OpenMP

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- A Running Example: SpMV
- 2 parallel pragma
- 3 Work sharing constructs
 - loops (for)
 - scheduling
 - task parallelism (task and taskwait)
- 4 Data sharing clauses
- SIMD constructs

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A running example: Sparse Matrix Vector Multiply (SpMV)

- sparse matrix: a matrix whose elements are mostly zeros
- i.e. the number of non-zero elements (nnz) \ll the number of all elements $(M \times N)$
 - \bullet M: the number of rows
 - \bullet N: the number of columns

Sparse matrices appear everywhere

- meshes in scientific simulation
 - $A_{i,j} =$ a weight connecting nodes i and j in the mesh
- graphs, which in turn appear in many applications
 - $A_{i,j}$ = the weight of the edge $i \to j$ (or $j \to i$)
 - Web, social network, road/traffic networks, citation networks, metabolic pathways, etc.
- many problems can be solved using SpMV
 - eigenvalues (including PageRank, graph partitioning, etc.)
 - partial differential equation
 - . . .

What makes "sparse" matrix different from ordinary (dense) matrix?

- the number of non-zero elements are so small that representing it as $M \times N$ array is too wasteful (or just impossible)
- → use a data structure that takes memory/computation only (or mostly) for non-zero elements (coordinate list, compressed sparse row, etc.)

Coordinate list (COO)

- represent a matrix as a list of $(i, j, A_{i,j})$'s
- data format:

```
struct coo {
int n_rows, n_cols, nnz;
/* nnz elements */
struct { i, j, Aij } * elems;
};
```

• SpMV (y = Ax)

```
for (k = 0; k < A.nnz; k++) {
   i,j,Aij = A.elems[k];
   y[i] += Aij * x[j];
}</pre>
```

Compressed sparse row (CSR)

- puts elements of a single row in a contiguous range
- an index (number) specifies where a particular row begins in the elems array
- $\bullet \rightarrow no \ need \ to \ have \ i \ for \ every \ single \ element$
- data format:

```
struct coo {
int n_rows, n_cols, nnz;
struct { j, Aij } * elems; // nnz elements
int * row_start; // n_rows elements
};
```

elems [row_start[i]] \cdots elems [row_start[i + 1]] are the elements in the ith row

• SpMV (y = Ax)

```
for (i = 0; i < A.n_rows; i++) {
  for (k = A.row_start[i]; k < A.row_start[i+1]; k++) {
    j,Aij = A.elems[k];
    y[i] += Aij * x[j];
  }
}</pre>
```

OpenMP

- de fact standard model for programming shared memory machines
- \bullet C/C++/Fortran + directives + APIs
 - by **#pragma** in C/C++
 - by comments in Fortran
- many free/vendor compilers, including GCC, LLVM, NVIDIA HPC SDK

OpenMP reference

- official home page: http://openmp.org/
- specification: http://openmp.org/wp/openmp-specifications/
- latest version is 5.0 (https://www.openmp.org/spec-html/5.0/openmp.html)
- section numbers below refer to those in OpenMP spec 5.0

Compiling OpenMP programs for multicores

• GCC and LLVM (clang/clang++): compile with -fopenmp

```
$ clang -Wall -fopenmp program.c
$ gcc -Wall -fopenmp program.c
```

• NVIDIA HPC SDK (nvc/nvc++): compile with -mp

```
1 $ nvc -Wall -mp program.c
```

• In this lecture, we use LLVM and NVIDIA HPC SDK, as they support OpenMP for multicore, GPU offloading, and CUDA

Running OpenMP programs

• run the executable specifying the number of threads with OMP_NUM_THREADS environment variable

```
$ OMP_NUM_THREADS=1 ./a.out # use 1 thread
$ OMP_NUM_THREADS=4 ./a.out # use 4 threads
```

- if OMP_NUM_THREADS is unspecified, it uses the number of available processors visible to OS, including hyperthreading
- see 2.6.1 "Determining the Number of Threads for a parallel Region" for more details and other ways to control the number of threads

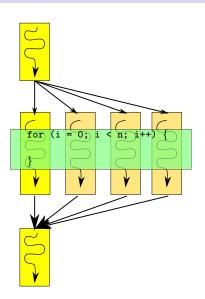
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Two pragmas you must know first

- #pragma omp parallel to launch a team of threads (2.6)
- then #pragma omp for to distribute iterations to threads (2.9.2)

Note: all OpenMP pragmas have the common format: #pragma omp ...

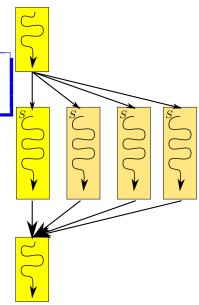


#pragma omp parallel

• basic syntax:

```
1 ... #pragma omp parallel S ...
```

- basic semantics:
 - create a team of OMP_NUM_THREADS threads
 - the current thread becomes the *master* of the team
 - S will be executed by each member of the team
 - the master thread waits for all to finish S and continue



parallel pragma example

```
#include <stdio.h>
int main() {
  printf("hello\n");

#pragma omp parallel
  printf("world\n");
  printf("bye\n");

return 0;
}
```

```
1 $ OMP_NUM_THREADS=1 ./a.out
2 hello
3 world
4 $ OMP_NUM_THREADS=4 ./a.out
5 hello
6 world
7 world
8 world
9 world
10 bye
```

Remarks: what does parallel do?

- you may assume an OpenMP thread \approx OS-supported thread (e.g., Pthread)
- that is, if you write this program

```
int main() {
    #pragma omp parallel
    worker();
}
```

and run it as follows,

```
1 $ OMP_NUM_THREADS=50 ./a.out
```

you will get 50 OS-level threads, each doing worker()

 $\bullet \Rightarrow$ specifying a number (> the hardware core count) causes more harm than good on CPUs

How to distribute work among threads?

- #pragma omp parallel creates threads, all executing the same statement
- it's not a means to parallelize work, per se, but just a means to create a number of similar threads
 - Single Program Multiple Data (SPMD) model
- so how to distribute (or partition) work among them?
 - do it yourself
 - 2 use work sharing constructs

Do it yourself: functions to get the number/id of threads

- omp_get_num_threads() (3.2.2): the number of threads in the current team
- omp_get_thread_num() (3.2.4): the current thread's id (0, 1, ...) in the team
- they are primitives with which you may partition work yourself by whichever ways you prefer
- e.g.,

```
#pragma omp parallel

f

int t = omp_get_thread_num();

int nt = omp_get_num_threads();

/* divide n iterations evenly amont nt threads */

for (i = t * n / nt; i < (t + 1) * n / nt; i++) {

...

}

}</pre>
```

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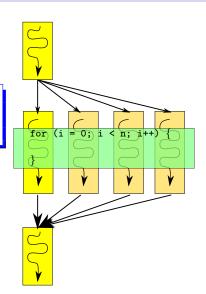
Work sharing constructs

- in theory, parallel construct is all you need to do things in parallel
- but it's too inconvenient
- \bullet OpenMP defines ways to partition work among threads $(work\ sharing\ constructs)$
 - for
 - task

#pragma omp for (work-sharing for)

• basic syntax (2.9.2):

- basic semantics: the threads in the team divde the iterations among them
- but how? \Rightarrow scheduling



#pragma omp for restrictions

- iterations are executed in any order may interleave
 - the program must not rely on the order in which they are executed
- strong syntactic restrictions apply (2.9.1); basically, the *iteration space must be easily identifiable at the beginning* of the loop
 - roughly, it must be of the form:

```
#pragma omp for
for(i = init; i < limit; i += incr)
S</pre>
```

except < and += may be other similar operators

• init, limit, and incr must be loop invariant

Parallelizing loop nests by collapse

• collapse(l) can be used to work-share nested loops. e.g.,

```
#pragma omp for collapse(2)
for (i = 0; i < n; i++)
for (j = 0; j < n; j++)
S</pre>
```

will partition n^2 iterations of the doubly-nested loop

- schedule clause applies to nested loops as if the nested loop is an equivalent flat loop
- restriction: the loop must be "perfectly nested" (the iteration space must be a rectangular and no intervening statement between different levels of the nest)

Parallel SpMV for CSR using #pragma omp for

• it only takes to work-share the outer for loop

```
// assume inside #pragma omp parallel
...

#pragma omp for
for (i = 0; i < A.n_rows; i++) {
    for (k = A.row_start[i]; k < A.row_start[i+1]; k++) {
        j,Aij = A.elems[k];
        y[i] += Aij * x[j];
    }
}</pre>
```

• note: the inner loop (k) is executed sequentially

Parallel SpMV COO using #pragma omp for?

• the following code does not work (why?)

```
// assume inside #pragma omp parallel
...

#pragma omp for
for (k = 0; k < A.nnz; k++) {
    i,j,Aij = A.elems[k];
    y[i] += Aij * x[j];
}</pre>
```

- for a similar reason, we cannot apply collapse to the CSR loop
- a possible remedy will be described later

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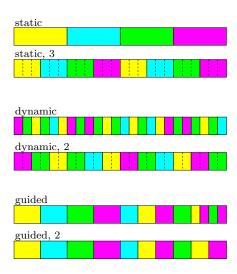
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Scheduling (2.9.2)

- schedule clause in work-sharing for loop determines how iterations are divided among threads
- There are three alternatives (static, dynamic, and guided)

static, dynamic, and guided

- schedule(static[,chunk]): predictable round-robin
- schedule(dynamic[,chunk]): each thread repeats fetching chunk iterations
- schedule(guided[,chunk]): threads grab many iterations in early stages; gradually reduce iterations to fetch at a time
- *chunk* specifies the minimum granularity (iteration counts)



Other scheduling options and notes

• schedule(runtime) determines the schedule by OMP_SCHEDULE environment variable. e.g.,

```
1 $ OMP_SCHEDULE=dynamic,2 ./a.out
```

• schedule(auto) or no schedule clause choose an implementation dependent default

Visualizing schedulers

See demo

Scheduling for SpMV on CSR

```
// assume inside #pragma omp parallel
...

#pragma omp for schedule(???)

for (i = 0; i < A.n_rows; i++) {
    for (k = A.row_start[i]; k < A.row_start[i+1]; k++) {
        j,Aij = A.elems[k];
        y[i] += Aij * x[j];
    }

}</pre>
```

- static? depending on the number of elements in rows, load imbalance may be significant
- dynamic/guided? load balancing will be better, but extremely dense rows may still be an issue
- the more robust strategy is to partition non-zeros, not rows

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Task parallelism in OpenMP

- OpenMP's initial focus was simple parallel loops
- since 3.0, it supports task parallelism
- but why it's necessary?
- aren't parallel and for all we need?

Limitation of parallel for

• what if you have a parallel loop inside another

• perhaps in a function?

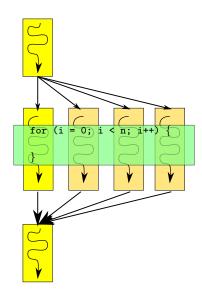
```
main() {
   for ( ... ) {
        ...
        g();
      }
   }
   g() {
      for (...) ...
   }
```

• what about parallel recursions?

```
1  qs() {
2   if (...) { ... }
3   else {
4    qs();
5    qs();
6   }
7  }
```

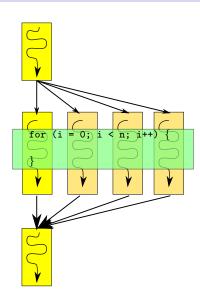
parallel for can't handle nested parallelism

 OpenMP generally ignores nested parallel pragma when enough threads have been created by the outer parallel pragma, for good reasons



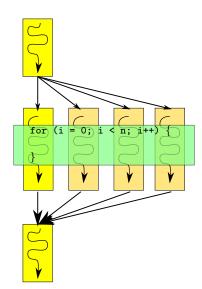
parallel for can't handle nested parallelism

- OpenMP generally ignores nested parallel pragma when enough threads have been created by the outer parallel pragma, for good reasons
- the fundamental limitation is its simplistic work-sharing mechanism



parallel for can't handle nested parallelism

- OpenMP generally ignores nested parallel pragma when enough threads have been created by the outer parallel pragma, for good reasons
- the fundamental limitation is its simplistic work-sharing mechanism
- *tasks* address these issues, by allowing tasks to be created at arbitrary points of execution (and a mechanism to distribute them across cores)



Task parallelism in OpenMP

- syntax:
 - task creates a task executing S (2.10.1)

```
 \begin{array}{c} {}_{1}\\ {}_{2}\\ \end{array} \end{array} \left[ \begin{array}{c} {}_{\text{pragma omp task}}\\ {}_{S}\\ \end{array} \right.
```

• taskwait waits for child tasks to finish (2.17.5)

```
#pragma omp taskwait
```

OpenMP task parallelism template

- don't forget to create a parallel region
- don't also forget to enter a master region, which says only the master executes the following statement and others "stand-by"

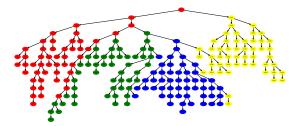
```
int main() {
#pragma omp parallel
#pragma omp master
// or #pragma omp single
ms(a, a + n, t, 0);
}
```

• and create tasks in the master region

```
void ms(a, a_end, t, dest) {
   if (n == 1) {
        ...
   } else {
        ...
   #pragma omp task
   ms(a, c, t, 1 - dest);
   #pragma omp task
   ms(c, a_end, t + nh, 1 - dest);
   #pragma omp task
   inc   inc
```

What are tasks good for?

- the strength of tasks as opposed to for loop is its flexibility
 - create tasks at any point during the computation
 - they get distributed to cores
- especially good for "nested parallelism" and "parallel recursions (divide and conquer)"



• even for loops, you may consider reformulating them into divide-and-conquer as an alternative dynamic load-balancing strategy

Pros/cons of various approaches

• static:

- partitioning iterations is simple and does not require communication
- mapping between work ↔ thread is deterministic and predictable (why it's important?)
- may cause load imbalance (leave some threads idle, even when other threads have many work to do)

• dynamic:

- less prone to load imbalance, if chunks are sufficiently small
- partitioning iterations needs communication (no two threads execute the same iteration) and may become a bottleneck
- mapping between iterations and threads is non-deterministic
- OpenMP's dynamic scheduler is inflexible in partitioning nested loops

Pros/cons of schedulers

- divide and conquer + tasks :
 - less prone to load imbalance, as in dynamic
 - distributing tasks needs communication, but efficient implementation techniques are known
 - mapping between work and thread is non-deterministic, as in dynamic
 - you can flexibly partition loop nests in various ways (e.g., keep the space to square-like)
 - need some coding efforts (easily circumvented by additional libraries; e.g., TBB's blocked_range2d and parallel_for)

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Data sharing

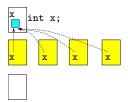
- parallel, for, task pragma accept clauses specifying which variables should be shared among threads or between the parent/child tasks (or otherwise privatized/replicated to each thread)
- 2.19 "Data Environments"
 - private
 - firstprivate
 - shared
 - reduction (only for parallel and for)
 - copyin

Data sharing/privatizing example

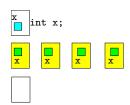
```
$ OMP_NUM_THREADS=2 ./a.out
S at 0x..777f494, P at 0x..80d0e28, L at 0x..80d0e2c
S at 0x..777f494, P at 0x..777f468, L at 0x..777f46c
```

Data sharing behavior

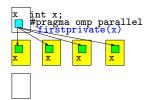
shared



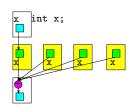
private



firstprivate



reduction



- definition: there is a race condition when concurrent threads access the same location and one of which writes to it
- a race condition almost always implies your program won't work
- even something as simple as this (some accumulations may be lost)

thread 1	thread 2
$x (123) \rightarrow t$	
$x \leftarrow 124$	

thread 1	thread 2
$x (123) \rightarrow t$	
	\mathbf{x} (123) $\rightarrow \mathbf{t}$
$x \leftarrow 124$	
	$x \leftarrow 124$

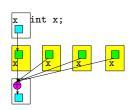
thread 1	thread 2
$x (123) \rightarrow t$	
/ 197	$x (123) \rightarrow t$
x ← 124	$x \leftarrow 124$

• The increment by a thread is "lost"

Two basic tools to resolve race conditions

- "make it atomic" #pragma omp atomic and #pragma omp critical: gaurantee the specified operation to be done atomically
- "all you need may be a reduction" reduction clause performs efficient reduction operations on behalf of you

thread 1	thread 2
$\begin{array}{c} x (123) \to t \\ x \leftarrow 124 \end{array}$	
	$\begin{array}{c} x (124) \to t \\ x \leftarrow 125 \end{array}$



#pragma omp critical

• syntax:

```
#pragma omp critical
statement
```

- effect: the execution of *statement* will not overlap with other executions of *statement* (or any other statement labeled #pragma omp critical, for that matter)
- note: most general, but likely to be slow

#pragma omp atomic

• syntax:

```
#pragma omp atomic
var = var op exp
```

op is a predefined operation such as +, -, *, ...

- effect: guarantee the read-update is done atomically (is not lost); that is, *var* is not updated by someone else between the read and update
- note: semantically, it is like

but typical implementations take advantage of atomic instructions supported by CPU, such as fetch-and-add or compare-and-swap

Reduction

• in general, "reduction" refers to ¹/₂ an operation to combine many ³ values into a single value. e.g., ⁴

```
• v = v_1 + \dots + v_n

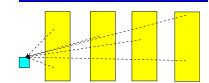
• v = \max(v_1, \dots, v_n)

• \dots
```

- simply sharing the variable (v) does not work (race condition)
- one way to fix is to make updates atomic, but it will be slow

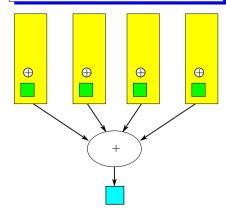
```
v = 0.0;
for (i = 0; i < n; i++) {
v += f(a + i * dt) * dt;
}</pre>
```

```
v = 0.0;
#pragma omp parallel for
for (i = 0; i < n; i++) {
#pragma omp atomic
v += f(a + i * dt) * dt;
}</pre>
```



Reduction clause in OpenMP

- a more efficient strategy:
 - let each thread work (reduce) on its private variable, and
 - when threads finish, combine their partial results into one
- reduction clause in OpenMP does just that (2.19.5)



Builtin reduction and user-defined reduction (2.9.2)

• reduction syntax:

```
#pragma omp parallel reduction(op:var,var,...)
S
```

- builtin reductions
 - op is one of +, *, -, &, ^, |, &&, and ||
 - (Since 3.1) min or max
- builtin reductions are limited to simple types and common operations → user-defined reductions (since 4.0)

Why do you want user-defined reductions?

- consider how to do reduction on 3-element vector
- e.g., how to parallelize this loop safely

```
typedef struct {
      double a[3];
    } vec_t;
4
    int main() {
      vec_t y;
6
      vec_init(&y);
                                      /* y = \{0,0,0\} */
    #pragma omp parallel
    #pragma omp for
      for (long i = 0; i < 10000; i++) {
10
        y.a[..] += 1;
11
12
    }
13
```

- you cannot say reduction(+:y.a[0], y.a[1], y.a[2]) (what if you have 100 elements?)
- we define a reduction operation on vec_t type instead

User-defined reduction

• syntax: (2.19.5.7)

(init statement)

```
#pragma omp declare reduction (name : type : combine_statement)

Or

#pragma omp declare reduction (name : type : combine_statement) initializer
```

• effect:

- you can specify reduction(name: var) for a variable of type type
- init_statement is executed by each thread before entering the loop, typically to initialize its private copy of var
- combine_statement is executed to merge a partial result to another variable

User-defined reduction: a simple example

• introduce reduction

```
#pragma omp declare reduction \
(vp : vec_t : vec_add(&omp_out,&omp_in)) \
initializer(vec_init(&omp_priv))
```

vec_add must be defined somewhere and not shown

• add reduction(vp : y) to the for loop

User-defined reduction: how it works

with

```
#pragma omp declare reduction \
(vp : vec_t : vec_add(&omp_out,&omp_in)) \
initializer(vec_init(&omp_priv))

#pragma omp for reduction(vp : y)
for (long i = 0; i < 10000; i++) {
    y.a[..] += 1;</pre>
```

```
\approx
```

```
vec_t y_priv; // thread—local copy of y
vec_init(&y_priv); // initializer

#pragma omp for
for (long i = 0; i < 10000; i++) {
    y_priv.a[..] += 1;
}

// merge the partial result into the shared variable
// actual implementation may be (is likely to be) different
vec_add(&y, &y_priv); // y += y_priv</pre>
```

User-defined reduction: limitations

- combine-statement can reference only two local variables (omp_in and omp_out)
 - it should reduce (merge) omp_in into omp_out (e.g., omp_out
 += omp_in)
- *init-statement* can reference only two local variables (omp_priv and omp_orig)
 - omp_priv: the private copy init-statement should initialize
 - omp_orig: the original shared variable
- \bullet \Rightarrow local contexts necessary for initialization and reduction must be encapsulated in the variables subject to reduction

An exercise: reduction on variable-length vectors

• a variable-length version of the previous example

```
typedef struct {
long n;  // number of elements (variable)
double * a; // n elements
} vec_t;
```

• and a reduction for it

• the point is you cannot reference n in the initializer

```
1
2 (!) #pragma omp declare reduction \
2  (vp : vec_t : vec_add(&omp_out,&omp_in)) \
3  initializer(vec_init(&omp_priv, n))
```

An exercise: reduction on variable-length vectors

- initializer can reference omp_orig to obtain the context (i.e. vector length in this example)
- \Rightarrow define a function, vec_init_from, which takes the shared y and initialize the private copy of y

```
int vec_init_from(vec_t * v, vec_t * orig) {
   long n = orig->n;
   double * a = (double *)malloc(sizeof(double) * n);
   for (long i = 0; i < n; i++) {
      a[i] = 0;
   }
   v->n = n;
   v->a = a;
   return 0;
}
```

• and say

```
#pragma omp declare reduction \
(vp : vec_t : vec_add(&omp_out,&omp_in)) \
initializer(vec_init_from(&omp_priv, &omp_orig))
```

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SIMD constructs

- simd pragma (2.9.3)
 - allows an explicit vectorization of for loops
 - syntax restrictions similar to omp for pragma apply
- declare simd pragma (2.9.3.3)
 - instructs the compiler to generate vectorized versions of a function
 - with it, loops with function calls can be vectorized

simd pragma

• basic syntax (similar to omp for):

```
#pragma omp simd clauses
for (i = ...; i < ...; i += ...)
S</pre>
```

- clauses
 - aligned(var, var, ... : align)
 - uniform(var,var,...) says variables are loop invariant
 - linear(var,var,...:stride) says variables have the specified stride between consecutive iterations

declare simd pragma

• basic syntax (similar to omp for):

```
#pragma omp declare simd clauses
function definition
```

- clauses
 - those for simd pragma
 - notinbranch
 - inbranch

SIMD pragmas, rationales

- most automatic vectorizers give up vectorization in many cases
 - conditionals (lanes may branch differently)
 - 2 inner loops (lanes may have different trip counts)
 - 3 function calls (function bodies are not vectorized)
 - 1 iterations may not be independent
- simd and declare simd directives should eliminate obstacles 3 and 4 and significantly enhance vectorization opportunities

A note on GCC OpenMP SIMD implementation

- GCC simd and declare simd ≈ existing auto vectorizer dependence analysis
- declare simd functions are first converted into a loop over all vector elements and then passed to the loop vectorizer

```
#pragma omp declare simd
float f(float x, float y) {
    return x + y;
}

#pragma omp declare simd
float f(float x, float y) {
    return x + y;
}

#pragma omp declare simd
float x = 0; i < 8; i++) {
    float x = vx[i], y = vy[i]
    r[i] = x + y;
}

#pragma omp declare simd
float x;
for (i = 0; i < 8; i++) {
    float x = vx[i], y = vy[i]
    r[i] = x + y;
}

#pragma omp declare simd
float n;
for (i = 0; i < 8; i++) {
    float x = vx[i], y = vy[i]
    return r;
}

#pragma omp declare simd
float n;
float x = vx[i], y = vy[i]
    return r;
}
</pre>
```

- the range of vectorizable loops in a recent version I investigated (7.3.0) seems very limited
 - innermost loop with no conditionals
 - doubly nested loop with a very simple inner loop

Strategies for SpMV

- parallelize only across different rows (a single row is processed sequentially)
 - especially natural for CSR
 - extremely long rows may limit speedup
- parallelize all non-zeros, with careful handling of y[i] +=
 - atomic accumulation (#pragma omp atomic)
 - reduction (#pragma omp reduction). you must have user-defined reduction
- divide rows until the number of non-zeros becomes small (e.g., ≤ 5000)
 - further divide a single row if a row contains many zeros
 - can be done naturally with tasks