Single Node Optimisation

Memory Optimisations

Reusing this material

epcc

archer2

Motivation

- Why is memory structure important?
  - With current hardware memory access has become the most significant resource impacting program performance.
    - Changing memory structures can have a big impact on code performance.
  - Memory structures are frequently global to the program
    - Different code sections communicate via memory structures.
    - The programming cost of changing a memory structure can be very high.

Programmer's perspective:

- Memory structures are the programmers responsibility
  - At best the compiler can add small amounts of padding in limited circumstances.
  - Compilers can (and hopefully will) try to make best use of the memory structures that you specify (e.g. uni-modular transformations)
- Changing the memory structures you specify may allow the compiler to generate better code.

Types of data structure

- Arrays
- Pointer arrays
- records/structures
- Trees and lists
- Objects

Arrays

- Arrays are large blocks of memory indexed by integer index
- Probably the most common data structure used in HPC codes
- Good for representing regularly discretised versions of dense continuous data

$$f(x,y,z) \rightarrow F[i][j][k]$$

Arrays

- Multi dimensional arrays use multiple indexes (shorthand)

```
REAL  A(100,100,100)          REAL A(1000000)
A (i,j,k) =  7.0                    A(i+100*j+10000*k) = 7.0

float  A[100][100][100];            float A[1000000];
A [i][j][k] =  7.0                  A[k+100*j+10000*i] = 7.0
```

- Address calculation requires computation but still relatively cheap.
- Compilers have better chance to optimise where dimension sizes are known at compile time.

Arrays

- Many codes loop over array elements
  - Data access pattern is regular and easy to predict
- Good spatial locality achieved by accessing neighbouring elements on consecutive iterations of the innermost loop.
- Unless loop nest order and array index order match the access pattern may not be optimal for cache re-use.
  - Compiler can potentially address these problems by transforming the loops.
  - But often can do a better job when provided with a more cache-friendly index order.

Bad spatial locality

```
do i=1,n
   do j=1,m
      a(i,j)=a(i,j)+b(i,j)
   end do
end do
```

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

Good spatial locality

```
do j=1,m
   do i=1,m
      a(i,j)=a(i,j)+b(i,j)
   end do
end do
```

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

Dynamic sized arrays (Fortran)

- Not always possible/desirable to fix array sizes at compile time
  - Fortran allows arrays to be dynamically sized based on subroutine arguments.
- Address calculation can still be optimised using CSE.
- Size of slowest moving index is not needed in address computation.
  - Fortran actually allows this dimension to be unspecified in subroutine arguments (assumed size arrays)

Dynamic sized arrays (C)

- C requires array dimensions to be known at compile time.
- However can make slowest dimension variable with pointers and **`typedef`**

```
typedef  float Mat[2][2];
Mat *data =(Mat *) malloc(n*sizeof(Mat));
for(i=0;i<n;i++){
  for(j=0;j<2;j++){
    for(k=0;k<2;k++){
        data[i][j][k] = 12.0;
    }
  }
}
```

Pointer arrays

- Alternative to multi-dimensional arrays
  - Pointer to: array of pointers to: array of pointers to: …. Data

```
float ***data;
data = (float ***) malloc(2*sizeof(float **));
for(i=0;i<2;i++){
  data[i]=(float **) malloc(2*sizeof(float *));
   for(j=0;j<2;j++){
      data[i][j] = (float *) malloc(n*sizeof(float));
      for(k=0;k<n;k++){
         data[i][j][k] = 12.0;
      }
   }
}
```

  - Note reverse index order to previous example!

Pointer arrays II

- In C the use-syntax is the same as for arrays
    - `a[i][j][k] = 7.0;`
  - But actually equivalent to
    - `p1 = a[i];`
    - `P2 = p1[j];`
    - `p2[k] = 7.0;`
- Advantage
  - The “columns” are allocated separately and need not be the same length
- Disadvantages
  - Need multiple memory accesses per element access.
  - Need more memory to store all the pointers
  - Less regular access pattern
  - Messy to create/destroy

Records/structures

- Collection of values (of varying types)
  - C structs
  - F90 user defined types
- Good for representing multi-valued data or sparse/scattered data.
- Related variables are stored close together may help cache use.
  - If a code section only uses a subset of the values cache use may suffer.
- Easy to add/re-order members without breaking code as members are referenced by name not position.
  - much harder to remove them.

Structures and the compiler

- Programmer only specifies what a structure contains.
- Compiler chooses layout within the structure.
- In C the compiler usually preserves the order of members but inserts padding between members if needed to meet alignment constraints
  - i.e. Doubles must be aligned on double-word boundaries.
  - Padding reduces cache-line utilisation so order members to reduce padding.
- Similarly in Fortran but can use SEQUENCE keyword to force deterministic layout.

Arrays of structs or structs of arrays?

```
struct Part{
  double x;
  double y;
  double z;
  int index;
  double mass;
}
Part data[numParts];
```

or

```
struct AllParts{
  double x[numParts];
  double y[numParts];
  double z[numParts];
  int index[numParts];
  double mass[numParts];
}
AllParts data;
```

Array of structs

Struct of arrays

Array of structs:

- May have good temporal locality if there is lots of computation on each struct
- May have poor spatial locality if computations don't
- Unfavourable for vector loads/stores
- Natural for OO design

Struct of arrays

- May have better spatial locality (use all data on cache line), but worse temporal locality
- More favourable for vector loads/stores
- Less natural for OO design

Arrays of structs of (short) arrays

```
struct FourVecParts{
  double x[4];
  double y[4];
  double z[4];
  int index[4];
  double mass[4];
}
FourVecParts data[(numParts+3)/4];
```

- Vector friendly without compromising temporal locality too much?
- Not at all natural from a design perspective!

Objects

- Usually implemented much the same as structures
- But objects are opaque
  - Language restricts access to the internal data.
  - Usually need to use special access functions.
- Much easier to change underlying data structure as this is only visible to small fraction of the program
- Access functions introduce additional overhead
  - Function calls
  - Memory copies
- Really only a problem for small low-level objects

Trees/lists

- Structures/Objects can contain pointers to other structures.
  - Can construct trees and lists etc.
- Very flexible and can grow dynamically
  - Same problems as pointer arrays.
    - Additional memory accesses to navigate data
    - Additional storage to store pointers
  - Access pattern is very hard to predict.
- Limited navigation
  - Can only follow access pattern supported by pointer structure
  - e.g. cannot jump to middle of a list without traversing half the nodes.

High level data structures

- Many modern languages have built in-support for high level data structures such as
  - Lists
  - Trees
  - Sets
  - Maps
  - Etc.
- May be available either as built-in data-types or as standard libraries.
  - Have the same intrinsic advantages/disadvantages as home made equivalents but typically better tested and optimised.

What can go wrong

- Poor cache/page use
  - Lack of spatial locality
  - Lack of temporal locality
- Unnecessary memory accesses
  - pointer chasing
  - array temporaries
- Aliasing problems
  - Use of pointers can inhibit code optimisation

Reducing memory accesses

- Memory accesses are often the most important limiting factor for code performance.
  - Many older codes were written when memory access was relatively cheap.

- Things to look for:
  - Unnecessary pointer chasing
    - pointer arrays that could be simple arrays
    - linked lists that could be arrays.
  - Unnecessary temporary arrays.
  - Tables of values that would be cheap to re-calculate.

Utilizing caches

- Want to avoid cache conflicts
  - This happens when too much related data maps to the same cache set.
  - Arrays or array dimensions proportional to (cache-size/set-size) can cause this.
  - Rarely a problem with 8- and 16-way associative caches modern processors
  - Lots of accesses in a loop to arrays with power-of-2 dimensions might still be bad
  - Can pad arrays to avoid this.

Utilizing caches II

- Want to use all of the data in a cache line
  - loading unwanted values is a waste of memory bandwidth.
  - structures are good for this
  - Or loop fastest over the corresponding index of an array.
- Place variables that are used together close together
  - Also have to worry about alignment with cache block boundaries.
- Avoid “gaps” in structures
  - In C structures may contain gaps to ensure the address of each variable is aligned with its size.

Bad Cache Alignment

CrayPAT profiling with `export PAT_RT_HWPC=2` (L1 and L2 metrics)

```
Time%                                           0.2%
Time                                       0.000003
Calls                                             1
PAPI_L1_DCA             455.433M/sec           1367 ops
DC_L2_REFILL_MOESI       49.641M/sec            149 ops
DC_SYS_REFILL_MOESI       0.666M/sec              2 ops
BU_L2_REQ_DC             74.628M/sec            224 req
User time                 0.000  secs          7804 cycles
Utilization rate                               97.9%
L1 Data cache misses     50.308M/sec            151 misses
LD & ST per D1 miss                            9.05 ops/miss
D1 cache hit ratio                             89.0%
LD & ST per D2 miss                          683.50 ops/miss
D2 cache hit ratio                             99.1%
L2 cache hit ratio                             98.7%
Memory to D1 refill       0.666M/sec              2 lines
Memory to D1 bandwidth   40.669MB/sec           128 bytes
L2 to Dcache bandwidth 3029.859MB/sec          9536 bytes
```

Good cache alignment

```
Time%                                          0.1%
Time                                      0.000002
Calls                                            1
PAPI_L1_DCA              689.986M/sec       1333 ops
DC_L2_REFILL_MOESI        33.645M/sec         65 ops
DC_SYS_REFILL_MOESI                            0 ops
BU_L2_REQ_DC              34.163M/sec         66 req
User time                  0.000 secs       5023 cycles
Utilization rate                              95.1%
L1 Data cache misses      33.645M/sec         65 misses
LD & ST per D1 miss                         20.51 ops/miss
D1 cache hit ratio                            95.1%
LD & ST per D2 miss                       1333.00 ops/miss
D2 cache hit ratio                           100.0%
L2 cache hit ratio                           100.0%
Memory to D1 refill                            0 lines
Memory to D1 bandwidth                         0 bytes
L2 to Dcache bandwidth  2053.542MB/sec      4160 bytes
```

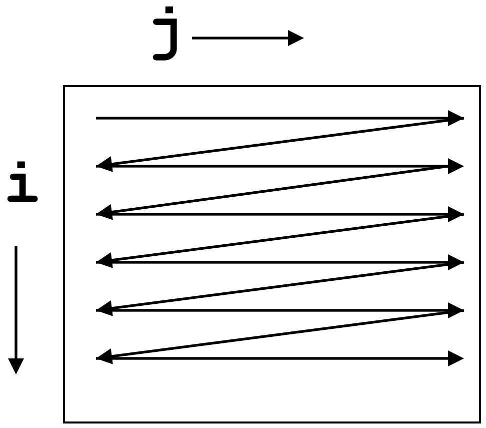
Cache blocking

- A combination of:
  - strip mining (also called loop blocking, loop tiling...)
  - loop interchange
- Designed to increase data reuse:
  - temporal reuse: reuse array elements already referenced
  - spatial reuse: good use of cache lines
- Many ways to block any given loop nest
  - Which loops should be blocked?
  - What block size(s) will work best?

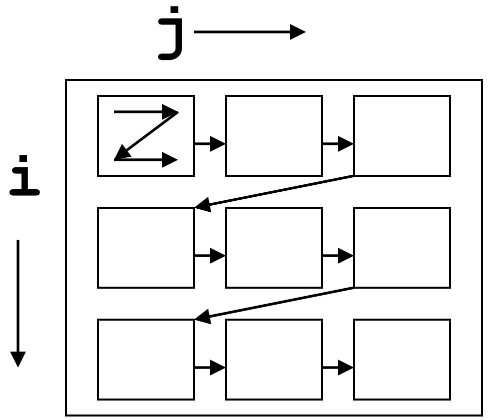
- Analysis can reveal which ways are beneficial
  - How big is your cache?
    - L1 is 512KB on AMD Rome.
  - How many cache lines can it hold?
    - each line typically 64B, so
  - How many cache lines are needed per loop iteration?
  - ...
- But trial-and-error is probably faster
  - or auto-tuning of the code

Loop tiling

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




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



Loop tiling for vectorisation

```
for (i=0;i<n;i++){
  for (j=1;j<n-1;j++){
     a[i][j]=(a[i][j-1] + a[i][j+1])/2.0 ;
  }
}
```

j loop won't vectorise due to dependencies

```
for (ii=0;ii<n;ii+=B){
  for (j=1;j<n-1;j++){
    for (i=ii;i<ii+B;i++){
       a[j][i]=(a[j-1][i] + a[j+1][i])/2.0 ;
    }
  }
}
```

i loop will vectorise
but note change of data layout

Further cache optimisations

- If multiple loop nests process a large array
  - First element of array will be out of cache when second loop nest starts

- Improving cache use
  - Consider fusing the loop nests
    - Completely: just have one loop nest
    - Partial: have one outer loop, containing multiple inner loops
  - Beware that too much fusion can result in lots of temporaries and cause the compiler to run out of registers....

Original code	Complete fusion	Partial fusing

do j = 1, Nj
 do i = 1, Ni
  a(i,j)=b(i,j)*2
 enddo
enddo
 	
do j = 1, Nj
 do i = 1, Ni
  a(i,j)=a(i,j)+1
 enddo
enddo
	do j = 1, Nj
	 do i = 1, Ni
	  a(i,j)=b(i,j)*2
	  a(i,j)=a(i,j)+1
	 enddo
	enddo
		do j = 1, Nj
		 do i = 1, Ni
		  a(i,j)=b(i,j)*2
		 enddo
		 do i = 1, Ni
		  a(i,j)=a(i,j)+1
		 enddo
		enddo

Further cache optimisations

- Perhaps cache block before fusing
  - Fuse one or more of the outer blocking loops
- If multiple subprograms process the array
  - Remove one or more outer loops (or all loops) from subprograms
  - Haul loop into parent routine, pass in index values instead
  - Might want to ensure that compiler is inlining this routine
  - This technique is very useful if you want to use OpenMP/OpenACC
- Beware of Fortran
  - array syntax often bad
    - `a(:,:)=b(:,:)*2`
    - `a(:,:)=a(:,:)+1`
  - compiler unlikely to fuse any loops

Original code

```
CALL sub1(a,b)
CALL sub2(a)

SUBROUTINE sub1(a)
 do j=1,Nj
  do i=1,Ni
   a(i,j)=b(i,j)*2
  enddo
 enddo
END SUBROUTINE sub1
```

After hauling

```
do j = 1, Nj
 CALL sub1(a,b,j)
 CALL sub2(a,j)
enddo

SUBROUTINE sub1(a,j)
 do i=1,Ni
  a(i,j)=b(i,j)*2
 enddo
END SUBROUTINE sub1
```

Optimising for TLB

- Aim to reuse data on a page
  - i.e. treat similarly to a cache
- Standard-sized pages are 4kB
  - But you can use larger "huge" pages
    - 128kB, 512kB, 2MB,... 64MB
  - Almost always benefit HPC applications
    - regular data accesses
    - huge pages give fewer TLB misses
  - Huge pages can also help communication performance

- To use huge pages (see `man intro_hugepages`)
  - Load chosen `craype-hugepages*` module
    - See `module avail craype-hugepages` for list of available options
    - 2M or 8M are usually most successful on Cray systems we've used
  - Compile as before
  - Make sure this module is also loaded in slurm jobscript
    - quick cheat: can load a different-sized hugepages module at runtime
      - compile-time module enables hugepages, runtime one determines actual size

Prefetch

- Some processors (including AMD Rome) prefetch automatically
- Regular access patterns are recognised and cache lines fetched in advance.
  - Usually only works for contiguous sequence of cache misses.
- Processor has a set of stream buffers
  - Each holds address of an active stream
  - Loads to the current block causes the next block to be prefetched and the stream address to be updated.
  - Streams are established by series of cache misses to consecutive locations

Using streams

- To utilize stream hardware use linear access patterns where possible
  - Only the order of cache block accesses needs to be linear, not each word access.
- Most loops will require multiple streams
  - If the loop requires more streams than are supported in hardware no prefetching will take place for some of the loads.
  - Consider splitting the loop.
- Prefetching typically cannot cross OS page boundaries
  - huge pages may help

Pointer aliasing

- Pointers are variables containing memory addresses.
  - Pointers are useful but can seriously inhibit code performance.
- Compilers try very hard to reduce memory accesses.
  - Only loading data from memory once.
  - Keep variables in registers and only update memory copy when necessary.
- Pointers could point anywhere, so to be safe compiler will:
  - Reload all values after write through pointer
  - Synchronize all variables with memory before read through pointer

Pointers and Fortran

- F77 had no pointers
- Arguments passed by reference (address)
  - Subroutine arguments are effectively pointers
  - But it is illegal Fortran if two arguments overlap
- F90/F95 has restricted pointers
  - Pointers can only point at variables declared as a "target" or at the target of another pointer
  - Compiler therefore knows more about possible aliasing problems
- Try to avoid F90 pointers for performance critical data structures.

Pointers and C

- In C pointers are unrestricted
  - Can therefore seriously inhibit performance
- Almost impossible to do without pointers
  - malloc requires the use of pointers.
  - Pointers used for call by reference. Alternative is call by value where all data is copied!
- Use the C99 **restrict** keyword where possible
- ...or else use compiler flags
  - CCE: **`-h restrict`**
  - AMD: **`-fstrict-aliasing`** (doesn't restrict argument aliasing)
  - GNU: **`-fstrict-aliasing -fargument-noalias -fargument-noalias-global`**
- Explicit use of scalar temporaries may also reduce the problem