Scientific Computing (PHYS 2109/Ast 3100 H)
I. Scientific Software Development

SciNet HPC Consortium
University of Toronto

Winter 2014

Lecture 6

- Debugging Basics
- Debugging with the command line: GDB
- Memory Checking: Valgrind

Debugging basics

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Help, my program doesn't work!

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$ gcc -O3 answer.c
$ ./a.out
Segmentation fault
```

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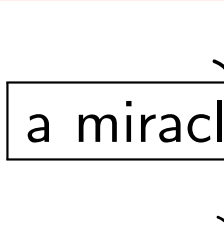

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↓

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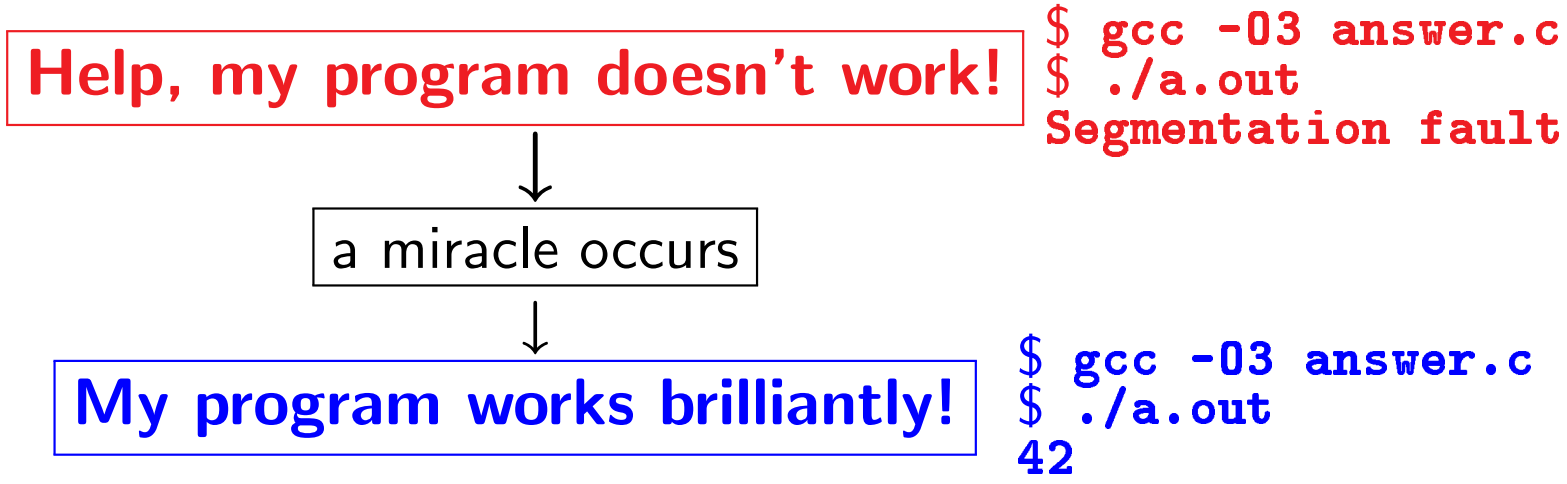

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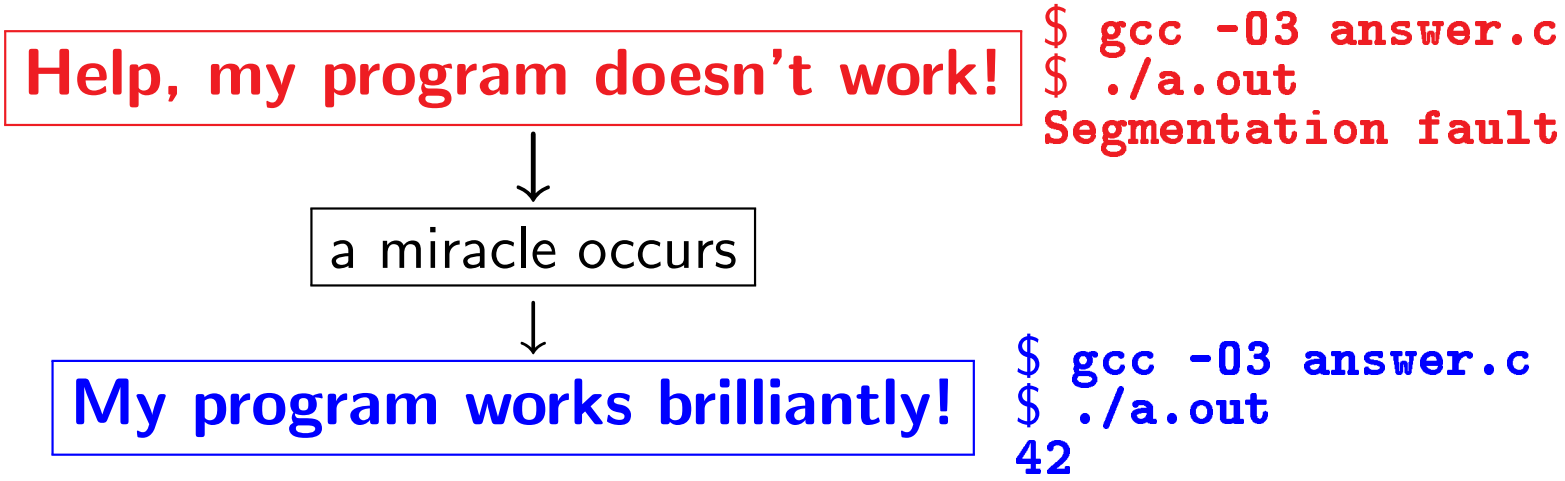
Debugging basics



- Unfortunately, "miracles" are not typically deterministic.

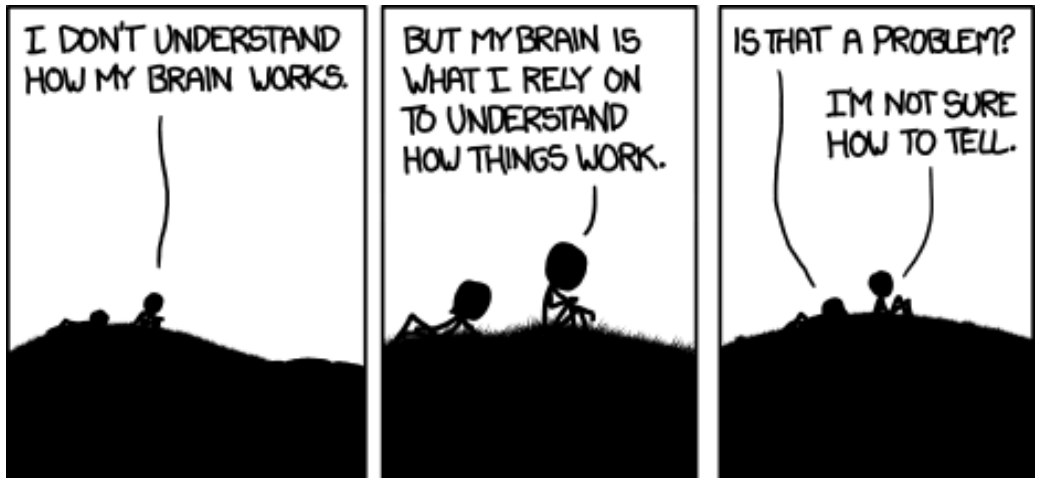
Debugging:

Methodical process of finding and fixing flaws in software

What is going on?

- All programs execute correclty.
- We just told it to do the wrong thing.
- Debugging is the art of reconciling your mental model of what the code is doing with what you actually told it to do.
- *Debugger:* program to help detect errors in other programs.
- **You are the real debugger.**

Debugging



http://imgs.xkcd.com/comics/debugger.png

Tips to avoid debugging

- Write better code.
  - simple, clear, straightfoward code.
  - modularity (avoid global variables and 10,000 line functions).
  - avoid "cute tricks", (no obfuscated C code winners).
- Don't write code, use existing libraries
- Write tests (simple) for each part

Debugging Workflow

- As soon as you are convinced there is a real problem, create the simplest situation in which it repeatedly occurs.
- This is science: model, hypothesis, experiment, conclusion.
- Try a smaller problem size, turning off different physical effects with options, etc, until you have a simple, fast, repeatable example.
- Try to narrow it down to a particular module/function/class.
- Integrated calculation: Write out intermediate results, inspect them.

Common symptoms

Errors at compile time

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Runtime errors

Common symptoms

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Runtime errors

- Floating point exceptions
- Segmentation fault
- Aborted
- Incorrect output (nans)

Common issues

Arithmetic	corner cases (`sqrt(-0.0)`), infinities
Memory access	Index out of range, uninitialized pointers.
Logic	Infinite loop, corner cases
Misuse	wrong input, ignored error, no initialization
Syntax	wrong operators/arguments
Resource starvation	memory leak, quota overflow
Parallel	race conditions, deadlock

Ways to debug

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  - Turn on compiler warnings: fix or understand them!

    ```
    $ gcc/g++ -Wall
    ```

  - Check your assumptions (e.g. use **`assert`**).

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- Inspect the exit code and read the error messages!
- Use a debugger
- Add print statements

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  - Check your assumptions (e.g. use **`assert`**).
- Inspect the exit code and read the error messages!
- Use a debugger
- Add print statements ←**No way to debug!**

What's wrong with using print statements?

Strategy

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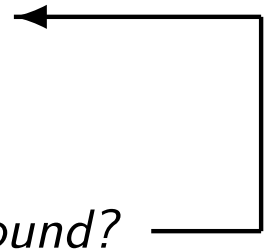

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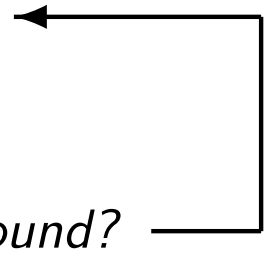

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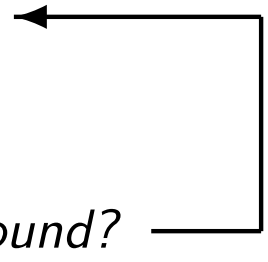

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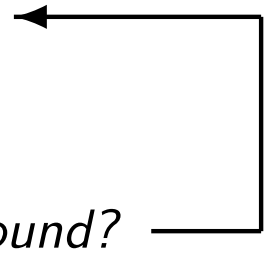

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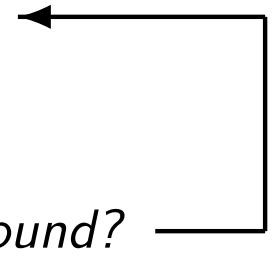

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Problems with this approach

- Time consuming
- Error prone
- Changes memory, timing...

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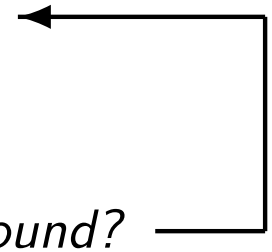

- Removing the extra code after the bug is fixed
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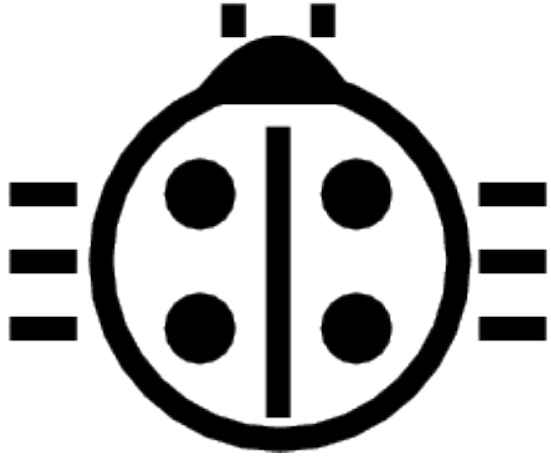
Problems with this approach

- Time consuming
- Error prone
- Changes memory, timing... **There's a better way!**

Symbolic debuggers



Symbolic debuggers

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1. Crash inspection
2. Function call stack
3. Step through code
4. Automated interruption
5. Variable checking and setting

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Use a graphical debugger or not?

- Local work station: graphical is convenient
- Remotely (SciNet): can be slow

In any case, graphical and text-based debuggers use the same concepts.

Symbolic debuggers

Preparing the executable

- Add required compilination flags:
  - `$ gcc/g++/gfortran -g -gstabs`
  - `$ icc/icpc/ifort -g -debug all`
  - `$ nvcc -g -G`
- Optional: switch off optimization `-O0`

Symbolic debuggers

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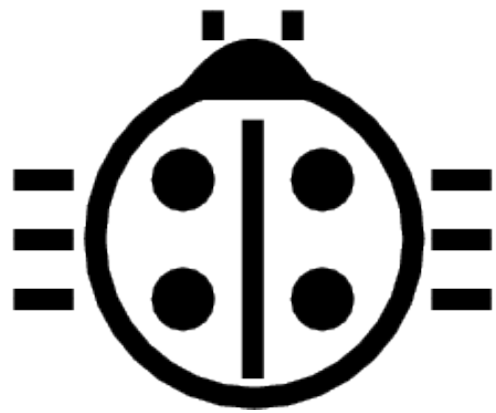
Command-line based symbolic debuggers: gdb

GDB



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What is GDB?

- Free, GNU license, symbolic debugger.
- Available on many systems.
- Been around for a while, but still developed and up-to-date
- Text based, but has a '-tui' option.

```
$ module load gcc
$ gcc -g -O0 example.c -o example
$ module load gdb
$ gdb -tui example
...
(gdb)_
```

GDB command summary

help	**h**	print description of
run	**r**	run from the start (+args)
backtrace/where	**ba**	function call stack
break	**b**	set breakpoint
delete	**d**	delete breakpoint
continue	**c**	continue
step	**s**	step into function
next	**n**	continue until next line
print	**p**	print variable
quit	**q**	quit
finish	**fin**	continue until function end
set variable	**set var**	change variable
down	**do**	go to called function
tbreak	**tb**	set temporary breakpoint
until	**unt**	continue until line/function
up	**up**	go to caller
watch	**wa**	stop if variable changes
quit	**q**	quit gdb

GDB basic building blocks

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GDB building block #1: Inspect crashes

Inspecting core files

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- NOTE: needs max core size set (**`ulimit -c <number>`**)
- gdb reads with **`gdb <executable> <corefile>`**
- it will show you where the program crashed

GDB building block #1: Inspect crashes

Inspecting core files

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GDB building block #1: Inspect crashes

Inspecting core files

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- gdb reads with **`gdb <executable> <corefile>`**
- it will show you where the program crashed

No core file?

- can start gdb as **`gdb <executable>`**
- type **`run`** to start program
- gdb will show you where the program crashed if it does.

GDB Exampe: Code

```
#include <iostream>
#include <cmath>
int main(int argc, char **argv) {
  int nmax; float *squares, sum;
  std::cin >> nmax;
  for (int i=1; i<=nmax; i++) {
    squares[i] = sqrt(i-2);
    sum += squares[i];
  }
  std::cout << sum;
  return 0;
}
```

GDB Example #1

```
$g++ -g -o square square.c
$./square
5000
Segmentation fault
```

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$g++ -g -o square square.c
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```
$gdb ./square core.12345
Program terminated with signal 11, Segmentation fault.
#0 0x0000000000400855 in main (argc=2,
argv=0x7fff6db1ac18) at square.c:12
12 squares[i] = sqrt( (i-2) );
(gdb)
```

GDB building block #2: Function call stack

Interrupting program

- Press Crtl-C while program is running in gdb
- gdb will show you where the program was.

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Stack trace

- From what functions was this line reached?
- What were the arguments of those function calls?

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Stack trace

- From what functions was this line reached?
- What were the arguments of those function calls?

gdb commands

backtrace	function call stack
continue	continue
down	go to called function
up	go to caller

GDB building block #3: Step through code

Stepping through code

- Line-by-line
- Choose to step into or over functions
- Can show surrounding lines or use **`-tui`**

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gdb commands

`list`	list part of code
`next`	continue until next line
`step`	step into function
`finish`	continue until function end
`until`	continue until line/function

GDB building block #4: Automatic interruption

Breakpoints

- **`break [file:]<line>|<function>`**
- each breakpoint gets a number
- when run, automatically stops there
- can add conditions, temporarily remote breaks, etc.

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Breakpoints

- **`break [file:]<line>|<function>`**
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Related gdb commands

`delete`	unset breakpoint
`condition`	break if condition met
`disable`	disable breakpoint
`enable`	enable breakpoint
`info breakpoints`	list breakpoints
`tbreak`	temporary breakpoint

GDB building block #5: Variables

Checking a variable

- Can print the value of a variable
- Can keep track of variable (print at prompt)
- Can stop the program when variable changes
- Can change a variable ("what if . . . ")

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gdb commands

`print`	print variable
`display`	print at every prompt
`set variable`	change variable
`watch`	stop if variable changes

GDB Exampe: Code (fixed)

```
#include <iostream>
#include <cmath>
int main(int argc, char **argv) {
  int nmax; float *squares, sum;
  std::cin >> nmax;
  squares = new float [nmax]; //allocate memory
  for (int i=1; i<=nmax; i++) {
    squares[i] = sqrt(i-2);
    sum += squares[i];
  }
  std::cout << sum;
  return 0;
}
```

GDB : Example #2

```
$gdb ./square
(gdb)
(gdb) list 15
10
11 for (int i=1; i<=nmax; i++) {
12 squares[i] = sqrt( (i-2) );
13 sum += squares[i];
14 }
15
16 std::cout << sum;
17 return 0;
18 }
19
(gdb) break 13
Breakpoint 1 at 0x4008ae:  file square.2.c, line 13.
```

GDB : Example #2 - continued

```
(gdb) run
Starting program:  ./square
20
Breakpoint 1, main (argc=1, argv=0x7fffffffdc48) at
square.2.c:13
13 sum += squares[i];
(gdb) print sum
$1 = 5.88011741e-39
(gdb) step
11 for (int i=0; i<nmax; i++) {
(gdb) print sum
$2 = -nan(0x400000)
(gdb) print squares[0]
$3 = -nan(0x400000)
(gdb) quit
```

Graphical symbolic debuggers

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Graphical symbolic debuggers

Features

- Nice, more intuitive graphical user interface
- Front to command-line based tools: Same concepts
- Need graphics support: X forwarding (or VNC)

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Available on SciNet: ddd and ddt

- ddd

```
$ module load gcc ddd
$ ddd <executable compiled with -g flag>
```

- ddt

```
$ module load ddt
$ ddt <executable compiled with -g flag>
(more later)
```

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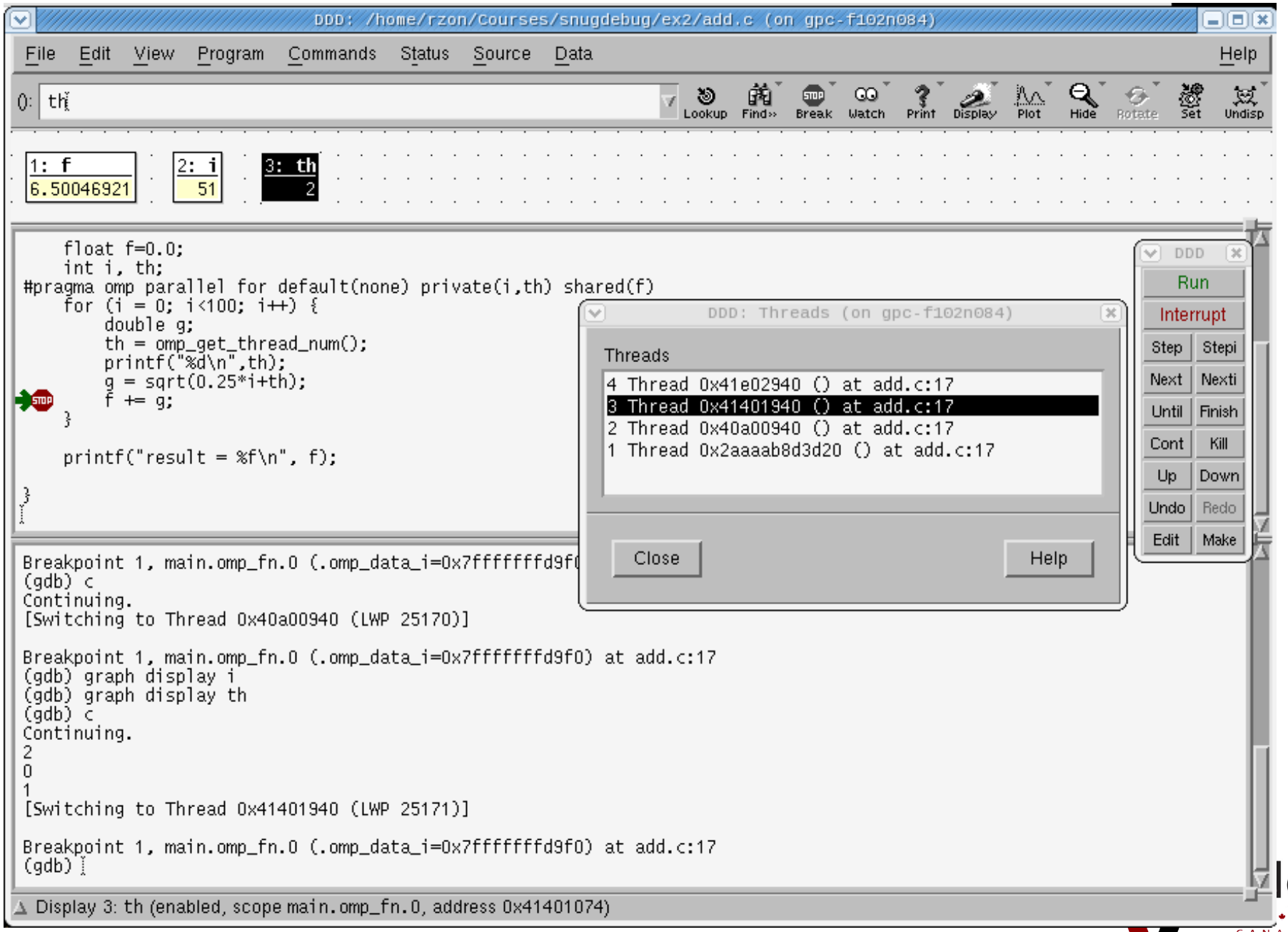
Graphical symbolic debuggers - ddd



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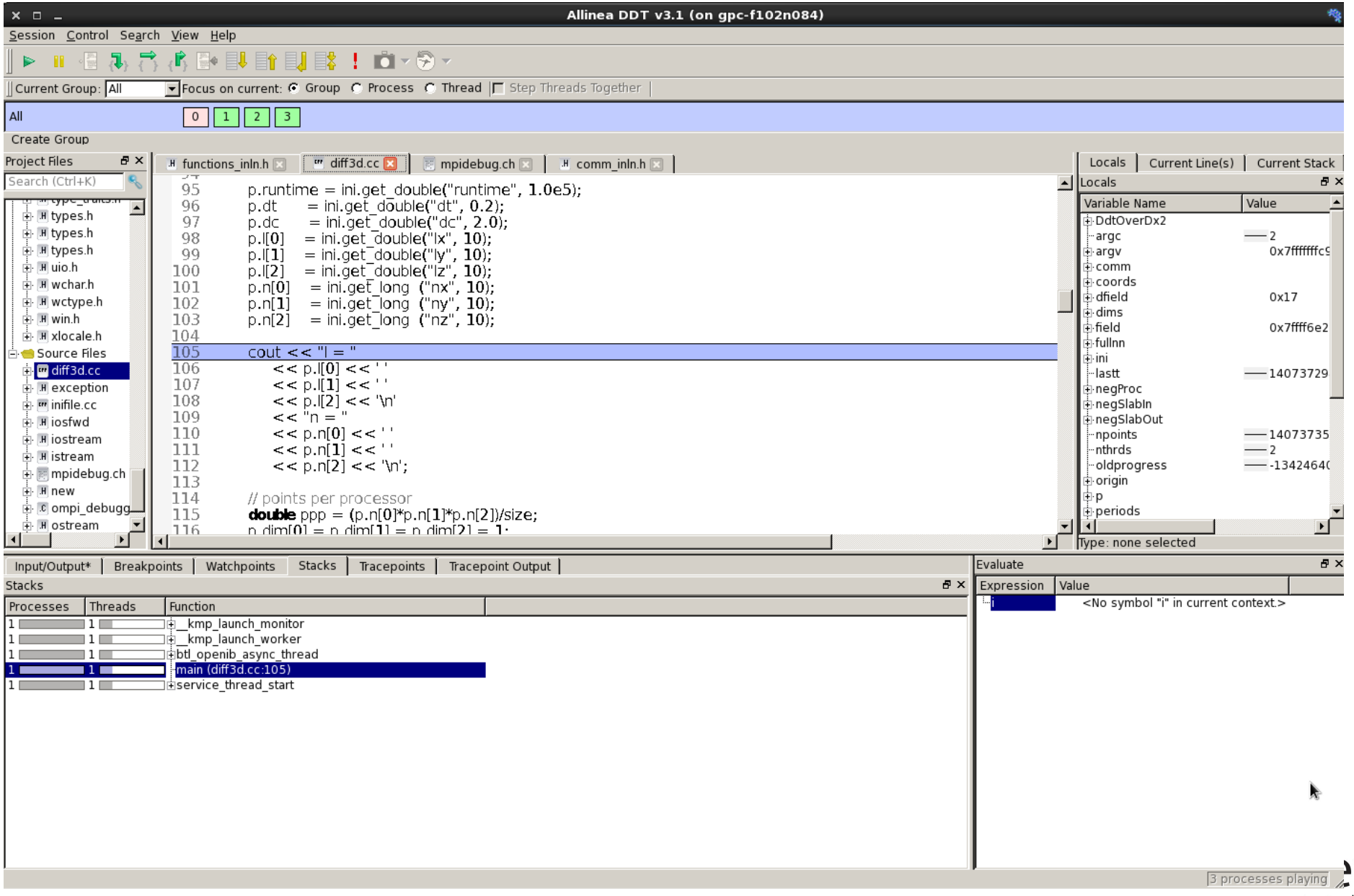

Memory Checking: Valgrind

- Memory errors do not always give segfaults
- Commonly have to go *way* out of bounds to get a segfault.
- Write into other variables - hard to find problem.
- Valgrind - intercepts each memory call and checks them (very thorough but slow).
- Finds illegal accesses, uninitialized values, memory leaks.
- Is typically very verbose.
- If you use external libraries, sometimes false positive

GDB Exampe: Code (fixed?)

```
#include <iostream>
#include <cmath>
int main(int argc, char **argv) {
  int nmax; float *squares, sum;
  std::cin >> nmax;
  squares = new float [nmax]; //allocate memory
  for (int i=1; i<=nmax; i++) {
    squares[i] = sqrt(i); //fixed nan's
    sum += squares[i];
  }
  std::cout << sum;
  return 0;
}
```

Memory Checking: Valgrind

valgrind --tool=memcheck ./square

```
==31550== Invalid write of size 4
==31550==    at 0x4008A5: main (square.c:8)
==31550==  Address 0x4c3b090 is 0 bytes after a block of size 80 alloc'd
==31550==    at 0x4A07152: operator new[](unsigned long) (vg_replace_mallo
==31550==    by 0x400875: main (square..c:6)
==31550==
==31550== Invalid read of size 4
==31550==    at 0x4008B6: main (square.c:9)
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Error:

i index from 1 to nmax

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Memory Checking: Valgrind

```
==31550== Conditional jump or move depends on uninitialised value(s)
==31550==    at 0x3A41243696: __mpn_extract_double (in /lib64/libc-2.12.so
==31550==    by 0x3A4124A4BD: __printf_fp (in /lib64/libc-2.12.so)
==31550==    by 0x3A41245B9F: vfprintf (in /lib64/libc-2.12.so)
==31550==    by 0x3A4126FA51: vsnprintf (in /lib64/libc-2.12.so)
==31550==    by 0x3A47E7EB4E: ??? (in /usr/lib64/libstdc++.so.6.0.13)
==31550==    by 0x3A47E80F22: std::ostreambuf_iterator<char, std::char_tra
==31550==    by 0x3A47E81248: std::num_put<char, std::ostreambuf_iterator<
==31550==    by 0x3A47E9487E: std::ostream& std::ostream::_M_insert<double
==31550==    by 0x4008E7: main (square.c:11)

==31550== Use of uninitialised value of size 8
```

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==31550==    by 0x3A4124A4BD: __printf_fp (in /lib64/libc-2.12.so)
==31550==    by 0x3A41245B9F: vfprintf (in /lib64/libc-2.12.so)
==31550==    by 0x3A4126FA51: vsnprintf (in /lib64/libc-2.12.so)
==31550==    by 0x3A47E7EB4E: ??? (in /usr/lib64/libstdc++.so.6.0.13)
==31550==    by 0x3A47E80F22: std::ostreambuf_iterator<char, std::char_tra
==31550==    by 0x3A47E81248: std::num_put<char, std::ostreambuf_iterator<
==31550==    by 0x3A47E9487E: std::ostream& std::ostream::_M_insert<double
==31550==    by 0x4008E7: main (square.c:11)

==31550== Use of uninitialised value of size 8
```

Error:

variable “sum” never initialized

GDB Exampe: Code (fixed?)

```
#include <iostream>
#include <cmath>
int main(int argc, char **argv) {
  int nmax; float *squares, sum(0); //init sum
  std::cin >> nmax;
  squares = new float [nmax]; //allocate memory
  for (int i=0; i<nmax; i++)//fixed i index {
    squares[i] = sqrt(i); //fixed nan's
    sum += squares[i];
  }
  std::cout << sum;
  return 0;
}
```

Memory Checking: Valgrind

```
==31550== HEAP SUMMARY:
==31550==     in use at exit: 80 bytes in 1 blocks
==31550==   total heap usage: 1 allocs, 0 frees, 80 bytes allocated
==31550==
==31550== LEAK SUMMARY:
==31550==    definitely lost: 80 bytes in 1 blocks
==31550==    indirectly lost: 0 bytes in 0 blocks
==31550==      possibly lost: 0 bytes in 0 blocks
==31550==    still reachable: 0 bytes in 0 blocks
==31550==         suppressed: 0 bytes in 0 blocks

==31550== ERROR SUMMARY: 204 errors from 113 contexts (suppressed: 6 from
```

Memory Checking: Valgrind

```
==31550== HEAP SUMMARY:
==31550==     in use at exit: 80 bytes in 1 blocks
==31550==   total heap usage: 1 allocs, 0 frees, 80 bytes allocated
==31550==
==31550== LEAK SUMMARY:
==31550==    definitely lost: 80 bytes in 1 blocks
==31550==    indirectly lost: 0 bytes in 0 blocks
==31550==      possibly lost: 0 bytes in 0 blocks
==31550==    still reachable: 0 bytes in 0 blocks
==31550==         suppressed: 0 bytes in 0 blocks

==31550== ERROR SUMMARY: 204 errors from 113 contexts (suppressed: 6 from
```

Error:

forgot to free dynamic memory squares

GDB Exampe: Code (fixed?)

```
#include <iostream>
#include <cmath>
int main(int argc, char **argv) {
  int nmax; float *squares, sum(0); //init sum
  std::cin >> nmax;
  squares = new float [nmax]; //allocate memory
  for (int i=0; i<nmax; i++) //fixed i index{
    squares[i] = sqrt(i); //fixed nan's
    sum += squares[i];
  }
  std::cout << sum;
  delete [] squares; //deallocate memory
  return 0;
}
```

Memory Checking: Valgrind

```
$  valgrind --tool=memcheck ./square
==31707== Memcheck, a memory error detector
==31707== Copyright (C) 2002-2012, and GNU GPL'd, by Julian Seward et al.
==31707== Using Valgrind-3.8.1 and LibVEX; rerun with -h for copyright inf
==31707== Command: ./square
==31707==
20
57.1938
==31707==
==31707== HEAP SUMMARY:
==31707==     in use at exit: 0 bytes in 0 blocks
==31707==   total heap usage: 1 allocs, 1 frees, 80 bytes allocated
==31707==
==31707== All heap blocks were freed -- no leaks are possible
==31707==
==31707== For counts of detected and suppressed errors, rerun with: -v
==31707== ERROR SUMMARY: 0 errors from 0 contexts (suppressed: 6 from 6)
```