

International Centre for Theoretical Physics



Debugging & Profiling

Ivan Girotto – igirotto@ictp.it

Information & Communication Technology Section (ICTS)

International Centre for Theoretical Physics (ICTP)







- Debugging
- Profiling
- Practical examples





What is Debugging ?!

- Identifying the cause of an error and correcting it
- Once you have identified defects, you need to:
 - find and understand the cause
 - remove the defect from your code
- In a large number of cases bug fixes are wrong:
 - they remove the symptom, but not the cause
- Improve productivity by getting it right the first time
- A lot of programmers don't know how to debug!
 - Doesn't add functionality & doesn't improve the science
- Debugging needs practice and experience:
 - understand the science and the tools





Errors are Opportunities

- Learn from the program you're working on:
 - Errors mean you didn't understand the program. If you knew it better, it wouldn't have an error. You would have fixed it already
- Learn about the kinds of mistakes you make:
 - If you wrote the program, you inserted the error
 - Once you find a mistake, ask yourself:
 - Why did you make it?
 - How could you have found it more quickly?
 - How could you have prevented it?
 - Are there other similar mistakes in the code?





The Nature of Bugs

- Straightforward bug to intercept and solve
- The program crashes unexpectedly
 - the problem can be easily reproduced (lucky)
 - bug whose causes are too complex to be reliably reproduced; it thus defies repair
 - bug disappears when debugging a problem (compiling with -g or adding prints)
- The produced numbers differ from what we expected
 - bug generated by an invalid operations
 - bug disappears when debugging a problem (compiling with -g or adding prints)





Main Reasons of Debugging

- Floating Point Exceptions (FPE)
 - Overflow
 - Invalid Number
 - Division by Zero
- Out of bound
- Segmentation Fault
- Not expected execution flow
- The Program Hangs





Purpose of a Debugger

- More information than print statements
- Allows to stop/start/single step execution
- Look at data and modify it
- 'Post mortem' analysis from core dumps
- Prove / disprove hypotheses
- No substitute for good thinking
- But, sometimes good thinking is not a substitute for effectively using a debugger!
- Easier to use with modular code





Approaches

- Print Messages and Variables \odot
- Compiler Debug Options
- Core analysis
- Run the Program with a Debugger
- Attach Debugger to a running process
- Ask for help!





Using a Debugger

- When compiling use -g option to include debug info in object (.o) and executable
- 1:1 mapping of execution and source code only when optimization is turned off
 - problem when optimization uncovers bug
- GNU compilers allow -g with optimization
 - not always correct line numbers
 - variables/code can be 'optimized away'
 - progress confusing with loop unrolling
- strip command removes debug info





Using gdb as a Debugger

- gdb ex01-c launches debugger, loads binary, stops with (gdb) prompt waiting for input:
- run starts executable, arguments are passed Running program can be interrupted (ctrl-c)
- gdb ./prog --args arg1 -flag passes all arguments to the run command inside gdb
- continue continues stopped program
- **finish** continues until the end of a subroutine
- **step** single steps through program line by line
- **next** single steps but doesn't step into subroutines





More Basic **gdb** Commands

- print displays contents of a known data object
- **display** is like print but shows updates every step
- where shows stack trace (of function calls)
- **up down** allows to move up/down on the stack
- break sets break point (unconditional stop), location indicated by file name+line no. or function
- watch sets a conditional break point (breaks when an expression changes, e.g. a variable)
- delete removes display or break points





Post Mortem Analysis

- Enable core dumps: ulimit -c unlimited
- Run executable until it crashes; will generate a file core or core.<pid> with memory image
- Load executable and core dump into debugger gdb myexe core.<pid>
- Inspect location of crash through commands: where, up, down, list
- Use directory to point to location of sources





Using valgrind

- Run valgrind -v ./exe to instrument and run
- --leak-check=full --track-origins=yes
- Output will list individual errors and summary
- With debug info present can resolve problems to line of code, otherwise to name of function
- Also monitors memory allocation / deallocation to flag memory leaks ("forgotten" allocations)
- Instrumentation slows down execution
- Can produce "false positives" (flag non-errors)





How to NOT do Debugging

- Find the error by guessing
- Change things randomly until it works (again)
- Don't keep track of what you changed
- Don't make a backup of the original
- Fix the error with the most obvious fix
- If wrong code gives the correct result, and changing it doesn't work, don't correct it.
- If the error is gone, the problem is solved. Trying to understand the problem, is a waste of time





Debugging Tools

- Source code comparison and management tools: diff, vimdiff, emacs/ediff, cvs/svn/git
 - Help you to find differences, origins of changes
- Source code analysis tools: compiler warnings, ftnchek, lint
 - Help you to find problematic code
 - Always enable warnings when programming
 - Always take warnings seriously (but not all)
 - Always compile/test on multiple platforms
- Bounds checking allows checking of (static) memory allocation violations (no malloc)





More Debugging Tools

- Using different compilers (Intel, GCC, Clang, ...)
- Debuggers and debugger frontends: gdb (GNU compilers), idb (Intel compilers), ddd (GUI), eclipse (IDE), and many more...
- **gprof** (profiler) as it can generate call graphs
- **valgrind**, an instrumentation framework
 - Memcheck: detects memory management problems
 - Cachegrind: cache profiler, detects cache misses
 - Callgrind: call graph creation tool





How to Report a Bug(?) to Others

- Research whether bug is known/fixed
 web search, mailing list archive, bugzilla
- Provide description on how to reproduce the problem. Find a minimal input to show bug.
- Always state hardware/software you are using (distribution, compilers, code version)
- Demonstrate, that you have invested effort
- Make it easy for others to help you!





Profiling

- Profiling usually means:
 - Instrumentation of code (e.g. during compilation)
 - Automated collection of timing data during execution
 - Analysis of collected data, breakdown by function
- Example: gcc -o some_exe.x -pg some_code.c
 - ./some_exe.x
 - gprof some_exe.x gmon.out
- Profiling is often incompatible with code optimization or can be misleading (inlining)





PERF – Hardware Assisted Profiling

- Modern x86 CPUs contain performance monitor tools included in their hardware
- Linux kernel versions support this feature which allows for very low overhead profiling without instrumentation of binaries
- **perf stat ./a.out** -> profile summary
- perf record ./a.out; perf report -i perf.data
- gprof like function level profiling (with coverage report and disassembly, if debug info present)



The Abdus Salam International Centre for Theoretical Physics



convergence	NOT a	chieved after	r 5 itera	tions: s	topping			
Writing outp	ut da	ta file c8_a	tm213_k111.	save				
init_run		93.79s CPU	93.79s	WALL (1	calls)		
electrons		961.37s CPU	961.37s	WALL (1	calls)		
Called by in	it ru	in•						
wfcinit		60 27c (DII	60 276		1	calle)		
notinit		69.37s CPU 4.76s CPU	4 760	WALL (1	calle)		
ροτιπιτ		4.768 CPU	4.705	WALL (1	carts)		
Called by el	ectro	ns:						
c_bands		883.32s CPU	883.32s	WALL (5	calls)		
sum_band		40.30s CPU	40.30s	WALL (5	calls)		
v_of_rho		1.10s CPU	1.10s	WALL (6	calls)		
c_bands sum_band v_of_rho mix_rho		1.51s CPU	1.51s	WALL (5	calls)		
Called by c_	Danas		A FA-	WALL C	11	11->		
Init_us_2		0.50s CPU 882.01s CPU	0.505	WALL (11			
cegterg		882.015 CPU	882.01S	WALL (5	calls)		
Called by *e	gtērg							
h_psi		259.11s CPU	259.11s	WALL (17	calls)		
q_psi	:	9.02s CPU	9.02s	WALL (11	calls)		
cdiaghg		259.11s CPU 9.02s CPU 401.37s CPU	401.37s	WALL (16	calls)		
Called by h_								
dilled by n_	pst:	22.44s (PU	22 446	WALL C	17	calle)		
aaa_vuspsi		22.445 CPU	22.445	WALL (17	carts)		
General rout	ines							
calbec		17.25s CPU	17.25s	WALL (17	calls)		
fft		0.52s CPU	0.52s	WALL (66	calls)		
ffts		0.63s CPU	0.63s	WALL (117	calls)		
fftw		231.61s CPU	231.61s	WALL (10260	calls)		
davcio		0.52s CPU 0.63s CPU 231.61s CPU 4.72s CPU	4.72s	WALL (5	calls)		
Parallel rou								
		63.50s CPU	62 540	WALL	10112	called		
		10.66s CPU	10 676	WALL (10752	calle)		
		10.005 CPU	10.675	WALL (10232	currs)		
EXX routines								
PWSCF	: 17	m42.94s CPU	17m42.94	s WALL				

convergence NOT achieved after 5 iterations: stopping

Writing output data file c8_atm213_k111.save

init_run		119.48s	CPU	119.48s	WALL	(1	calls)
electrons		1369.53s	CPU	1369.53s	WALL	(1	calls)
Called by i	nit_r	un:						
								calls)
potinit		2 . 15s	CPU	2 . 15s	WALL	(1	calls)
Called by e	lectr	ons:						
c_bands		1289.41s	CPU	1289.41s	WALL			calls)
sum_band		56.06s	CPU	56.06s		(5	calls)
v_of_rho		1.39s	CPU	1.39s		(6	calls)
mix_rho		1.23s	CPU	1.23s	WALL	(5	calls)
init_us_2		0.13s	CPU	0.13s	WALL	(11	calls)
cegterg		1288.89s	CPU	1288.89s	WALL	(5	calls)
Called by *	eater	'a:						
h_psi	:	409.59s	CPU	409.59s	WALL	(calls)
q_psi		2.35s	CPU	2.35s	WALL	Ċ	11	calls)
cdiaghg	:	528.61s	CPU	528.61s	WALL	Ċ		calls)
Called by h	_psi:							
			CPU	32 . 96s	WALL	C	17	calls)
General rou	tines							
calbec		31.22s	CPU	31.22s	WALL	(17	calls)
fft		0.62s	CPU	0.62s	WALL	Ċ	66	calls)
ffts		Ø.86s	CPU	Ø.86s	WALL	Ċ	117	calls)
fftw		376.02s	CPU	376.04s	WALL	(82004	calls)
davcio		6.38s			WALL	(5	calls)
Parallel ro	utine	es						
fft_scatter		81.64s	CPU	81.65s	WALL	(82187	calls)
PWSCF	: 2	24m57.48s (CPU	24m57.48	s WALL			
	electrons Called by i wfcinit potinit Called by e c_bands sum_band v_of_rho mix_rho Called by c init_us_2 cegterg Called by * h_psi g_psi cdiaghg Called by h add_vuspsi General rou calbec fft ffts fftw davcio Parallel rou	electrons : Called by init_r wfcinit : potinit : Called by electr c_bands : sum_band : v_of_rho : mix_rho : Called by c_band init_us_2 : cegterg : Called by *egter h_psi : g_psi : cdiaghg : Called by h_psi: add_vuspsi : General routines called by h_psi: add_vuspsi : General routines called i y h_psi: add_vuspsi : General routines fft : fft	electrons : 1369.53s Called by init_run: wfcinit : 98.55s potinit : 2.15s Called by electrons: c_bands : 1289.41s sum_band : 56.06s v_of_rho : 1.39s mix_rho : 1.23s Called by c_bands: init_us_2 : 0.13s cegterg : 1288.89s Called by c_bands: init_us_2 : 0.13s cegterg : 1288.89s Called by *egterg: h_psi : 409.59s g_psi : 2.35s cdiaghg : 528.61s Called by h_psi: add_vuspsi : 32.96s General routines calbec : 31.22s fft : 0.62s ffts : 0.86s fftw : 376.02s davcio : 6.38s Parallel routines fft_scatter : 81.64s	electrons : 1369.53s CPU Called by init_run: wfcinit : 98.55s CPU potinit : 2.15s CPU Called by electrons: bands : 1289.41s CPU sum_band : 56.06s CPU v_of_rho : 1.39s CPU mix_rho : 1.23s CPU Called by c_bands: init_us_2 : 0.13s CPU Called by c_bands: init_us_2 : 0.13s CPU Called by *egterg: h_psi : 409.59s CPU g_psi : 2.35s CPU Called by h_psi: add_vuspsi : 32.96s CPU Called by h_si: add_vuspsi : 31.22s CPU fft : 0.62s CPU ffts : 0.86s CPU ffts : 0.86s CPU ffts : 0.86s CPU fftw : 376.02s CPU davcio : 6.38s CPU	electrons : 1369.53s CPU 1369.53s Called by init_run: wfcinit : 98.55s CPU 98.55s potinit : 2.15s CPU 2.15s Called by electrons: : 2.15s CPU 2.15s Called by electrons: : : 1289.41s CPU 1289.41s Sum_band : 56.06s CPU 1.39s mix_rho : 1.39s v_of_rho : 1.39s CPU 1.39s mix_rho : 1.23s Called by c_bands: : 1.23s CPU 1.23s 0.13s called by c_bands: : 1.23s CPU 1.23s Called by c_bands: : 1.23s CPU 1.23s Called by c_bands: : 1.23s CPU 0.13s cgeterg : 1288.89s CPU 1288.89s Called by *egterg: . . 2.35s CPU 2.35s h_psi : 2.35s CPU 2.35s 2.35s <t< td=""><td>electrons:1369.53s (PU1369.53s WALLCalled by init_run: wfcinit:98.55s (PU 2.15s WALLpotinit:2.15s (PU 2.15s WALLCalled by electrons: c_bands:2.15s (PU 2.15s WALLCalled by electrons: c_bands:1289.41s (PU 56.06s (PU 1.39s (PU 1.39s WALLCalled by c_bands: init_us_2:1.23s (PU 1.39s (PU 1.23s WALLCalled by c_bands: init_us_2:0.13s (PU 2.35s WALLCalled by c_bands: init_us_2:0.13s (PU 2.35s WALLCalled by c_bands: init_us_2:0.13s (PU 2.35s WALLCalled by *egterg: h_psi:2.35s (PU 2.35s WALLCalled by *egterg: h_psi:2.35s (PU 2.35s WALLCalled by h_psi: add_vuspsi:32.96s (PU 32.96s WALLCalled by h_psi: calbec:31.22s WALLGeneral routines calbec:31.22s WALLFfts:0.86s (PU 0.62s WALLffts:0.86s (PU 0.62s WALLffts:0.86s (PU 0.63s WALLfftw:376.02s (PU 0.63s WALLParallel routines fft_scatter:81.65s WALL</td><td>Called by init_run: wfcinit : 98.55s (PU 98.55s WALL (potinit : 2.15s (PU 2.15s WALL (Called by electrons: c_bands : 1289.41s (PU 1289.41s WALL (sum_band : 56.06s (PU 56.06s WALL (v_of_rho : 1.39s (PU 1.39s WALL (mix_rho : 1.23s (PU 1.39s WALL (Called by c_bands: init_us_2 : 0.13s (PU 0.13s WALL (Called by c_bands: init_us_2 : 0.13s (PU 1288.89s WALL (Called by *egterg: h_psi : 409.59s (PU 1288.89s WALL (Called by *egterg: h_psi : 2.35s (PU 2.35s WALL (Called by h_psi: add_vuspsi : 32.96s (PU 32.96s WALL (Called by h_psi: add_vuspsi : 31.22s (PU 31.22s WALL (fft : 0.62s (PU 0.62s WALL (ffts : 0.86s (PU 0.86s WALL (fftw : 376.02s (PU 376.04s WALL (Parallel routines fft_scatter : 81.64s (PU 81.65s WALL (</td><td>electrons : 1369.53s CPU 1369.53s WALL (1 Called by init_run: wfcinit : 98.55s CPU 98.55s WALL (1 potinit : 2.15s CPU 2.15s WALL (1 Called by electrons: : 2.15s CPU 1289.41s WALL (5 c_bands : 1289.41s CPU 1289.41s WALL (5 sum_band : 56.06s CPU 56.06s WALL (5 v_of_rho : 1.39s CPU 1.39s WALL (5 called by c_bands: init_us_2 : 0.13s CPU 1.23s WALL (5 called by c_bands: init_us_2 : 0.13s CPU 1.23s WALL (5 called by c_bands: init_us_2 : 0.13s WALL (11 cegterg : 1288.89s CPU 1288.89s WALL (17 g_psi : 2.35s CPU 2.35s WALL (<t< td=""></t<></td></t<>	electrons:1369.53s (PU1369.53s WALLCalled by init_run: wfcinit:98.55s (PU 2.15s WALLpotinit:2.15s (PU 2.15s WALLCalled by electrons: c_bands:2.15s (PU 2.15s WALLCalled by electrons: c_bands:1289.41s (PU 56.06s (PU 1.39s (PU 1.39s WALLCalled by c_bands: init_us_2:1.23s (PU 1.39s (PU 1.23s WALLCalled by c_bands: init_us_2:0.13s (PU 2.35s WALLCalled by c_bands: init_us_2:0.13s (PU 2.35s WALLCalled by c_bands: init_us_2:0.13s (PU 2.35s WALLCalled by *egterg: h_psi:2.35s (PU 2.35s WALLCalled by *egterg: h_psi:2.35s (PU 2.35s WALLCalled by h_psi: add_vuspsi:32.96s (PU 32.96s WALLCalled by h_psi: calbec:31.22s WALLGeneral routines calbec:31.22s WALLFfts:0.86s (PU 0.62s WALLffts:0.86s (PU 0.62s WALLffts:0.86s (PU 0.63s WALLfftw:376.02s (PU 0.63s WALLParallel routines fft_scatter:81.65s WALL	Called by init_run: wfcinit : 98.55s (PU 98.55s WALL (potinit : 2.15s (PU 2.15s WALL (Called by electrons: c_bands : 1289.41s (PU 1289.41s WALL (sum_band : 56.06s (PU 56.06s WALL (v_of_rho : 1.39s (PU 1.39s WALL (mix_rho : 1.23s (PU 1.39s WALL (Called by c_bands: init_us_2 : 0.13s (PU 0.13s WALL (Called by c_bands: init_us_2 : 0.13s (PU 1288.89s WALL (Called by *egterg: h_psi : 409.59s (PU 1288.89s WALL (Called by *egterg: h_psi : 2.35s (PU 2.35s WALL (Called by h_psi: add_vuspsi : 32.96s (PU 32.96s WALL (Called by h_psi: add_vuspsi : 31.22s (PU 31.22s WALL (fft : 0.62s (PU 0.62s WALL (ffts : 0.86s (PU 0.86s WALL (fftw : 376.02s (PU 376.04s WALL (Parallel routines fft_scatter : 81.64s (PU 81.65s WALL (electrons : 1369.53s CPU 1369.53s WALL (1 Called by init_run: wfcinit : 98.55s CPU 98.55s WALL (1 potinit : 2.15s CPU 2.15s WALL (1 Called by electrons: : 2.15s CPU 1289.41s WALL (5 c_bands : 1289.41s CPU 1289.41s WALL (5 sum_band : 56.06s CPU 56.06s WALL (5 v_of_rho : 1.39s CPU 1.39s WALL (5 called by c_bands: init_us_2 : 0.13s CPU 1.23s WALL (5 called by c_bands: init_us_2 : 0.13s CPU 1.23s WALL (5 called by c_bands: init_us_2 : 0.13s WALL (11 cegterg : 1288.89s CPU 1288.89s WALL (17 g_psi : 2.35s CPU 2.35s WALL (<t< td=""></t<>

This run was terminated on: 12:25:36 120ct2012

Ivan Girotto - igirotto@ictp.it Trieste, 10th March 2016

Debugging & Profiling





Profiling in Python

- individual functions:
 - import cProfile
 - cProfile.run('some_func()', 'profile.tmp')
- whole script:
 - python -m cProfile [-o output_file] [-s sort_order] myscript.py
- Analyze profile file:
 - import pstats
 - p = pstats.Stats('profile.tmp')
 - p.strip_dirs().sort_stats(-1).print_stats()
- More info at <u>http://docs.python.org/2/library/profile.html</u>





Time embedded in code

In this example, we just have to run the script run.sh provided in the zipfile.

```
from timeit import default_timer as timer
#mathnative
start = timer() #starting the clock
N =1000000
x=range(N)
s=sum(x)
end = timer() # stopping the clock
print(end - start) , "seconds [native library]"
mav@fkopp:~/hands-on/codes/time $ ls
run.sh time0.py time1.py
mav@fkopp:~/hands-on/codes/time $ ./run.sh
comparing numpy vs native without profiler
0.0467429161072 seconds [native library]
0.00434994697571 seconds [numpy library]
mav@fkopp:~/hands-on/codes/time $
```





To measure using cprofile

The command to run the profiler is:

python -m cProfile yourcode > yourcode.txt

Here, we are writting the output in yourcode.txt. In the example presented here, we compare the Romberg integration using two ways: coding all the Romberg integration and using scipy (library). The integral to be evaluated is $\int_{0.5}^{1} tan(x) dx$.





Debugging Python

- typically very easy to do interactively with "print()" and "exit()" statements in the code
- More featureful debugger available in module "pdb", see:
 - <u>http://docs.python.org/2.7/library/pdb.html</u>





IAE



• <u>PERF wiki</u>