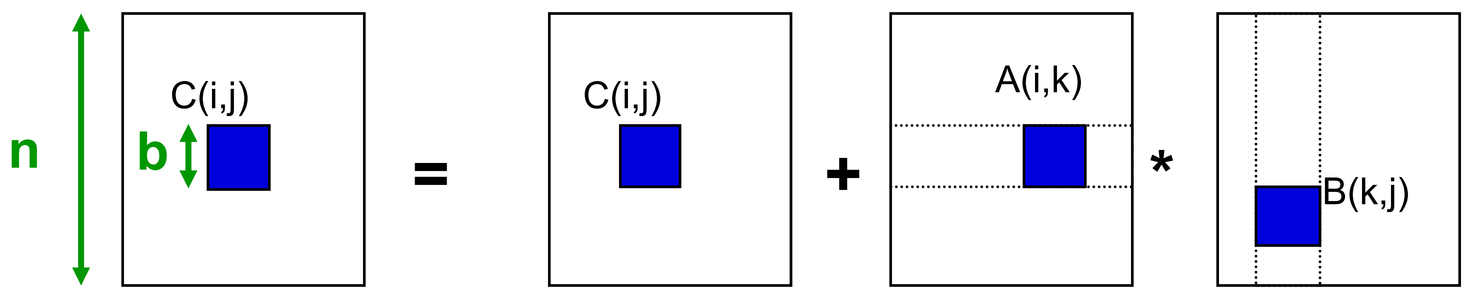
for i = 1 to N
  for j = 1 to N
    {read block C(i,j) into fast memory}
    for k = 1 to N
      {read block A(i,k) into fast memory}
      {read block B(k,j) into fast memory}
      C(i,j) = C(i,j) + A(i,k) * B(k,j) {do a matrix multiply on blocks}
    {write block C(i,j) back to slow memory}

cache does this automatically

3 nested loops inside

block size = loop bounds

N=n/b



$$m = N * N \left((n/N)^2 + N * ((n/N)^2 + (n/N)^2) + (n/N)^2 \right) = (2N+2)\, n^2$$

Tiling for registers (managed by you/compiler) or caches (hardware)

Blocked (Tiled) Matrix Multiply

Recall:

m is amount memory traffic between slow and fast memory

matrix has nxn elements, and NxN blocks each of size bxb

f is number of floating point operations, $2n^3$ for this problem

q = f / m is our measure of algorithm efficiency in the memory system

So:

$m = N*n^2$ read each block of B N^3 times ($N^3 * b^2 = N^3 * (n/N)^2 = N*n^2$)

$+ N*n^2$ read each block of A N^3 times

$+ 2n^2$ read and write each block of C once

$= (2N + 2) * n^2$

So computational intensity q = ?

Another way: If initially we assume each matrix as N by N elements (the blocks are each one element) then B and A each get read N times, and C is read/written 2 times. Since each element/block is size of $(n/N)^2$ so m is $N^3 (n/N)^2 + N^3 (n/N)^2 + 2 N^2 (n/N)^2$

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$= (2N + 2) * n^2$

So computational intensity $q = f / m = 2n^3 / ((2N + 2) * n^2)$

$\approx n / N = b$ for large n

So we can improve performance by increasing the blocksize b

Can have a much better computational intensity than matrix-vector multiply (q=2)

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Follow the exact process you did for the non blocked version with the difference that now an element is extended to be a b by b block.

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Why not increase b to a very large number?

So we can improve performance by increasing the blocksize b

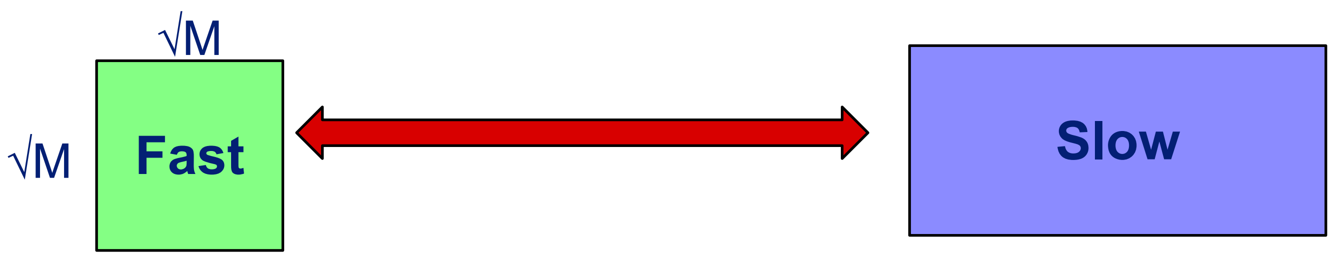
Can have a much better computational intensity than matrix-vector multiply (q=2)

Limits to Optimizing Matrix Multiply

- The tiled matrix multiply analysis assumes that three tiles/blocks fit into fast memory at once.

- If M_{fast} is the size of fast memory then the previous analysis shows that the blocked algorithm has computational intensity:

$$q \approx b \leq (M_{fast}/3)^{1/2}$$



Basic Linear Algebra Subroutines (BLAS)

- Industry standard interface (evolving)
    - www.netlib.org/blas,   www.netlib.org/blas/blast--forum
- Vendors, others supply optimized implementations
- History
    - BLAS1 (1970s): 15 different operations
        - vector operations: dot product, saxpy ($y=\alpha*x+y$), etc
        - $m=2*n$, $f=2*n$, $q = f/m$ = computational intensity ~1 or less

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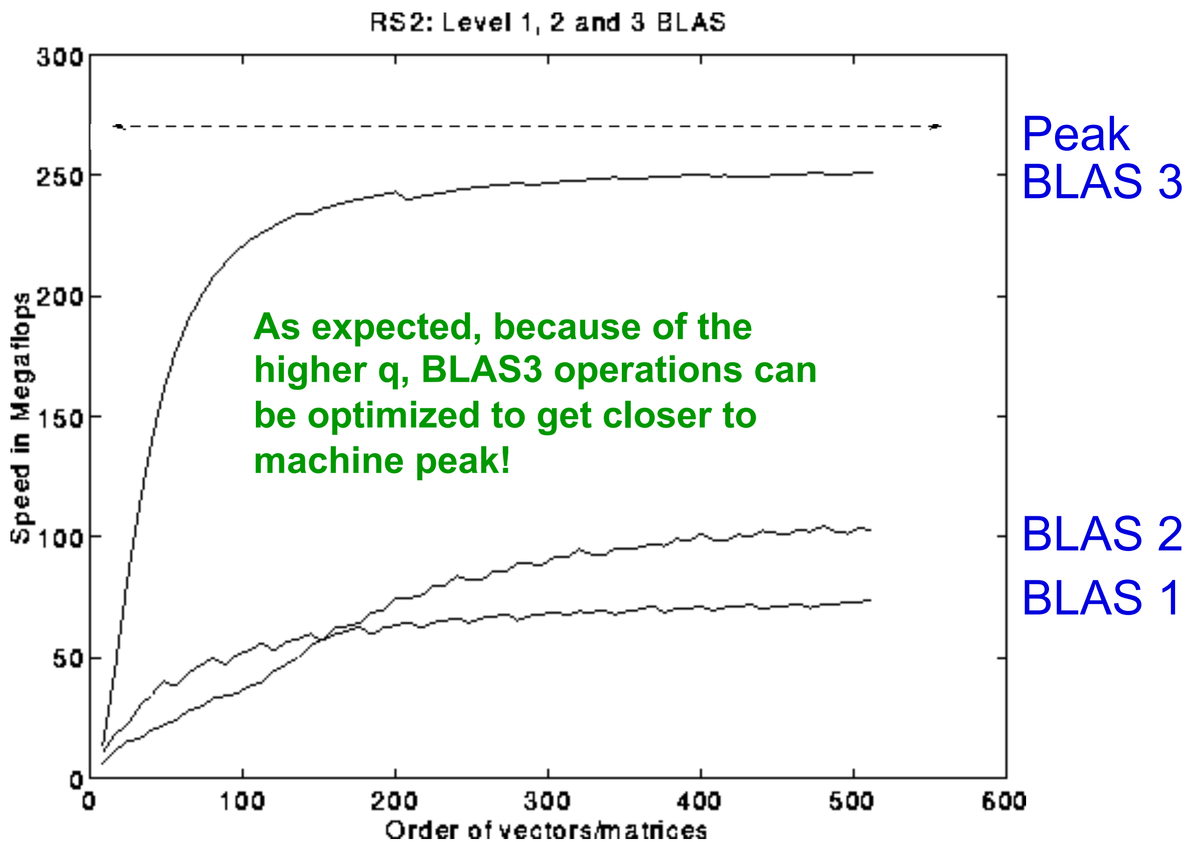
  - BLAS3 (late 1980s): 9 different operations (such as matrix-matrix multiply or solving a triangular system or matrix factorization and so on)
    - matrix-matrix operations: matrix matrix multiply, etc
    - m <= 3n^2, f=O(n^3), so q=f/m can possibly be as large as n, so BLAS3 is potentially much faster than BLAS2
- Good algorithms use BLAS3 when possible (LAPACK & ScaLAPACK)
  - See `www.netlib.org/{lapack,scalapack}`

BLAS speeds on an IBM RS6000/590

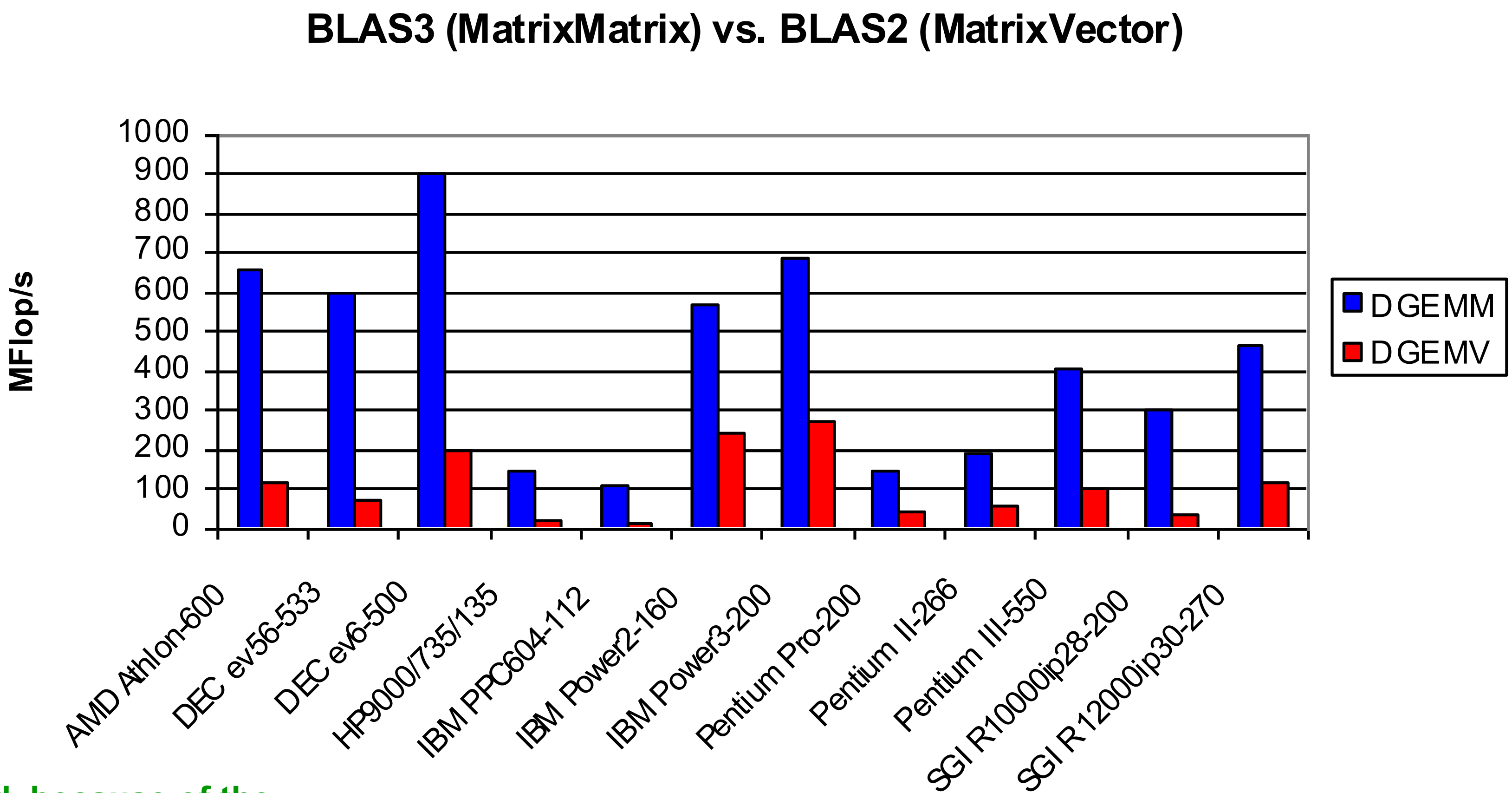
Peak speed = 266 Mflops



BLAS 3 (n-by-n matrix matrix multiply) vs
BLAS 2 (n-by-n matrix vector multiply) vs
BLAS 1 (saxpy of n vectors)

Dense Linear Algebra: BLAS2 vs. BLAS3

- BLAS2 and BLAS3 have very different computational intensity, and therefore different performance



As expected, because of the higher q, BLAS3 operations can be optimized to get closer to machine peak!

Data source: Jack Dongarra