The Abdus Salam
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Debugging & Profiling with Open Source SW Tools

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OUTLINE

- 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

Lot of time debugging. We did learn also from it, but I have the feeling we could have learnt more things about Quantum Espresso if we hadn't had to be debugging for so long (some of the bugs we had were due to our lack of excellence in programming skills and were not specific to QE issues) (Cit. feedback from a ICTP Activity)

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 ☺
- 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

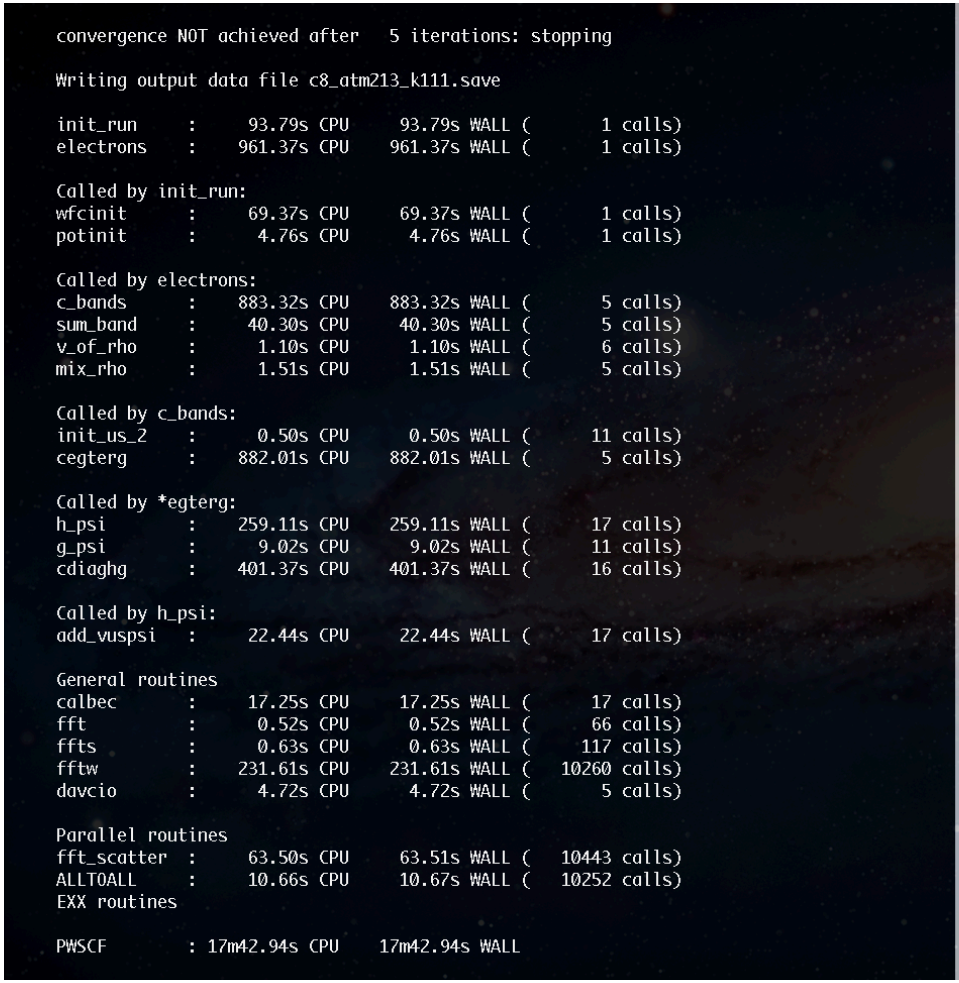
- Using different compilers (Intel, GCC, Clang, ...)
- Debuggers and debugger frontends:
  gdb (GNU compilers), **idb** (Intel compilers), **ddd** (GUI), **eclipse** (IDE), and many more...
- **gprof** (profiler) as it can generate call graphs
- **valgrind,** an instrumentation framework
  - Memcheck: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

How to Report a Bug(?) to Others

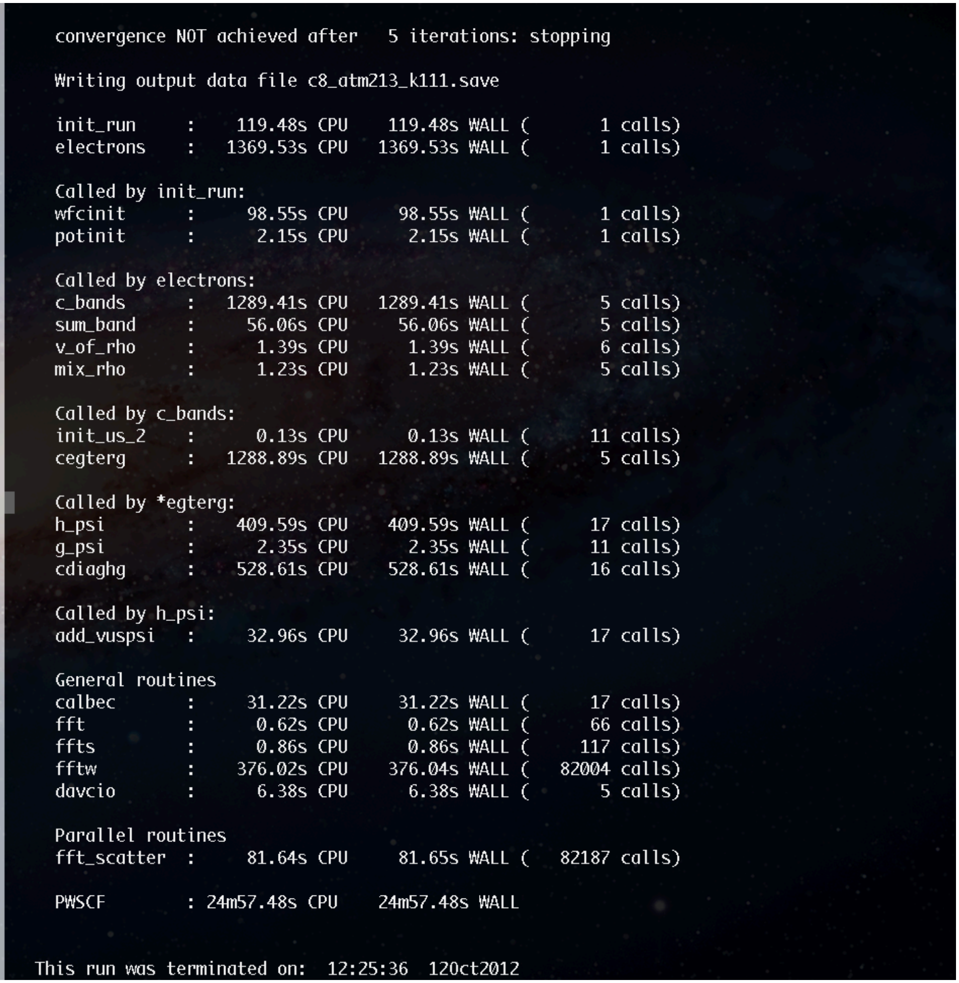
- Research whether bug is known/fixed
  - web search, mailing list archive, bugzilla
- Provide description on how to reproduce the problem. Find a minimal input to show bug.
- Always state hardware/software you are using (distribution, compilers, code version)
- Demonstrate, that you have invested effort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



```
     convergence NOT achieved after   5 iterations: stopping

     Writing output data file c8_atm213_k111.save

     init_run     :     93.79s CPU     93.79s WALL (       1 calls)
     electrons    :    961.37s CPU    961.37s WALL (       1 calls)

     Called by init_run:
     wfcinit      :     69.37s CPU     69.37s WALL (       1 calls)
     potinit      :      4.76s CPU      4.76s WALL (       1 calls)

     Called by electrons:
     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)
     mix_rho      :      1.51s CPU      1.51s WALL (       5 calls)

     Called by c_bands:
     init_us_2    :      0.50s CPU      0.50s WALL (      11 calls)
     cegterg      :    882.01s CPU    882.01s WALL (       5 calls)

     Called by *egterg:
     h_psi        :    259.11s CPU    259.11s WALL (      17 calls)
     g_psi        :      9.02s CPU      9.02s WALL (      11 calls)
     cdiaghg      :    401.37s CPU    401.37s WALL (      16 calls)

     Called by h_psi:
     add_vuspsi   :     22.44s CPU     22.44s WALL (      17 calls)

     General routines
     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       :      4.72s CPU      4.72s WALL (       5 calls)

     Parallel routines
     fft_scatter  :     63.50s CPU     63.51s WALL (   10443 calls)
     ALLTOALL     :     10.66s CPU     10.67s WALL (   10252 calls)
     EXX routines

     PWSCF        : 17m42.94s CPU    17m42.94s 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 init_run:
     wfcinit      :     98.55s CPU     98.55s WALL (       1 calls)
     potinit      :      2.15s CPU      2.15s WALL (       1 calls)

     Called by electrons:
     c_bands      :   1289.41s CPU   1289.41s WALL (       5 calls)
     sum_band     :     56.06s CPU     56.06s WALL (       5 calls)
     v_of_rho     :      1.39s CPU      1.39s WALL (       6 calls)
     mix_rho      :      1.23s CPU      1.23s WALL (       5 calls)

     Called by c_bands:
     init_us_2    :      0.13s CPU      0.13s WALL (      11 calls)
     cegterg      :   1288.89s CPU   1288.89s WALL (       5 calls)

     Called by *egterg:
     h_psi        :    409.59s CPU    409.59s WALL (      17 calls)
     g_psi        :      2.35s CPU      2.35s WALL (      11 calls)
     cdiaghg      :    528.61s CPU    528.61s WALL (      16 calls)

     Called by h_psi:
     add_vuspsi   :     32.96s CPU     32.96s WALL (      17 calls)

     General routines
     calbec       :     31.22s CPU     31.22s WALL (      17 calls)
     fft          :      0.62s CPU      0.62s WALL (      66 calls)
     ffts         :      0.86s CPU      0.86s WALL (     117 calls)
     fftw         :    376.02s CPU    376.04s WALL (   82004 calls)
     davcio       :      6.38s CPU      6.38s WALL (       5 calls)

     Parallel routines
     fft_scatter  :     81.64s CPU     81.65s WALL (   82187 calls)

     PWSCF        : 24m57.48s CPU    24m57.48s WALL


   This run was terminated on:  12:25:36  12Oct2012
```