Debugging in Serial & Parallel

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Part I

Basic (Serial) Debugging

Software for Debugging

The most common method for debugging (by far) is the “instrumentation” method:

- One “instruments” the code with print statements to check values and follow the execution of the program
- Not exactly sophisticated - one can certainly debug code in this way, but wise use of software debugging tools can be more effective

Debugging Tools

Debugging tools are abundant, but we will focus merely on some of the most common attributes to give you a bag of tricks that can be used when dealing with common problems.

Basic Capabilities

Common attributes:

- Divided into command-line or graphical user interfaces
- Usually have to recompile (**“-g”** is almost a standard option to enable debugging) your code to utilize most debugger features
- Invocation by name of debugger and executable (e.g. **gdb ./a.out [core]**)

Running Within

Inside a debugger (be it using a command-line interface (CLI) or graphical front-end), you have some very handy abilities:

- Look at source code listing (very handy when isolating an IEEE exception)
- Line-by-line execution
- Insert stops or “breakpoints” at certain functional points (i.e., when critical values change)
- Ability to monitor variable values
- Look at “stack trace” (or “backtrace”) when code crashes

Command-line debugging example

Consider the following code example:

```
#include <stdio.h>
#include <stdlib.h>

int indx;

void initArray(int nelem_in_array, int *array);
void printArray(int nelem_in_array, int *array);
int squareArray(int nelem_in_array, int *array);

int main(void) {
  const int nelem = 10;
  int *array1, *array2, *del;

  /* Allocate memory for each array */
  array1 = (int *)malloc(nelem*sizeof(int));
  array2 = (int *)malloc(nelem*sizeof(int));
  del = (int *)malloc(nelem*sizeof(int));

  /* Initialize array1 */
  initArray(nelem, array1);

  for (indx = 0; indx < nelem; indx++) {
    array1[indx] = indx + 2;
  }
```



```
  /* Print the elements of array1 */
  printf("array1 = ");
  printArray(nelem, array1);

  /* Copy array1 to array2 */
  array2 = array1;

  /* Pass array2 to the function 'squareArray( )' */
  squareArray(nelem, array2);

  /* Compute difference between elements of array2 and array1 */
  for (indx = 0; indx < nelem; indx++) {
    del[indx] = array2[indx] - array1[indx];
  }

  /* Print the computed differences */
  printf("The difference in the elements of array2 and array1 are:  ");
  printArray(nelem, del);

  free(array1);
  free(array2);
  free(del);
  return 0;
}
```

```c
void initArray(const int nelem_in_array, int *array) {
  for (indx = 0; indx < nelem_in_array; indx++) {
    array[indx] = indx + 1;
  }
}

int squareArray(const int nelem_in_array, int *array) {
  int indx;
  for (indx = 0; indx < nelem_in_array; indx++){
    array[indx] *= array[indx];
  }
  return *array;
}

void printArray(const int nelem_in_array, int *array){
  printf("\n( ");
  for (indx = 0; indx < nelem_in_array; indx++){
    printf("%d  ", array[indx]);
  }
  printf(")\n");
}
```


Ok, now let's compile and run this code:

```
[rush:~/d_debug]$ gcc -g -o array-ex array-ex.c
[rush:~/d_debug]$ ./array-ex
array1 =
( 2  3  4  5  6  7  8  9  10  11  )
The difference in the elements of array2 and array1 are:
( 0  0  0  0  0  0  0  0  0  0  )
*** glibc detected *** ./array-ex: double free or corruption (fasttop): 0x0000000001cc7010 ***
======= Backtrace: =========
/lib64/libc.so.6[0x3e1be760e6]
./array-ex[0x400710]
/lib64/libc.so.6(__libc_start_main+0xfd)[0x3e1be1ecdd]
./array-ex[0x4004d9]
======= Memory map: ========
...
```

Not exactly what we expect, is it? Array2 should contain the squares of the values in array1, and therefore the difference should be $i^2 - i$ for $i = [2, 11]$.

Now let us run the code from within **gdb**. Our goal is to set a **breakpoint** where the squared arrays elements are computed, then step through the code:

```
[rush:~/d_debug]$ gdb -quiet array-ex
Reading symbols from /ifs/user/jonesm/d_debug/array-ex...done.
(gdb) l 34
29
30    /* Copy array1 to array2 */
31    array2 = array1;
32
33    /* Pass array2 to the function 'squareArray( )' */
34    squareArray(nelem, array2);
35
36    /* Compute difference between elements of array2 and array1 */
37    for (indx = 0; indx < nelem; indx++) {
38      del[indx] = array2[indx] - array1[indx];
(gdb) b 34
Breakpoint 1 at 0x400660: file array-ex.c, line 34.
(gdb) run
Starting program: /ifs/user/jonesm/d_debug/array-ex
array1 =
( 2  3  4  5  6  7  8  9  10  11  )

Breakpoint 1, main () at array-ex.c:34
34    squareArray(nelem, array2);
```



```
(gdb) s
squareArray (nelem_in_array=10, array=0x601010) at array-ex.c:59
59    for (indx = 0; indx < nelem_in_array; indx++){
(gdb) p indx
$1 = 10
(gdb) s
60      array[indx] *= array[indx];
(gdb) p indx
$2 = 0
(gdb) display indx
1: indx = 0
(gdb) display array[indx]
2: array[indx] = 2
(gdb) s
59    for (indx = 0; indx < nelem_in_array; indx++){
2: array[indx] = 4
1: indx = 0
(gdb) s
60      array[indx] *= array[indx];
2: array[indx] = 3
1: indx = 1
```

Ok, that is instructive, but no closer to finding the bug.

So, what have we learned so far about the command-line debugger:

- Useful for peaking inside source code
- (break) Breakpoints
- (s) Stepping through execution
- (p) Print values at selected points (can also use handy printf syntax as in C)
- (display) Displaying values for monitoring while stepping through code
- (bt) Backtrace, or 'Stack Trace' - haven't used this yet, but certainly will

Digging Out the Bug

What we have learned is enough - look more closely at the line where the differences between array1 and array2 are computed:

```
(gdb) l 38
33          /* Pass array2 to the function 'squareArray( )' */
34          squareArray(nelem, array2);
35
36          /* Compute difference between elements of array2 and array1 */
37          for (indx = 0; indx < nelem; indx++) {
38            del[indx] = array2[indx] - array1[indx];
39          }
40
41          /* Print the computed differences */
42          printf("The difference in the elements of array2 and array1 are:  ");
(gdb) b 37
Breakpoint 1 at 0x400611: file array-ex.c, line 37.
(gdb) run
Starting program: /san/user/jonesm/u2/d_debug/array-ex
array1 =
( 2  3  4  5  6  7  8  9  10  11  )
```



```
Breakpoint 1, main () at array-ex.c:37
37          for (indx = 0; indx < nelem; indx++) {
(gdb) disp indx
1: indx = 10
(gdb) disp array1[indx]
2: array1[indx] = 49
(gdb) disp array2[indx]
3: array2[indx] = 49
(gdb) s
38            del[indx] = array2[indx] - array1[indx];
3: array2[indx] = 4
2: array1[indx] = 4
1: indx = 0
(gdb) s
37          for (indx = 0; indx < nelem; indx++) {
3: array2[indx] = 4
2: array1[indx] = 4
1: indx = 0
(gdb) s
38            del[indx] = array2[indx] - array1[indx];
3: array2[indx] = 9
2: array1[indx] = 9
1: indx = 1
```


Now that isn't right - array1 was **not** supposed to change. Let us go back and look more closely at the call to `squareArray` ...

```
(gdb) l
32
33        /* Pass array2 to the function 'squareArray( )' */
34        squareArray(nelem, array2);
35
36        /* Compute difference between elements of array2 and array1 */
37        for (indx = 0; indx < nelem; indx++) {
38          del[indx] = array2[indx] - array1[indx];
39        }
40
41        /* Print the computed differences */
(gdb) b 34
Breakpoint 2 at 0x400605: file array-ex.c, line 34.
(gdb) run
The program being debugged has been started already.
Start it from the beginning? (y or n) y

Starting program: /ifs/user/jonesm/d_debug/array-ex
array1 =
( 2  3  4  5  6  7  8  9  10  11  )

Breakpoint 2, main () at array-ex.c:34
34        squareArray(nelem, array2);
3: array2[indx] = 49
2: array1[indx] = 49
1: indx = 10
(gdb) disp array2
4: array2 = (int *) 0x501010
(gdb) disp array1
5: array1 = (int *) 0x501010
```


Yikes, array1 and array2 point to the same memory location! See, pointer errors like this don't happen too often in Fortran ... Now , of course, the bug is obvious - but aren't they all obvious **after** you find them?

The Fix Is In

Just as an afterthought, what we ought to have done in the first place was copy `array1` into `array2`:

```
/* Copy array1 to array2 */
/* array2 = array1; */
for (indx=0; indx<nelem; indx++) {
  array2[indx]=array1[indx];
}
```

which will finally produce the right output:

```
(gdb) run
Starting program: /home/jonesm/d_debug/ex1
array1 =
( 2  3  4  5  6  7  8  9  10  11  )
The difference in the elements of array2 and array1 are:
( 2  6  12  20  30  42  56  72  90  110  )

Program exited normally.
(gdb)
```


Array Indexing Errors

Array indexing errors are one of the most common errors in both sequential and parallel codes - and it is not entirely surprising:

- Different languages have different indexing defaults
- Multi-dimensional arrays are pretty easy to reference out-of-bounds
- Fortran in particular lets you use very complex indexing schemes (essentially arbitrary!)

Example: Indexing Error

```c
#include <stdio.h>
#define N 10
int main(int argc, char *argv[]) {
   int arr[N];
   int i,odd_sum,even_sum;

   for(i=1;i<(N-1);++i) {
      if(i<=4) {
        arr[i]=(i*i)%3;
      } else {
        arr[i]=(i*i)%5;
      }
   }
   odd_sum=0;
   even_sum=0;
   for(i=0;i<(N-1);++i) {
     if(i%2==0) {
       even_sum += arr[i];
     } else {
       odd_sum += arr[i];
     }
   }
   printf("odd_sum=%d, even_sum=%d\n",odd_sum,even_sum);
}
```


Now, try compiling with **gcc** and running the code:

```
[rush:~/d_debug]$ gcc -O -g -o ex2 ex2.c
[rush:~/d_debug]$ ./ex2
odd_sum=5, even_sum=671173703
```

Ok, that hardly seems reasonable (does it?) Now, let's run this example from within **gdb** and set a breakpoint to examine the accumulation of values to `even_sum`.


```
(gdb) l 16
11              arr[i]=(i*i)%5;
12            }
13         }
14         odd_sum=0;
15         even_sum=0;
16         for(i=0;i<(N-1);++i) {
17           if(i%2==0) {
18             even_sum += arr[i];
19           } else {
20             odd_sum += arr[i];
(gdb) b 16
Breakpoint 1 at 0x40051e: file ex2.c, line 16.
(gdb) run
Starting program: /ifs/user/jonesm/d_debug/ex2

Breakpoint 1, main (argc=Variable "argc" is not available.
) at ex2.c:16
16         for(i=0;i<(N-1);++i) {
(gdb) p arr
$1 = {671173696, 1, 1, 0, 1, 0, 1, 4, 4, 0}
```


So we see that our original example code missed initializing the first element of the array, and the results were rather erratic (in fact they will likely be compiler and flag dependent).

Initialization is just one aspect of things going wrong with array indexing - let us examine another common problem ...

The (Infamous) Seg Fault

This example I “borrowed” from Norman Matloff (UC Davis), who has a nice article (well worth the time to read): “Guide to Faster, Less Frustrating Debugging,” which you can find easily enough on the web:

http://heather.cs.ucdavis.edu/~matloff/unix.html

Main code: **findprimes.c**

```c
/*
   prime-number finding program - will (after bugs are fixed) report a list of
   all primes which are less than or equal to the user-supplied upper bound
*/
#include <stdio.h>

#define MaxPrimes 50
int Prime[MaxPrimes],    /* Prime[I] will be 1 if I is prime, 0 otherwise */
    UpperBound;          /* we will check up through UpperBound for primeness */
void CheckPrime(int K); /* prototype for CheckPrime function */
int main()
{
  int N;

  printf("enter upper bound\n");
  scanf("%d",UpperBound);

  Prime[2] = 1;

  for (N = 3; N <= UpperBound; N += 2)
    CheckPrime(N);
  if (Prime[N]) printf("%d is a prime\n",N);
}
```


Function `FindPrime`:

```c

void CheckPrime(int K) {
  int J;

  /* the plan:  see if J divides K, for all values J which are
  (a) themselves prime (no need to try J if it is nonprime), and
  (b) less than or equal to sqrt(K) (if K has a divisor larger
      than this square root, it must also have a smaller one,
      so no need to check for larger ones) */

  J = 2;
  while (1)  {
    if (Prime[J] == 1)
      if (K % J == 0)  {
         Prime[K] = 0;
         return;
      }
    J++;
  }

  /* if we get here, then there were no divisors of K, so it is
     prime */
  Prime[K] = 1;
}
```

so now if we compile and run this code ...


```
[rush:~/d_debug]$ gcc -g -o findprimes_orig findprimes_orig.c
[rush:~/d_debug]$ ./findprimes_orig
enter upper bound
20
Segmentation fault (core dumped)
[rush:~/d_debug]$ ulimit -c
0
```

Ok, let’s fire up **gdb** and see where this code crashed:

```
[rush:~/d_debug]$ gdb -quiet ./findprimes_orig
Reading symbols from /ifs/user/jonesm/d_debug/findprimes_orig...done.
(gdb) run
Starting program: /ifs/user/jonesm/d_debug/findprimes_orig
enter upper bound
20

Program received signal SIGSEGV, Segmentation fault.
0x0000003e1be56ed0 in _IO_vfscanf_internal () from /lib64/libc.so.6
Missing separate debuginfos, use: debuginfo-install glibc-2.12-1.107.el6.x86_64
(gdb) bt
#0  0x0000003e1be56ed0 in _IO_vfscanf_internal () from /lib64/libc.so.6
#1  0x0000003e1be646cd in __isoc99_scanf () from /lib64/libc.so.6
#2  0x00000000004005a0 in main () at findprimes_orig.c:16
```

Now, the `scanf` intrinsic is probably pretty safe from internal bugs, so the error is likely coming from our usage:

```
(gdb) list 16
11 int main()
12 {
13   int N;
14
15   printf("enter upper bound\n");
16   scanf("%d",UpperBound);
17
18   Prime[2] = 1;
19
20   for (N = 3; N <= UpperBound; N += 2)
```

Yeah, pretty dumb - `scanf` needs a pointer argument, i.e. `scanf("%d",&UpperBound)`, and that takes care of the first bug ... but let's keep running from within **gdb**


```
[rush:~/d_debug]$ gcc -g -o findprimes findprimes.c
[rush:~/d_debug]$ gdb findprimes
(gdb) run
Starting program: /ifs/user/jonesm/d_debug/findprimes
enter upper bound
20

Program received signal SIGSEGV, Segmentation fault.
0x0000000000400586 in CheckPrime (K=3) at findprimes.c:37
37          if (Prime[J] == 1)
(gdb) bt
#0  0x0000000000400586 in CheckPrime (K=3) at findprimes.c:37
#1  0x0000000000400547 in main () at findprimes.c:21
(gdb) l 37
32             than this square root, it must also have a smaller one,
33             so no need to check for larger ones) */
34
35         J = 2;
36         while (1)  {
37           if (Prime[J] == 1)
38             if (K % J == 0)  {
39               Prime[K] = 0;
40               return;
41             }
(gdb)
```


very often we get seg faults on trying to reference an array "out-of-bounds," so have a look at the value of `J`:

```
(gdb) l 37
32             than this square root, it must also have a smaller one,
33             so no need to check for larger ones) */
34
35         J = 2;
36         while (1)  {
37           if (Prime[J] == 1)
38             if (K % J == 0)  {
39               Prime[K] = 0;
40               return;
41             }
(gdb) p J
$1 = 376
```

Oops! That is just a tad outside the bounds (50). Kind of forgot to put a cap on the value of `J` ...

Fixing the last bug:

```
(gdb) list 40
35         J = 2;
36         /* while (1)  { */
37         for (J=2; J*J <= K; J++) {
38           if (Prime[J] == 1)
39             if (K % J == 0)  {
40               Prime[K] = 0;
41               return;
42             }
43           /* J++; */
44         }
```

Ok, now let us try to run the code:

```
[rush:~/d_debug]$ gcc -g -o findprimes findprimes.c
[rush:~/d_debug]$ ./findprimes
enter upper bound
20
[rush:~/d_debug]$
```

Oh, fantastic - no primes between 1 and 20? Not hardly ...

Ok, so now we will set a couple of breakpoints - one at the call to `FindPrime` and the second where a successful prime is to be output:


```
(gdb) l
16          scanf("%d",&UpperBound);
17
18          Prime[2] = 1;
19
20          for (N = 3; N <= UpperBound; N += 2)
21            CheckPrime(N);
22          if (Prime[N]) printf("%d is a prime\n",N);
23        }
24
25        void CheckPrime(int K) {
(gdb) b 20
Breakpoint 1 at 0x40052d: file findprimes.c, line 20.
(gdb) b 22
Breakpoint 2 at 0x400550: file findprimes.c, line 22.
(gdb) run
Starting program: /ifs/user/jonesm/d_debug/findprimes
enter upper bound
20
Breakpoint 1, main () at findprimes.c:20
20          for (N = 3; N <= UpperBound; N += 2)
(gdb) c
Continuing.

Breakpoint 2, main () at findprimes.c:22
22          if (Prime[N]) printf("%d is a prime\n",N);
(gdb) p N
$1 = 21
(gdb)
```


Another gotcha - misplaced (or no) braces. Fix that:

```
(gdb) l
16          scanf("%d",&UpperBound);
17
18          Prime[2] = 1;
19
20          for (N = 3; N <= UpperBound; N += 2) {
21            CheckPrime(N);
22            if (Prime[N]) printf("%d is a prime\n",N);
23          }
24        }
25
(gdb) run
Starting program: /ifs/user/jonesm/d_debug/findprimes
enter upper bound
20
3 is a prime
5 is a prime
7 is a prime
11 is a prime
13 is a prime
17 is a prime
19 is a prime

Program exited with code 025.
(gdb)
```

Ah, the sweet taste of success ... (even better, give the program a return code!)

Debugging Life Itself

Well, ok, not exactly debugging life itself; rather the **game of life**. Mathematician John Horton Conway's **game of life**[1], to be exact. This example will basically be similar to the prior examples, but now we will work in Fortran, and debug some integer arithmetic errors.

And the context will be slightly more interesting.

[1] see, for example, Martin Gardner's article in *Scientific American*, **223**, pp. 120-123 (1970).

Game of Life

The **Game of Life** is one of the better known examples of **cellular automatons** (CA), namely a discrete model with a finite number of states, often used in theoretical biology, game theory, etc. The rules are actually pretty simple, and can lead to some rather surprising self-organizing behavior. The universe in the game of life:

- Universe is an infinite 2D grid of cells, each of which is alive or dead
- Cells interact only with nearest neighbors (including on the diagonals, which makes for eight neighbors)

Rules of Life

The rules in the game of life:

- Any live cell with fewer than two neighbours dies, as if by loneliness
- Any live cell with more than three neighbours dies, as if by overcrowding
- Any live cell with two or three neighbours lives, unchanged, to the next generation
- Any dead cell with exactly three neighbours comes to life

An initial pattern is evolved by simultaneously applying the above rules to the entire grid, and subsequently at each "tick" of the clock.

Sample Code - Game of Life

```
program life
  !
  ! Conway game of life (debugging example)
  !
  implicit none
  integer, parameter :: ni=1000, nj=1000, nsteps = 100
  integer :: i, j, n, im, ip, jm, jp, nsum, isum
  integer, dimension(0:ni,0:nj) :: old, new
  real :: arand, nim2, njm2
  !
  !  initialize elements of "old" to 0 or 1
  !
  do j = 1, nj
     do i = 1, ni
        CALL random_number(arand)
        old(i,j) = NINT(arand)
     enddo
  enddo
  nim2 = ni - 2
  njm2 = nj - 2
```



```
  !
  ! time iteration
  !
  time_iteration: do n = 1, nsteps
     do j = 1, nj
        do i = 1, ni
           !
           ! periodic boundaries,
           !
           im = 1 + (i+nim2) - ((i+nim2)/ni)*ni   ! if i=1, ni
           ip = 1 + i - (i/ni)*ni                  ! if i=ni, 1
           jm = 1 + (j+njm2) - ((j+njm2)/nj)*nj   ! if j=1, nj
           jp = 1 + j - (j/nj)*nj                  ! if j=nj, 1
           !
           ! for each point, add surrounding values
           !
           nsum =  old(im,jp) + old(i,jp) + old(ip,jp) &
                 + old(im,j )             + old(ip,j ) &
                 + old(im,jm) + old(i,jm) + old(ip,jm)
```

```fortran
          !
          ! set new value based on number of "live" neighbors
          !
          select case (nsum)
          case (3)
             new(i,j) = 1
          case (2)
             new(i,j) = old(i,j)
          case default
             new(i,j) = 0
          end select
       enddo
    enddo
    !
    ! copy new state into old state
    !
    old = new
    print*, 'Tick ',n,' number of living: ',sum(new)
 enddo time_iteration
 !
 ! write number of live points
 !
 print*, 'number of live points = ', sum(new)
end program life
```


Initial Run ...

```
[bono:~/d_debug]$ ifort -g -o life life.f90
[bono:~/d_debug]$ ./life
 Tick           1  number of living:       342946
 Tick           2  number of living:       334381
 Tick           3  number of living:       291022
 Tick           4  number of living:       263356
 Tick           5  number of living:       290940
 Tick           6  number of living:       322733
 :
 :
 Tick          99  number of living:            0
 Tick         100  number of living:            0
 number of live points =            0
```

Hmm, everybody dies! What kind of life is that? ... well, not a correct one, in this context, at least. Undoubtedly the problem lies within the neighbor calculation, so let us take a closer look at the execution ...


```
(gdb) l 30
25            do j = 1, nj
26               do i = 1, ni
27                  !
28                  ! periodic boundaries
29                  !
30                  im = 1 + (i+nim2) - ((i+nim2)/ni)*ni ! if i=1, ni
31                  ip = 1 + i - (i/ni)*ni               ! if i=ni, 1
32                  jm = 1 + (j+njm2) - ((j+njm2)/nj)*nj ! if j=1, nj
33                  jp = 1 + j - (j/nj)*nj               ! if j=nj, 1
(gdb) b 25
Breakpoint 1 at 0x402e23: file life.f90, line 25.
(gdb) run
Starting program: /ifs/user/jonesm/d_debug/life

Breakpoint 1, life () at life.f90:25
25            do j = 1, nj
Current language:  auto; currently fortran
(gdb) s
26               do i = 1, ni
(gdb) s
30                  im = 1 + (i+nim2) - ((i+nim2)/ni)*ni ! if i=1, ni
(gdb) s
31                  ip = 1 + i - (i/ni)*ni               ! if i=ni, 1
(gdb) print im
$1 = 1
(gdb) print (i+nim2)/1000
$2 = 0.999
```


Ok, so therein lay the problem - `nim2` and `njm2` should be integers, not real values ... fix that:

```fortran
program life
  !
  ! Conway game of life (debugging example)
  !
  implicit none
  integer, parameter :: ni=1000, nj=1000, nsteps = 100
  integer :: i, j, n, im, ip, jm, jp, nsum, isum, nim2, njm2
  integer, dimension(0:ni,0:nj) :: old, new
  real :: arand
```

and things become a bit more reasonable:

```
[bono:~/d_debug]$ ifort -g -o life life.f90
[bono:~/d_debug]$ ./life
 Tick           1  number of living:       272990
 Tick           2  number of living:       253690
 :
 :
 Tick          99  number of living:        95073
 Tick         100  number of living:        94664
 number of live points =        94664
```

Diversion - Demo life

http://www.radicaleye.com/lifepage

http://en.wikipedia.org/wiki/Conway's_Game_of_Life

Interesting repository of Conway's life and cellular automata references.

Core Files

Core files can also be used to instantly analyze problems that caused a code failure bad enough to "dump" a core file. Often the computer system has been set up in such a way that the default is **not** to output core files, however:

```
[rush:~/d_debug]$ ulimit -a
core file size          (blocks, -c) 0
data seg size           (kbytes, -d) unlimited
scheduling priority             (-e) 0
file size               (blocks, -f) unlimited
pending signals                 (-i) 2066355
max locked memory       (kbytes, -l) 33554432
max memory size         (kbytes, -m) unlimited
open files                      (-n) 1024
pipe size            (512 bytes, -p) 8
POSIX message queues     (bytes, -q) 819200
real-time priority              (-r) 0
stack size              (kbytes, -s) unlimited
cpu time               (seconds, -t) 900
max user processes              (-u) 1024
virtual memory          (kbytes, -v) unlimited
file locks                      (-x) unlimited
```

for **bash** syntax.

Systems administrators set the core file size limit to zero by default for a good reason - these files generally contain the entire memory image of an application process when it dies, and that can be very large. End-users are also notoriously bad about leaving these files laying around ...

Having said that, we can up the limit, and produce a core file that can later be used for analysis.

Core File Example

Ok, so now we can use one of our previous examples, and generate a core file:

```
[rush:~/d_debug]$ ulimit -c unlimited
[rush:~/d_debug]$ gcc -g -o findprimes_orig findprimes_orig.c
[rush:~/d_debug]$ ./findprimes_orig
enter upper bound
20
Segmentation fault (core dumped)
[rush:~/d_debug]$ ls -l core*
-rw------- 1 jonesm ccrstaff 196608 Sep 16 13:22 core.38729
```

this example core file is not at all large (it is a simple code with very little stored data - generally the core file size will reflect the size of the application in terms of its memory use when it crashed). Analyzing it is very similar to when running this example “live” in gdb:

```
[rush:~/d_debug]$ gdb -quiet findprimes_orig core.38729
Reading symbols from /ifs/user/jonesm/d_debug/findprimes_orig...done.
[New Thread 38729]
...
Core was generated by `./findprimes_orig'.
Program terminated with signal 11, Segmentation fault.
#0  0x0000003e1be56ed0 in _IO_vfscanf_internal () from /lib64/libc.so.6
Missing separate debuginfos, use: debuginfo-install glibc-2.12-1.107.el6.x86_64
(gdb) bt
#0  0x0000003e1be56ed0 in _IO_vfscanf_internal () from /lib64/libc.so.6
#1  0x0000003e1be646cd in __isoc99_scanf () from /lib64/libc.so.6
#2  0x00000000004005a0 in main () at findprimes_orig.c:16
(gdb) l 16
11 int main()
12 {
13   int N;
14
15   printf("enter upper bound\n");
16   scanf("%d",UpperBound);
17
18   Prime[2] = 1;
19
20   for (N = 3; N <= UpperBound; N += 2)
```


Summary on Core Files

So why would you want to use a core file rather than interactively debug?

- Your bug may take quite a while to manifest itself
- You have to debug inside a batch queuing system where interactive use is difficult or curtailed
- You want to capture a “picture” of the code state when it crashes

More Comannd-line Debugging Tools

We focused on **gdb**, but there are command-line debuggers that accompany just about every available compiler product:

pgdbg
: part of the PGI compiler suite, defaults to a GUI, but can be run as a command line interface (CLI) using the **-text** option

idb
: part of the Intel compiler suite, defaults to CLI (has a special option **-gdb** for using gdb command syntax)

Run-time Compiler Checks

Most compilers support **run-time** checks than can quickly catch common bugs. Here is a handy short-list (contributions welcome!):

- For Intel fortran, “**-check bounds -traceback -g**” will automate bounds checking, and enable extensive traceback analysis in case of a crash (leave out the **bounds** option to get a crash report on any IEEE exception, format mismatch, etc.)
- For PGI compilers, **-Mbounds -g** will do bounds checking
- For GNU compilers, **-fbounds-check -g** should also do bounds checking, but is only currently supported for Fortran and Java front-ends.

Run-time Compiler Checks(cont'd)

WARNING

It should be noted that run-time error checking can very much slow down a code's execution, so it is not something that you will want to use all of the time.

Serial Debugging GUIs

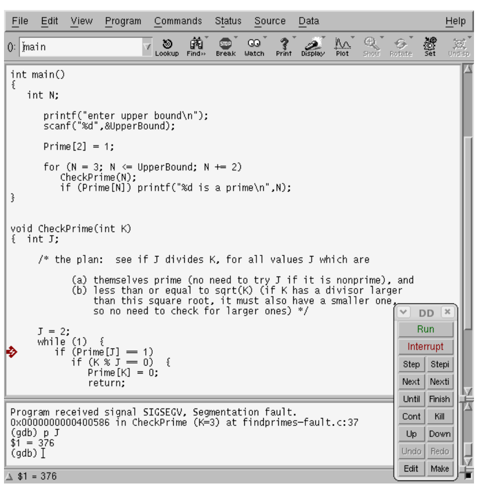
There are, of course, a matching set of GUIs for the various debuggers. A short list:

- **ddd** a graphical front-end for the venerable **gdb**
- **pgdbg** GUI for the PGI debugger
- **idb -gui** GUI for Intel compiler suite debugger

It is very much a matter of preference whether or not to use the GUI. I find the GUI to be constraining, but it does make navigation easier.

DDD Example

Running one of our previous examples using `ddd` ...



More Information on Debuggers

More information on the tools that we have used/mentioned (**man** pages are also a good place to start):

- **gdb** User Manual:
  `http://www.gnu.org/software/gdb/documentation`
- **ddd** User Manual:
  `https://www.gnu.org/software/ddd/manual/`
- **idb** Manual:
  `http://www.intel.com/software/products/compilers/docs/linux/idb_manual_l.html`
- **pgdbg** Guide (locally on CCR systems):
  `file:///util/pgi/linux86-64/[version]/doc/index.htm`

Source Code Checking Tools

Now, in a completely different vein, there are tools designed to help identify errors pre-compilation, namely by running it through the source code itself.

splint is a tool for statically checking C programs: `http://www.splint.org`

ftncheck is a tool that checks only (alas) `FORTRAN 77` codes: `http://www.dsm.fordham.edu/~ftnchek/`

I can't say that I have found these to be particulary helpful, though.

Memory Allocation Tools

Memory allocation problems are very common - there are some tools designed to help you catch such errors at run-time:

efence , or Electric Fence, tries to trap any out-of-bounds references (see **man efence**)

valgrind is a suite of tools for anlayzing and profiling binaries (see **man valgrind**) - there is a user manual available at (watch out for version dependencies): `http://valgrind.org/docs/manual`

valgrind I have seen used with good success, but not particularly in the HPC arena.

Strace

strace is a powerful tool that will allow you to trace **all** system calls and signals made by a particular binary, whether or not you have source code. Can be attached to already running processes. A powerful low-level tool. You can learn a lot from it, but is often a tool of last resort for user applications in HPC due to the copious quantity of extraneous information it outputs.

Strace Example

As an example of using **strace**, let's peek in on a running MPI process (part of a 32 task job on **U2**):

```
[c06n15:~]$ ps -u jonesm -Lf
UID          PID  PPID   LWP  C NLWP STIME TTY        TIME CMD
jonesm   23964 16284 23964 92    2 14:34 ?      00:04:11 /util/nwchem/nwchem-5.0/bin/
jonesm   23964 16284 23965 99    2 14:34 ?      00:04:30 /util/nwchem/nwchem-5.0/bin/
jonesm   23987 23986 23987  0    1 14:37 pts/0 00:00:00 -bash
jonesm   24128 23987 24128  0    1 14:39 pts/0 00:00:00 ps -u jonesm -Lf
[c06n15:~]$ strace -p 23965
Process 23965 attached - interrupt to quit
:
lseek(45, 691535872, SEEK_SET)          = 691535872
read(45, "\0\0\0\0\0\0\0\0\2\273\f[\250\207V\276\376K&]\331\230d"..., 524288)=524288
gettimeofday({1161107631, 126604}, {240, 1161107631}) = 0
gettimeofday({1161107631, 128553}, {240, 1161107631}) = 0
:
:
select(47, [3 4 6 7 8 9 42 43 44 46], [4], NULL, NULL) = 2 (in [4], out [4])
write(4, "\0\0\0\0\0\0\0\0\0\0\0\0\0\0\0\0\0\0\0\0\0\0\0\0\0"..., 2932) = 2932
writev(4, [{"\0\0\0\0\0\0\0\17\0\0\0\37\0\0\0\0\0\0\0,\0\0\0\0\0\0\0"..., 32},
{"\1\0\0\0\0\0\0\0\37\0\0\0\17\0\0\0\37\0\0\0,\0\1\0000u"..., 44}], 2) = 76
```

Part II

Advanced (Parallel) Debugging

Wither Goest the GUI?

Using a GUI-based debugger gets considerably more difficult when dealing with debugging an MPI-based parallel code (not so much on the OpenMP side), due to the fact that you are now dealing with multiple processes scattered across different machines.

The **TotalView** debugger is the premier product in this arena (it has both CLI and GUI support) - but it is **very** expensive, and not present in all environments. We will start out using our same toolbox as before, and see that we can accomplish much without spending a fortune. The methodologies will be equally applicable to the fancy commercial products.

Process Checking

First on the agenda - parallel processing involves multiple processes/threads (or both), and the first rule is to make sure that they are ending up where you think that they should be (needless to say, all too often they do not).

- Use `MPI_Get_processor_name` to report back on where processes are running
- Use `ps` to monitor processes as they run (useful flags: `ps u -L`), even on remote nodes (rsh/ssh into them)

Process Checking Example

```
[rush:/projects/jonesm/d_nwchem/d_siosi6]$ squeue --user jonesm
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            436728     debug   siosi6   jonesm  R       0:23      2 d09n29s02,d16n02
[rush:/projects/jonesm/d_nwchem/d_siosi6]$ ssh d16n02
[d16n02:~]$ ps -u jonesm -o pid,ppid,lwp,nlwp,psr,pcpu,rss,time,comm
  PID  PPID   LWP NLWP PSR %CPU    RSS     TIME COMMAND
 9665  9633  9665    5   0 98.4 1722040 00:01:12 nwchem-openib-i
 9666  9633  9666    4   4 98.6 1365672 00:01:12 nwchem-openib-i
 9667  9633  9667    4   1 98.2 1370000 00:01:12 nwchem-openib-i
 9668  9633  9668    4   5 98.7 1358960 00:01:13 nwchem-openib-i
 9669  9633  9669    4   2 98.7 1352112 00:01:13 nwchem-openib-i
 9670  9633  9670    4   6 98.7 1360200 00:01:13 nwchem-openib-i
 9671  9633  9671    4   3 98.7 1359828 00:01:13 nwchem-openib-i
 9672  9633  9672    4   7 98.7 1361228 00:01:13 nwchem-openib-i
 9751  9749  9751    1   7  0.0   2136 00:00:00 sshd
 9752  9751  9752    1   0  0.0   2040 00:00:00 bash
 9828  9752  9828    1   5  0.0   1204 00:00:00 ps
```

or you can script it (I called this script `job_ps`):

```
#!/bin/sh
#
# Shell script to take a single argument (Slurm job id) and launch a
#  ps command on each node in the job
#
QST=`which squeue`
if [ -z $QST ]; then
   echo "ERROR: no squeue in PATH: PATH="$PATH
   exit
fi
#
case $# in
0) echo "single SLURM_JOBID required."; exit ;; # no args, exit
1) jobid=$1 ;;
*) echo "single SLURM_JOBID required."; exit ;; # too many args, exit
esac
#
# get node listing
#
nodelist=`$QST --job $jobid --format="%i %N" | tail -1 | awk '{print $2}'`
echo "nodelist = $nodelist"
if [[ "$nodelist" == "" ]]; then
   echo "Job is not running yet, retry later."
   exit
fi
```



```
nodelist=`nodeset -e $nodelist`
echo "expanded nodelist = $nodelist"
#
# define ps command
#MYPS="ps -aeLf | awk '{if (\$5 > 10) print \$1, \$2, \$3, \$4, \$5, \$9, \$10}'"
MYPS="ps -u jonesm -L -o pid,ppid,lwp,nlwp,psr,pcpu,rss,time,comm"
#MYPS="ps -u jonesm -Lf"
echo "MYPS = $MYPS"

for node in $nodelist ; do
    echo "NODE = $node, my CPU/thread Usage:"
    ssh $node $MYPS
done
```



```
[rush:/projects/jonesm/d_nwchem/d_siosi6]$ job_ps 436728
nodelist = d09n29s02,d16n02
expanded nodelist = d16n02 d09n29s02
MYPS = ps -u jonesm -o pid,ppid,lwp,nlwp,psr,pcpu,rss,time,comm
NODE = d16n02, my CPU/thread Usage:
  PID  PPID   LWP NLWP PSR %CPU    RSS     TIME COMMAND
 9665  9633  9665    5   0 98.2 1748340 00:03:32 nwchem-openib-i
 9666  9633  9666    4   4 98.7 1479024 00:03:33 nwchem-openib-i
 9667  9633  9667    4   1 98.6 1479352 00:03:33 nwchem-openib-i
 9668  9633  9668    4   5 98.6 1466844 00:03:33 nwchem-openib-i
 9669  9633  9669    4   2 98.9 1461372 00:03:33 nwchem-openib-i
 9670  9633  9670    4   6 99.1 1474016 00:03:34 nwchem-openib-i
 9671  9633  9671    4   3 98.8 1470640 00:03:33 nwchem-openib-i
 9672  9633  9672    4   7 98.6 1474296 00:03:33 nwchem-openib-i
 9921  9919  9921    1   4  0.0   2132 00:00:00 sshd
 9922  9921  9922    1   5  2.0   1204 00:00:00 ps
NODE = d09n29s02, my CPU/thread Usage:
  PID  PPID   LWP NLWP PSR %CPU    RSS     TIME COMMAND
27963 27959 27963    1   4  0.0   1396 00:00:00 slurm_script
28145 27963 28145    5   3  0.0   7024 00:00:00 srun
28149 28145 28149    1   5  0.0    800 00:00:00 srun
28182 28167 28182    5   0 97.5 1750904 00:03:32 nwchem-openib-i
28183 28167 28183    4   4 98.0 1477128 00:03:33 nwchem-openib-i
28184 28167 28184    4   1 98.5 1472524 00:03:34 nwchem-openib-i
28185 28167 28185    4   5 98.3 1456200 00:03:34 nwchem-openib-i
28186 28167 28186    4   2 98.4 1488400 00:03:34 nwchem-openib-i
28187 28167 28187    4   6 98.1 1459120 00:03:33 nwchem-openib-i
28188 28167 28188    4   3 98.6 1470960 00:03:35 nwchem-openib-i
28189 28167 28189    4   7 98.4 1465752 00:03:34 nwchem-openib-i
28372 28370 28372    1   3  0.0   2148 00:00:00 sshd
28373 28372 28373    1   4  1.0   1204 00:00:00 ps
```



```
[rush:/projects/jonesm/d_nwchem/d_siosi6]$ job_ps 436749
nodelist = d09n29s02,d16n02
expanded nodelist = d16n02 d09n29s02
MYPS = ps -u jonesm -Lf
NODE = d16n02, my CPU/thread Usage:
UID        PID  PPID   LWP  C NLWP STIME TTY          TIME CMD
jonesm   11416 11382 11416 98    5 17:01 ?        00:00:59 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11416 11382 11441  0    5 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11416 11382 11442  0    5 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11416 11382 11454  0    5 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11416 11382 11465  0    5 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11417 11382 11417 99    4 17:01 ?        00:00:59 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11417 11382 11445  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11417 11382 11446  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11417 11382 11460  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11418 11382 11418 99    4 17:01 ?        00:00:59 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11418 11382 11439  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11418 11382 11440  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11418 11382 11455  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11419 11382 11419 99    4 17:01 ?        00:00:59 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11419 11382 11449  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11419 11382 11450  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11419 11382 11458  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11420 11382 11420 98    4 17:01 ?        00:00:59 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11420 11382 11451  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11420 11382 11452  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11420 11382 11457  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11421 11382 11421 99    4 17:01 ?        00:00:59 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11421 11382 11447  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11421 11382 11448  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11421 11382 11459  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11422 11382 11422 99    4 17:01 ?        00:00:59 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11422 11382 11437  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11422 11382 11438  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11422 11382 11453  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11423 11382 11423 99    4 17:01 ?        00:00:59 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11423 11382 11443  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11423 11382 11444  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11423 11382 11456  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm   11489 11487 11489  0    1 17:02 ?        00:00:00 sshd: jonesm@notty
jonesm   11490 11489 11490  2    1 17:02 ?        00:00:00 ps -u jonesm -Lf
%
```

```
NODE = d09n29s02, my CPU/thread Usage:
UID         PID  PPID   LWP  C NLWP STIME TTY          TIME CMD
jonesm    29706 29702 29706  0    1 17:01 ?        00:00:00 /bin/bash /var/spool/slurmd/job436749/slurm_script
jonesm    29883 29706 29883  0    5 17:01 ?        00:00:00 srun --mpi=pmi2 -n 16 -K /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi
jonesm    29883 29706 29889  0    5 17:01 ?        00:00:00 srun --mpi=pmi2 -n 16 -K /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi
jonesm    29883 29706 29891  0    5 17:01 ?        00:00:00 srun --mpi=pmi2 -n 16 -K /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi
jonesm    29883 29706 29892  0    5 17:01 ?        00:00:00 srun --mpi=pmi2 -n 16 -K /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi
jonesm    29883 29706 29895  0    5 17:01 ?        00:00:00 srun --mpi=pmi2 -n 16 -K /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi
jonesm    29888 29883 29888  0    1 17:01 ?        00:00:00 srun --mpi=pmi2 -n 16 -K /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi
jonesm    29921 29905 29921 96    5 17:01 ?        00:00:59 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29921 29905 29958  0    5 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29921 29905 29959  0    5 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29921 29905 29967  0    5 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29921 29905 29984  0    5 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29922 29905 29922 97    4 17:01 ?        00:01:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29922 29905 29960  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29922 29905 29961  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29922 29905 29972  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29923 29905 29923 97    4 17:01 ?        00:01:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29923 29905 29954  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29923 29905 29955  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29923 29905 29966  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29924 29905 29924 97    4 17:01 ?        00:01:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29924 29905 29956  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29924 29905 29957  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29924 29905 29968  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29925 29905 29925 97    4 17:01 ?        00:01:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29925 29905 29964  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29925 29905 29965  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29925 29905 29973  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29926 29905 29926 97    4 17:01 ?        00:01:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29926 29905 29950  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29926 29905 29951  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29926 29905 29953  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29927 29905 29927 97    4 17:01 ?        00:01:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29927 29905 29962  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29927 29905 29963  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29927 29905 29971  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29928 29905 29928 97    4 17:01 ?        00:01:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29928 29905 29969  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29928 29905 29970  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    29928 29905 29974  0    4 17:01 ?        00:00:00 /util/nwchem/nwchem-6.1.1/bin/nwchem-openib-impi siosi6-incore.nw
jonesm    30009 30007 30009  0    1 17:02 ?        00:00:00 sshd: jonesm@notty
jonesm    30010 30009 30010  2    1 17:02 ?        00:00:00 ps -u jonesm -Lf
```


Using Serial Debuggers in Parallel?

Yes, you can certainly run debuggers designed for use in sequential codes in parallel. They are even quite effective. You may just have to jump through a few extra hoops to do so ...

Attaching GDB to Running Processes

The simplest way to use a CLI-based debugger in parallel is to “attach” it to already running processes, namely:

- Find the parallel processes using the `ps` command (may have to ssh into remote nodes if that is where they are running)
- Invoke `gdb` on each process ID:

```
[rush:~]$ ps -u jonesm
  PID TTY          TIME CMD
 1772 ?        00:00:00 sshd
 1773 pts/30   00:00:00 bash
25814 ?        00:00:01 sshd
25815 pts/167  00:00:00 bash
34507 pts/169  00:00:00 mpirun
34512 pts/169  00:00:00 mpiexec.hydra
34513 pts/169  00:00:00 pmi_proxy
34517 pts/169  00:00:04 pp.gdb
34518 pts/169  00:00:04 pp.gdb
[rush:~/d_hw/d_pp]$ gdb -quiet pp.gdb -p 34517
Reading symbols from /ifs/user/jonesm/d_hw/d_pp/pp.gdb...done.
Attaching to program: /ifs/user/jonesm/d_hw/d_pp/pp.gdb, process 34517
...
(gdb)
```


Of course, unless you put an explicit waiting point inside your code, the processes are probably happily running along when you attach to them, and you will likely want to exert some control over that.

First, using our above example, I was running two mpi tasks on the CCR cluster front end. After attaching gdb to each process, they paused, and we can easily release them using *continue*

```
[rush:~/d_hw/d_pp]$ gdb -quiet pp.gdb -p 34517
Reading symbols from /ifs/user/jonesm/d_hw/d_pp/pp.gdb...done.
Attaching to program: /ifs/user/jonesm/d_hw/d_pp/pp.gdb, process 34517
...
(gdb) c
Continuing.
```


and on the second process:

```
[rush:~/d_hw/d_pp]$ gdb -quiet pp.gdb -p 34518
Reading symbols from /ifs/user/jonesm/d_hw/d_pp/pp.gdb...done.
Attaching to program: /ifs/user/jonesm/d_hw/d_pp/pp.gdb, process 34518
...
(gdb) c
Continuing.
```

and we used the (c) continue command to let the execution pick up again where we (temporarily) interrupted it.

Using a “Waiting Point”

You can insert a “waiting point” into your code to ensure that execution waits until you get a chance to attach a debugger:

```fortran
  integer :: gdbWait=0
...
...
  CALL MPI_COMM_RANK(MPI_COMM_WORLD,myid,ierr)
  CALL MPI_COMM_SIZE(MPI_COMM_WORLD,Nprocs,ierr)
  ! dummy pause point for gdb instertion
  do while (gdbWait /=1)
  end do
```


and then you will find the waiting at that point when you attach `gdb`, and you can release it at your leisure (after setting breakpoints, etc.):

```
[rush:~/d_hw/d_pp]$ gdb -quiet pp.gdbwait -p 80444
Reading symbols from /ifs/user/jonesm/d_hw/d_pp/pp.gdbwait...done.
Attaching to program: /ifs/user/jonesm/d_hw/d_pp/pp.gdbwait, process 80444
...
0x0000000000400df2 in pp () at pp.f90:42
42    do while (gdbWait /=1)
(gdb) set gdbWait=1
(gdb) c
Continuing.
```

```
[rush:~/d_hw/d_pp]$ gdb -quiet pp.gdbwait -p 80445
Reading symbols from /ifs/user/jonesm/d_hw/d_pp/pp.gdbwait...done.
Attaching to program: /ifs/user/jonesm/d_hw/d_pp/pp.gdbwait, process 80445
...
pp () at pp.f90:42
42    do while (gdbWait /=1)
(gdb) set gdbWait=1
(gdb) c
Continuing.
```

Using GDB Within MPI Task Launcher

Last, but not least, you can usually launch `gdb` through your MPI task launcher. For example, using the `Intel MPI` task launcher, `mpirun/mpiexec` (note that this generally pauses at `MPI_Init`):

```
[rush:~/d_hw/d_pp]$ mpirun -np 2 -gdb ./pp.gdb
mpigdb: np = 2
mpigdb: attaching to 22615 ./pp.gdb f07n05
mpigdb: attaching to 22616 ./pp.gdb f07n05
[0,1] (mpigdb) list 40
[0,1] 35    if (ierr /= 0) then
[0,1] 36       print*, 'Unable to intialize MPI.'
[0,1] 37       STOP
[0,1] 38    end if
[0,1] 39    CALL MPI_COMM_RANK(MPI_COMM_WORLD,myid,ierr)
[0,1] 40    CALL MPI_COMM_SIZE(MPI_COMM_WORLD,Nprocs,ierr)
[0,1] 41    ! dummy pause point for gdb insertion
[0,1] 42    !do while (gdbWait /=1)
[0,1] 43    !end do
[0,1] 44    if (Nprocs /= 2) then
[0,1] (mpigdb) c
[0,1] Continuing.
Hello from proc  0 of  2                          f07n05
Number Averaged for Sigmas:       2
Hello from proc  1 of  2                          f07n05
```


More Using GDB With MPI Task Launcher

```
[0,1] (mpigdb) list 84
[0,1] 79          do i=my_low,my_high,2
[0,1] 80             partial_sum_p = partial_sum_p + 1.0_dp/(2.0_dp*i-1.0_dp)
[0,1] 81             partial_sum_m = partial_sum_m - 1.0_dp/(2.0_dp*i+1.0_dp)
[0,1] 82          end do
[0,1] 83          partial_sum = partial_sum_p + partial_sum_m
[0,1] 84          CALL MPI_REDUCE(partial_sum,sum,1,MPI_DOUBLE_PRECISION,MPI_SUM,0, &
[0,1] 85               MPI_COMM_WORLD,ierr)
[0,1] 86          t1 = MPI_Wtime()
[0,1] 87          time_delta = time_delta + (t1-t0)
[0,1] 88       end do
[0,1] (mpigdb) b 83
[0,1] Breakpoint 1 at 0x401161: file pi-mpi.f90, line 83.
[0,1] (mpigdb) run
[0,1] Continuing.
    Greetings from proc    0 of    2 f07n05
      Nterms    Nperproc    Nreps         error     time/rep
    Greetings from proc    1 of    2 f07n05
[0,1]
[0,1] Breakpoint 1, pimpi () at pi-mpi.f90:83
[0,1] 83          partial_sum = partial_sum_p + partial_sum_m
[0,1] (mpigdb) p my_low
[0]  $1 = 1
[1]  $1 = 65
[0,1] (mpigdb) p my_high
[0]  $2 = 64
[1]  $2 = 128
```


Using Serial Debuggers in Parallel

So you can certainly use serial debuggers in parallel - in fact it is a pretty handy thing to do. Just keep in mind:

- Don't forget to compile with debugging turned on
- You can always attach to a running code (and you can instrument the code with that purpose in mind)
- Beware that not all task launchers are equally friendly towards built-in support for serial debuggers

The TotalView Debugger

The "premier" parallel debugger, TotalView:

- Sophisticated commercial product (think many $$ ...)
- Designed especially for HPC, multi-process, multi-thread
- Has both GUI and CLI
- Supports C/C++, Fortran 77/90/95, mixtures thereof
- The "official" debugger of DOE's **Advanced Simulation and Computing** (ASC) program

Using TotalView at CCR

Pretty simple to start using TotalView on the CCR systems:

1. Generally you want to load the latest version:

```
[d16n03:~]$ module avail totalview
```

2. Make sure that your X DISPLAY environment is working if you are going to use the GUI.
3. The current CCR license supports 2 concurrent users up to 8 processors (precludes usage on nodes with more than 8 cores until/unless this license is upgraded).

The DDT Debugger

Allinea's commercial parallel debugger, DDT:

- Sophisticated commercial product (think many $$ ...)
- Designed especially for HPC, multi-process, multi-thread
- Has both GUI and CLI
- Supports C/C++, Fortran 77/90/95, mixtures thereof
- CCR has a 32-token license for DDT (including CUDA and MAP profiler support)
- To find the latest installed version, `module avail ddt`

Current Recommendations

CCR has licenses for Allinea's DDT and TotalView (although the current TotalView license is very small and outdated and will be either upgraded or dropped in favor of DDT). Both are quite expensive, but stay tuned for further developments. Note that the open-source **eclipse** project also has a parallel tools platform that can be used in combination with C/C++ and Fortran:

http://www.eclipse.org/ptp