How to Write Fast Numerical Code

Spring 2012

Lecture 5

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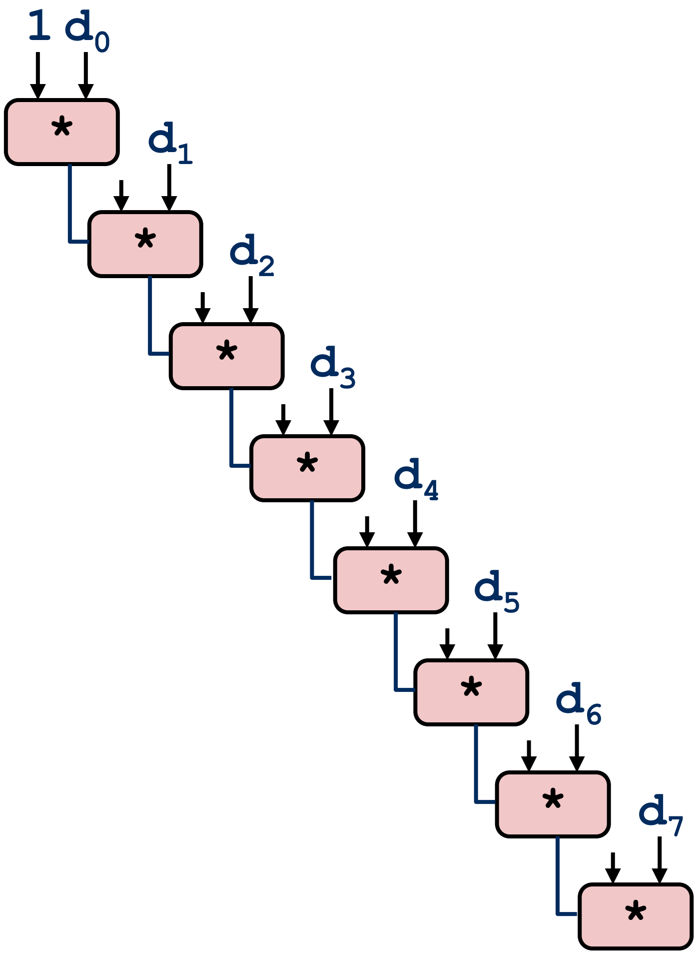
Technicalities

- Research project: Time to finalize!
- Find partner: fastcode-forum@lists.inf.ethz.ch
- Lost on finding a project? Talk to me (e.g., office hours tomorrow)

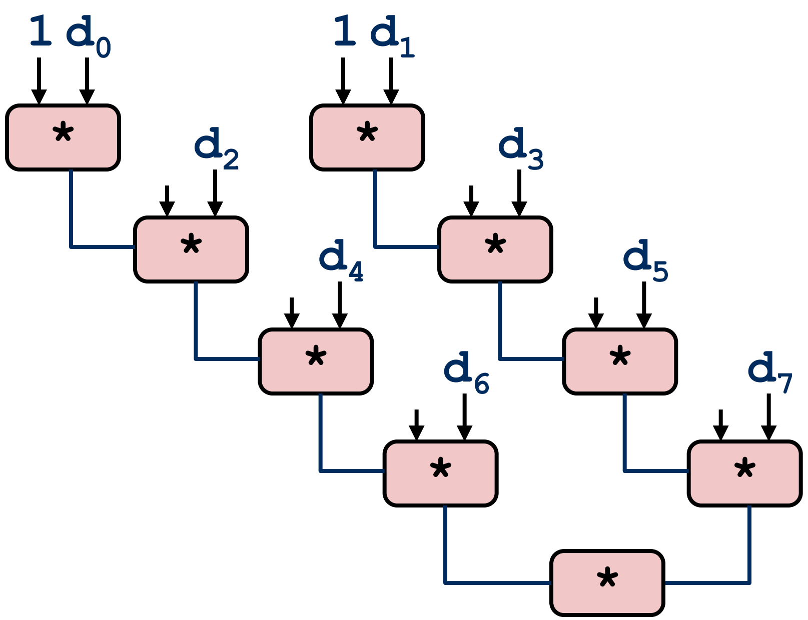
- Exam: Fr Apr 27th

Last Time: ILP

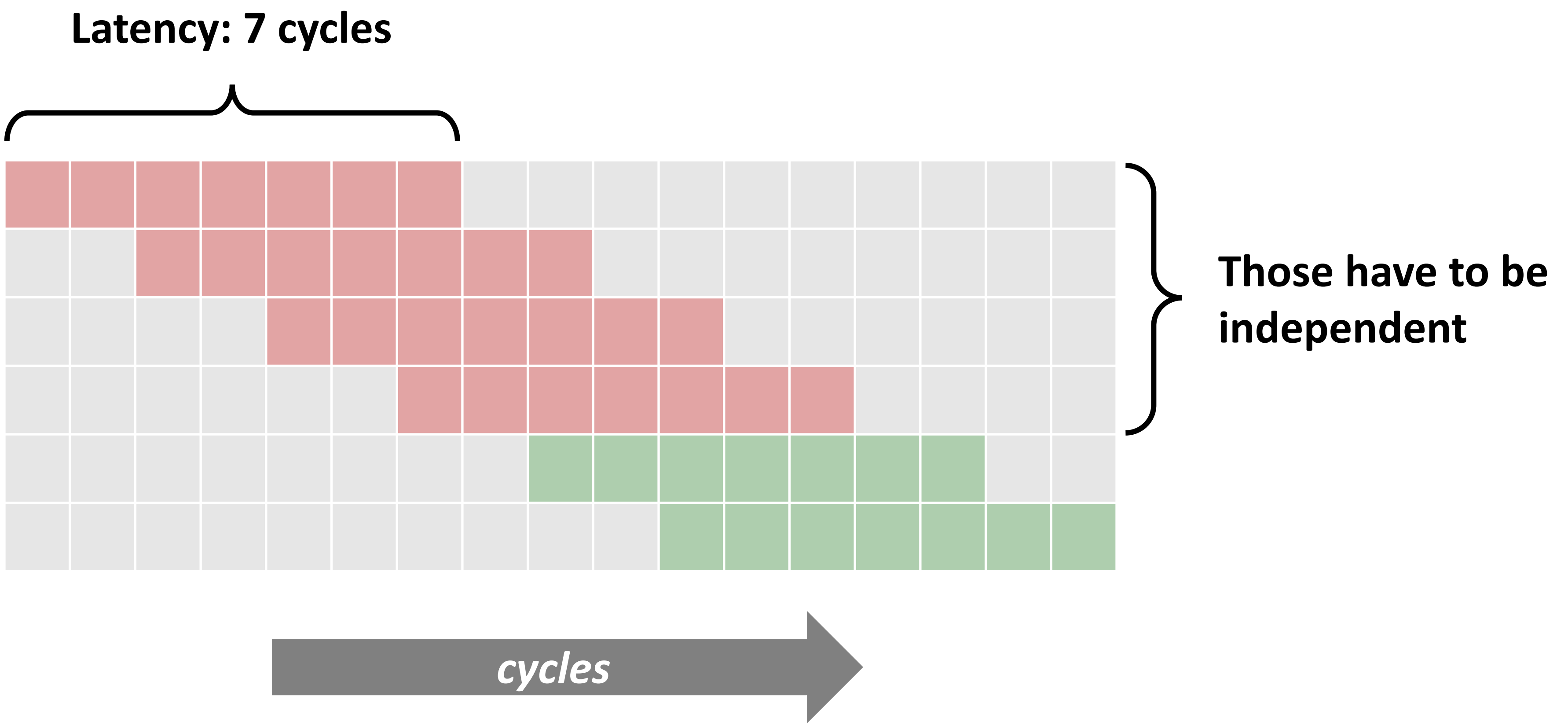
- Latency/throughput (Pentium 4 fp mult: 7/2)



Twice as fast



Last Time: How Many Accumulators?



Based on this insight: K = #accumulators = ceil(latency/cycles per issue)

Compiler Limitations

```
void combine4(vec_ptr v, data_t *dest)
{
  int i;
  int length = vec_length(v);
  data_t *d  = get_vec_start(v);
  data_t t   = IDENT;
  for (i = 0; i < length; i++)
    t = t OP d[i];
  *dest = t;
}
```

```
void unroll2_sa(vec_ptr v, data_t *dest)
{
    int length = vec_length(v);
    int limit  = length-1;
    data_t *d  = get_vec_start(v);
    data_t x0  = IDENT;
    data_t x1  = IDENT;
    int i;
    /* Combine 2 elements at a time */
    for (i = 0; i < limit; i+=2)
       x0 = x0 OP d[i];
       x1 = x1 OP d[i+1];
    /* Finish any remaining elements */
    for (; i < length; i++)
           x0 = x0 OP d[i];
    *dest = x0 OP x1;
}
```

- **Associativity law does not hold for floats: illegal transformation**
- **No good way of handling choices (e.g., number of accumulators)**
- ***More examples of limitations today***

Today

- **Measuring performance & benchmarking**
  Section 3.2 in the tutorial
  http://spiral.ece.cmu.edu:8080/pub-spiral/abstract.jsp?id=100
- **Optimizing compilers and optimization blockers**
  - Overview
  - Removing unnecessary procedure calls
  - Code motion
  - Strength reduction
  - Sharing of common subexpressions
  - Optimization blocker: Procedure calls
  - Optimization blocker: Memory aliasing
  - Summary

Chapter 5 in ***Computer Systems: A Programmer's Perspective****, 2nd edition, Randal E. Bryant and David R. O'Hallaron, Addison Wesley 2010*

Benchmarking

- ***First:*** **Verify your code!**
- **Measure runtime (in [s] or [cycles]) for a set of relevant input sizes**
  - seconds: actual runtime
  - cycles: abstracts from CPU frequency
- **Usually: Compute and show performance (in [flop/s] or [flop/cycle])**
- ***Careful:*** **Better performance ≠ better runtime (why?)**
  - Op count could differ
  - Never show in one plot performance of two algorithms with substantially different op count

How to measure runtime?

- **C clock()**
  - process specific, low resolution, very portable
- **gettimeofday**
  - measures wall clock time, higher resolution, somewhat portable
- **Performance counter (e.g., TSC on Intel)**
  - measures cycles (i.e., also wall clock time), highest resolution, not portable
- **Careful:**
  - measure only what you want to measure
  - ensure proper machine state
    (e.g., cold or warm cache = input data is or is not in cache)
  - measure enough repetitions
  - check how reproducible; if not reproducible: fix it
- ***Getting proper measurements is not easy at all!***

Example: Timing MMM

- Assume **MMM(A,B,C,n)** computes
  C = C + AB, A,B,C are nxn matrices

```
double time_MMM(int n)
{ // allocate
  double *A=(double*)malloc(n*n*sizeof(double));
  double *B=(double*)malloc(n*n*sizeof(double));
  double *C=(double*)malloc(n*n*sizeof(double));

  // initialize
  for (int i = 0; i < n*n; i++){
    A[i] = B[i] = C[i] = 0.0;
  }

  init_MMM(A,B,C,n); // if needed

  // warm up cache (for warm cache timing)
  MMM(A,B,C,n);

  // time
  ReadTime(t0);
  for (int i = 0; i < TIMING_REPETITIONS; i++)
    MMM(A,B,C,n);
  ReadTime(t1);

  // compute runtime
  return (double)((t1-t0)/TIMING_REPETITIONS);
}
```

Problems with Timing

- Too few iterations: inaccurate non-reproducible timing
- Too many iterations: system events interfere
- Machine is under load: produces side effects
- Multiple timings performed on the same machine
- Bad data alignment of input/output vectors: align to multiples of cache line (on Core: address is divisible by 64)
- Time stamp counter (if used) can overflow (on 32-bit architectures)
- Machine was not rebooted for a long time: state of operating system causes problems
- Computation is input data dependent: choose representative input data
- Computation is inplace and data grows until an exception is triggered (computation is done with NaNs)
- You work on a computer that has dynamic frequency scaling (e.g., turbo boost)
- *Always check whether timings make sense, are reproducible*

Benchmarks in Writing

- **Specify experimental setup**
  - platform
  - compiler and version
  - compiler flags used
- **Plot: Very readable**
  - Title, x-label, y-label should be there
  - Fonts large enough
  - Enough contrast (no yellow on white please)
  - Proper number format
    - ***No:*** *13.254687;* ***yes:*** *13.25*
    - ***No:*** *2.0345e-05 s;* ***yes:*** *20.3 μs*
    - ***No:*** *100000 B;* ***maybe:*** *100,000 B;* ***yes:*** *100 KB*

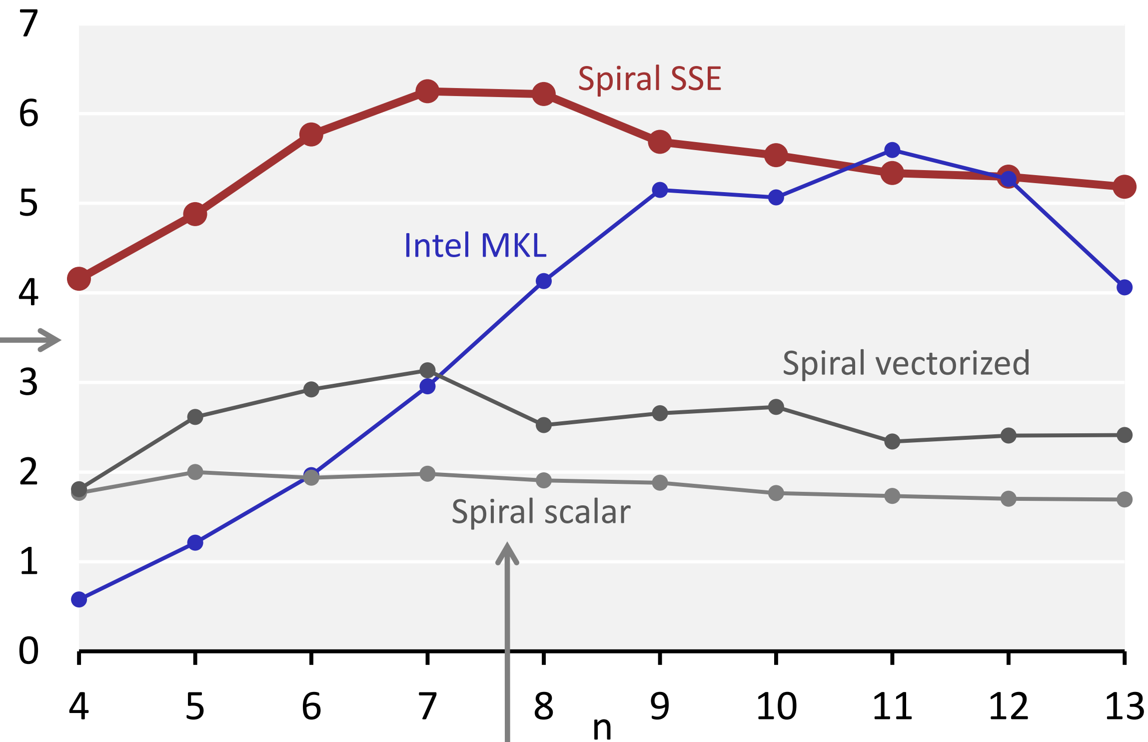
Left alignment

Attractive font (sans serif, avoid Arial)
Calibri, Helvetica, Gill Sans MT, …

DFT 2^n (single precision) on Pentium 4, 2.53 GHz

[Gflop/s]

Horizontal y-label



Main line possibly emphasized (red, thicker)

No y-axis (superfluous)

Background/grid inverted for better layering

No legend; makes decoding easier

Today

- **Measuring performance & benchmarking**
- **Optimizing compilers and optimization blockers**
  - Overview
  - Removing unnecessary procedure calls
  - Code motion
  - Strength reduction
  - Sharing of common subexpressions
  - Optimization blocker: Procedure calls
  - Optimization blocker: Memory aliasing
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Optimizing Compilers

-O

- **Always use optimization flags:**
  - gcc: *default is no optimization* (-O0)!
  - icc: some optimization is turned on
- **Good choices for gcc/icc: -O2, -O3, -march=xxx, -mSSE3, -m64**
  - Read in manual what they do
  - Try to understand the differences
- **Try different flags and maybe different compilers**

Example (On Core 2 Duo)

```
double a[4][4];
double b[4][4];
double c[4][4];

/* Multiply 4 x 4 matrices c = a*b + c */
void mmm(double *a, double *b, double *c) {
  int i, j, k;

  for (i = 0; i < 4; i++)
    for (j = 0; j < 4; j++)
      for (k = 0; k < 4; k++)
        c[i*4+j] += a[i*4 + k]*b[k*4 + j];
}
```

- **Compiled without flags:**
  ~1300 cycles
- **Compiled with -O3 -m64 -march=… -fno-tree-vectorize**
  ~150 cycles

Prevents use of SSE

Optimizing Compilers

- **Compilers are *good* at: mapping program to machine**
  - register allocation
  - code selection and ordering (instruction scheduling)
  - dead code elimination
  - eliminating minor inefficiencies
- **Compilers are *not good* at: algorithmic restructuring**
  - For example to increase ILP, locality, etc.
  - Cannot deal with choices
- **Compilers are *not good* at: overcoming "optimization blockers"**
  - potential memory aliasing
  - potential procedure side-effects

Limitations of Optimizing Compilers

- *If in doubt, the compiler is conservative*
- **Operate under fundamental constraints**
  - Must not change program behavior under any possible condition
  - Often prevents it from making optimizations when would only affect behavior under pathological conditions
- **Most analysis is performed only within procedures**
  - Whole-program analysis is too expensive in most cases
- **Most analysis is based only on *static* information**
  - Compiler has difficulty anticipating run-time inputs
  - Not good at evaluating or dealing with choices

Organization

- Instruction level parallelism (ILP): an example
- **Optimizing compilers and optimization blockers**
  - Overview
  - *Removing unnecessary procedure calls*
  - Code motion
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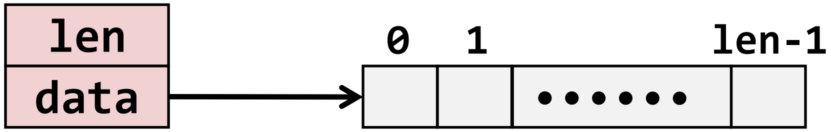
Example: Data Type for Vectors

```c
/* data structure for vectors */
typedef struct{
  int len;
  double *data;
} vec;
```




```c
/* retrieve vector element and store at val */
int get_vec_element(vec *v, int idx, double *val)
{
  if (idx < 0 || idx >= v->len)
    return 0;
  *val = v->data[idx];
  return 1;
}
```

Example: Summing Vector Elements

```
/* retrieve vector element and store at val */
int get_vec_element(vec *v, int idx, double *val)
{
  if (idx < 0 || idx >= v->len)
    return 0;
  *val = v->data[idx];
  return 1;
}
```

```
/* sum elements of vector */
double sum_elements(vec *v, double *res)
{
  int i;
  n = vec_length(v);
  *res = 0.0;
  double t;

  for (i = 0; i < n; i++) {
    get_vec_element(v, i, &t);
    *res += t;
  }
  return res;
}
```

Overhead for every fp +:

- One fct call
- One <
- One >=
- One ||
- One memory variable access

Slowdown:

probably 10x or more

Removing Procedure Call

```
/* sum elements of vector */
double sum_elements(vec *v, double *res)
{
  int i;
  n = vec_length(v);
  *res = 0.0;
  double t;

  for (i = 0; i < n; i++) {
    get_vec_element(v, i, &t);
    *res += t;
  }
  return res;
}
```

```
/* sum elements of vector */
double sum_elements(vec *v, double *res)
{
  int i;
  n = vec_length(v);
  *res = 0.0;
  double *data = get_vec_start(v);

  for (i = 0; i < n; i++)
     *res += data[i];
  return res;
}
```

Removing Procedure Calls

- **Procedure calls can be very expensive**
- **Bound checking can be very expensive**
- **Abstract data types can easily lead to inefficiencies**
  - Usually avoided for in superfast numerical library functions

- ***Watch your innermost loop!***
- ***Get a feel for overhead versus actual computation being performed***

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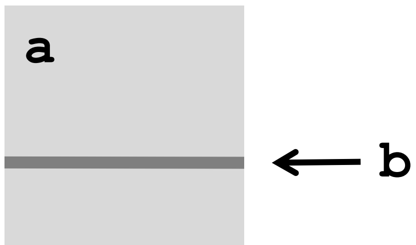
Compiler is likely to do that

Code Motion

- **Reduce frequency with which computation is performed**
  - If it will always produce same result
  - Especially moving code out of loop (loop-invariant code motion)
- **Sometimes also called precomputation**

```
void set_row(double *a, double *b,
   int i, int n)
{
  int j;
  for (j = 0; j < n; j++)
    a[n*i+j] = b[j];
}
```

```
  int j;
  int ni = n*i;
  for (j = 0; j < n; j++)
    a[ni+j] = b[j];
```



Organization

- Instruction level parallelism (ILP): an example
- **Optimizing compilers and optimization blockers**
  - Overview
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  - ***Strength reduction***
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Compiler is likely to do that

Strength Reduction

- **Replace costly operation with simpler one**
- **Example: Shift/add instead of multiply or divide** `16*x → x << 4`
  - Utility machine dependent
- **Example: Recognize sequence of products**

```
for (i = 0; i < n; i++)
  for (j = 0; j < n; j++)
    a[n*i + j] = b[j];
```

→

```
int ni = 0;
for (i = 0; i < n; i++) {
  for (j = 0; j < n; j++)
    a[ni + j] = b[j];
  ni += n;
}
```

Organization

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Compiler is likely to do that

Share Common Subexpressions

- **Reuse portions of expressions**
- **Compilers often not very sophisticated in exploiting arithmetic properties**

3 mults: i*n, (i–1)*n, (i+1)*n

```
/* Sum neighbors of i,j */
up    = val[(i-1)*n + j  ];
down  = val[(i+1)*n + j  ];
left  = val[i*n     + j-1];
right = val[i*n     + j+1];
sum   = up + down + left + right;
```

1 mult: i*n

```
int inj = i*n + j;
up      = val[inj - n];
down    = val[inj + n];
left    = val[inj - 1];
right   = val[inj + 1];
sum     = up + down + left + right;
```

Organization

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  - ***Optimization blocker: Procedure calls***
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Optimization Blocker #1: Procedure Calls

- **Procedure to convert string to lower case**

```
void lower(char *s)
{
  int i;
  for (i = 0; i < strlen(s); i++)
    if (s[i] >= 'A' && s[i] <= 'Z')
      s[i] -= ('A' - 'a');
}
```

$O(n^2)$ instead of $O(n)$

```
/* My version of strlen */
size_t strlen(const char *s)
{
  size_t length = 0;
  while (*s != '\0') {
    s++;
    length++;
  }
  return length;
}
```

$O(n)$

Improving Performance

```
void lower(char *s)
{
  int i;
  for (i = 0; i < strlen(s); i++)
    if (s[i] >= 'A' && s[i] <= 'Z')
      s[i] -= ('A' - 'a');
}
```

```
void lower(char *s)
{
  int i;
  int len = strlen(s);
  for (i = 0; i < len; i++)
    if (s[i] >= 'A' && s[i] <= 'Z')
      s[i] -= ('A' - 'a');
}
```

- **Move call to `strlen` outside of loop**
- **Since result does not change from one iteration to another**
- **Form of code motion/precomputation**

Optimization Blocker: Procedure Calls

- **Why couldn't compiler move `strlen` out of inner loop?**
  - Procedure may have side effects
- ***Compiler usually treats procedure call as a black box that cannot be analyzed***
  - Consequence: conservative in optimizations
- **In this case the compiler may actually do it if `strlen` is recognized as built-in function**

Organization

- Instruction level parallelism (ILP): an example
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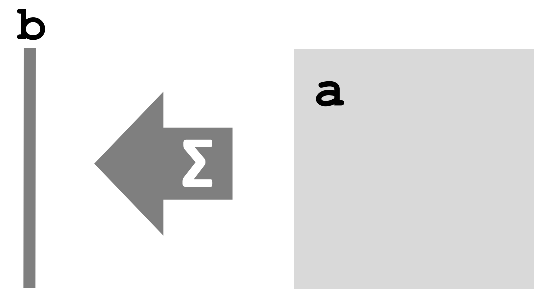
  - Optimization blocker: Procedure calls
  - *Optimization blocker: Memory aliasing*
  - Summary

Optimization Blocker: Memory Aliasing

```
/* Sums rows of n x n matrix a
   and stores in vector b  */
void sum_rows1(double *a, double *b, int n) {
  int i, j;

  for (i = 0; i < n; i++) {
    b[i] = 0;
    for (j = 0; j < n; j++)
      b[i] += a[i*n + j];
  }
}
```

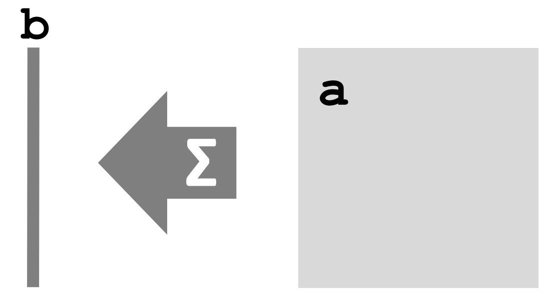


- Code updates `b[i]` (= memory access) on every iteration

Optimization Blocker: Memory Aliasing

```
/* Sums rows of n x n matrix a
   and stores in vector b  */
void sum_rows1(double *a, double *b, int n) {
  int i, j;

  for (i = 0; i < n; i++) {
    b[i] = 0;
    for (j = 0; j < n; j++)
      b[i] += a[i*n + j];
  }
}
```




```
/* Sums rows of n x n matrix a
   and stores in vector b  */
void sum_rows2(double *a, double *b, int n) {
  int i, j;

  for (i = 0; i < n; i++) {
    double val = 0;
    for (j = 0; j < n; j++)
      val += a[i*n + j];
    b[i] = val;
  }
}
```

Does compiler optimize this?

No!

Why?

Reason: Possible Memory Aliasing

- If memory is accessed, compiler assumes the possibility of side effects
- Example:

```
/* Sums rows of n x n matrix a
   and stores in vector b  */
void sum_rows1(double *a, double *b, int n) {
  int i, j;

  for (i = 0; i < n; i++) {
    b[i] = 0;
    for (j = 0; j < n; j++)
      b[i] += a[i*n + j];
  }
}
```

```
double A[9] =
  { 0,   1,   2,
    4,   8,  16},
   32,  64, 128};

double B[3] = A+3;

sum_rows1(A, B, 3);
```

Value of B:

```
init:  [4,  8,  16]

i = 0: [3,  8,  16]

i = 1: [3, 22,  16]

i = 2: [3, 22, 224]
```

Removing Aliasing

```
/* Sums rows of n x n matrix a
   and stores in vector b  */
void sum_rows2(double *a, double *b, int n) {
  int i, j;

  for (i = 0; i < n; i++) {
    double val = 0;
    for (j = 0; j < n; j++)
      val += a[i*n + j];
    b[i] = val;
  }
}
```

- **Scalar replacement:**
  - Copy array elements ***that are reused*** into temporary variables
  - Perform computation on those variables
  - Enables register allocation and instruction scheduling
  - Assumes no memory aliasing (otherwise possibly incorrect)

Optimization Blocker: Memory Aliasing

- **Memory aliasing:**
  Two different memory references write to the same location
- **Easy to have happen in C**
  - Since allowed to do address arithmetic
  - Direct access to storage structures
- **Hard to analyze = compiler cannot figure it out**
  - Hence is conservative
- **Solution: Scalar replacement in innermost loop**
  - Copy memory variables that are reused into local variables
  - Basic scheme:

    Load: *t1 = a[i], t2 = b[i+1], ….*

    Compute: *t4 = t1 * t2; ….*

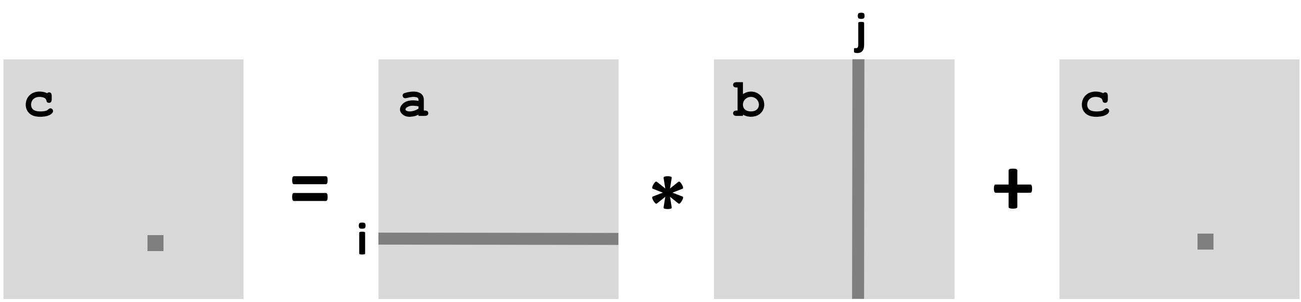
    Store: *a[i] = t12, b[i+1] = t7, …*

More Difficult Example

```
c = (double *) calloc(sizeof(double), n*n);

/* Multiply n x n matrices c = a*b + c   */
void mmm(double *a, double *b, double *c, int n) {
  int i, j, k;

  for (i = 0; i < n; i++)
    for (j = 0; j < n; j++)
      for (k = 0; k < n; k++)
        c[i*n+j] += a[i*n + k]*b[k*n + j];
}
```



- **Which array elements are reused?**
- **All of them!** ***But how to take advantage?***

Step 1: Blocking (Here: 2 x 2)

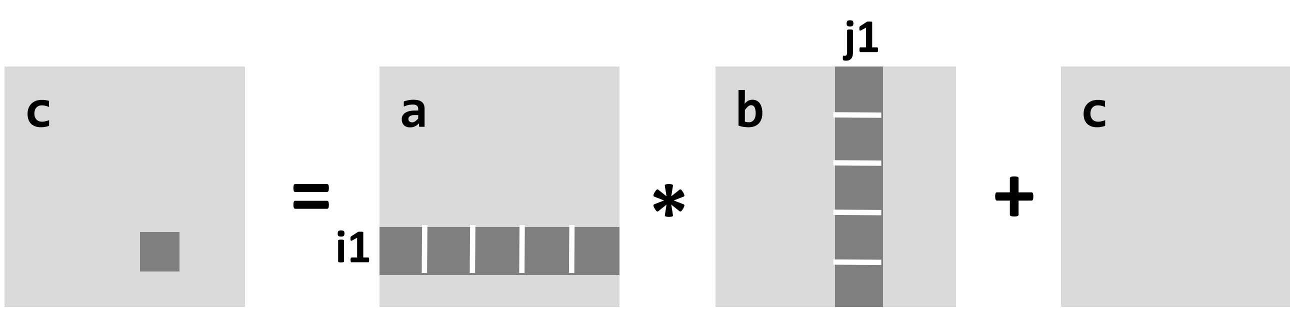
Blocking, also called tiling = partial unrolling + loop exchange

Assumes associativity (= compiler will not do it)

```
c = (double *) calloc(sizeof(double), n*n);

/* Multiply n x n matrices c = a*b + c  */
void mmm(double *a, double *b, double *c, int n) {
  int i, j, k;

  for (i = 0; i < n; i+=2)
    for (j = 0; j < n; j+=2)
      for (k = 0; k < n; k+=2)
        for (i1 = i; i1 < i+2; i1++)
          for (j1 = j; j1 < j+2; j1++)
            for (k1 = k; k1 < k+2; k1++)
              c[i1*n+j1] += a[i1*n + k1]*b[k1*n + j1];
}
```



Step 2: Unrolling Inner Loops

```
c = (double *) calloc(sizeof(double), n*n);

/* Multiply n x n matrices c = a*b + c  */
void mmm(double *a, double *b, double *c, int n) {
  int i, j, k;

  for (i = 0; i < n; i+=2)
    for (j = 0; j < n; j+=2)
      for (k = 0; k < n; k+=2)
        <body>
}
```

```
<body>:
c[i*n + j]           = a[i*n + k]*b[k*n + j] + a[i*n + k+1]*b[(k+1)*n + j]
                       + c[i*n + j]
c[(i+1)*n + j]       = a[(i+1)*n + k]*b[k*n + j] + a[(i+1)*n + k+1]*b[(k+1)*n + j]
                       + c[(i+1)*n + j]
c[i*n + (j+1)]       = a[i*n + k]*b[k*n + (j+1)] + a[i*n + k+1]*b[(k+1)*n + (j+1)]
                       + c[i*n + (j+1)]
c[(i+1)*n + (j+1)] = a[(i+1)*n + k]*b[k*n + (j+1)]
                       + a[(i+1)*n + k+1]*b[(k+1)*n + (j+1)] + c[(i+1)*n + (j+1)]
```

- **Every array element `a[…]`, `b[…]`, `c[…]` used twice**
- **Now scalar replacement can be applied**
  (so again: loop unrolling is done with a purpose)

Can Compiler Remove Aliasing?

```
for (i = 0; i < n; i++)
  a[i] = a[i] + b[i];
```

Potential aliasing: Can compiler do something about it?

Compiler can insert runtime check:

```
if (a + n < b || b + n < a)
  /* further optimizations may be possible now */
  ...
else
  /* aliased case */
  ...
```

Removing Aliasing With Compiler

- **Globally with compiler flag:**
  - `-fno-alias, /Oa`
  - `-fargument-noalias, /Qalias-args-` (function arguments only)
- **For one loop: pragma**

```
void add(float *a, float *b, int n) {
  #pragma ivdep
  for (i = 0; i < n; i++)
    a[i] = a[i] + b[i];
}
```

- **For specific arrays: restrict (needs compiler flag `-restrict, /Qrestrict`)**

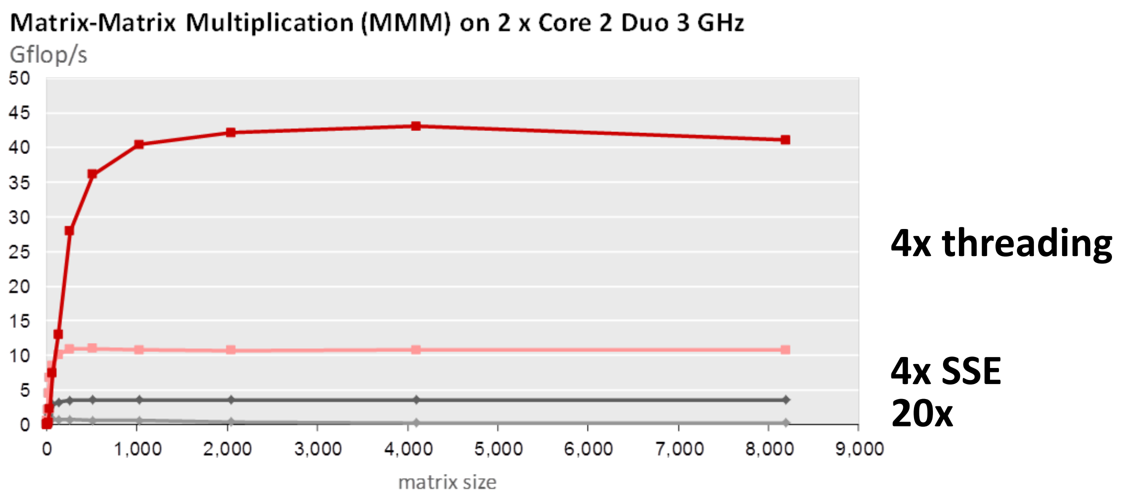
```
void add(float *restrict a, float *restrict b, int n) {
  for (i = 0; i < n; i++)
    a[i] = a[i] + b[i];
}
```

Organization

- Instruction level parallelism (ILP): an example
- **Optimizing compilers and optimization blockers**
  - Overview
  - Removing unnecessary procedure calls
  - Code motion
  - Strength reduction
  - Sharing of common subexpressions
  - Optimization blocker: Procedure calls
  - Optimization blocker: Memory aliasing
  - ***Summary***

Summary

- ***One can easily loose 10x, 100x in runtime or even more***



- **What matters besides operation count:**
  - Coding style (unnecessary procedure calls, unrolling, reordering, …)
  - Algorithm structure (instruction level parallelism, locality, …)
  - Data representation (complicated structs or simple arrays)

Summary: Optimize at Multiple Levels

- **Algorithm:**
  - Evaluate different algorithm choices
  - Restructuring may be needed (ILP, locality)
- **Data representations:**
  - Careful with overhead of complicated data types
  - Best are arrays
- **Procedures:**
  - Careful with overhead
  - They are black boxes for the compiler
- **Loops:**
  - Often need to be restructured (ILP, locality)
  - Unrolling often necessary to enable other optimizations
  - Watch the innermost loop bodies

Numerical Functions

- **Use arrays if possible**
- **Unroll to some extent**
  - To make ILP explicit
  - To enable scalar replacement and hence register allocation for variables that are reused