Coding, Debugging, and Profiling

Dr. Peter Woitke

- age of ~10: first CASIO programmable calculator
- age of ~12: first computer (Spectrum ZX81): **BASIC**, **Assembler** (chess)
- ATARI ST: many things in **GFA-Basic**, including science, games, computer go (European computer go champion 2000 & 2001 with "*GoAhead*")
- LINUX: **F77** (my science) and **C**-programming (compter go "*Suzie*")
- 2003-2009: **F90 + MPI** FLASH hydrodymics + dust formation + MC RT, running on parallel super-computers
- 2009-now: **F90 + OpenMP** disc simulation software *"ProDiMo"*
  - astrochemistry, radiative transfer, heating & cooling → observations
  - ~100 users world-wide, ~5 programmers, **SVN**-based
- since 2015: various science **F90** projects, **GIT**-based, for example "*GGchem*"
  using **python** for making plots
- since 2012: AS3013 Computational Astrophysics (**F90, python**)
  AS4012 Stars and nebulae II (**Mathematica**, **python**)

Resources

- https://software.intel.com/en-us/parallel-studio-xe/choose-download/student-linux-fortran
  - **ifort** : the INTEL FORTRAN compiler
  - **idb** : the INTEL DEBUGGE
  - **vtune** : the INTEL PROFILER
- free Linux
  - **gfortran** : the GNU FORTRAN compiler
  - **gdb** : the GNU DEBUGGER (not graphical)
  - **gprof** : the GNU PROFILING Library (not graphical)
  - **gprof2dot.py**, use with **dot** binary (→ package XDot)
- from http://www-star.st-and.ac.uk/~pw31/CodeCake.tgz:
  short example programs
  - debug.f90
  - bench.f90 and bench.py

Debugging

- good for: **(1) find problems,**
  (2) better understand your code
- you need a ***reproducible problem*** (which occurs after *t* < some minutes)
- ***most frequent problems***:
  — incorrect variable declaration (rank / dimension / type)
  — incorrect argument lists (rank / dimension / type)
  — index errors
  — NaN production
  — forgotten / wrong initialisation
- use debugging ***compiler flags***:

```
gfortran: -g -O0 -fbacktrace -fcheck=all -Wall -pedantic
          -Wimplicit-interface
   ifort: -g -O0 -traceback -fpe0 -check all -warn all -fp-stack-check
          -gen-interfaces -warn interfaces
```

- try ***different compilers*** (!)
- use ***"print & stop"***
- ***graphical debuggers:*** **idb**, there is also ddd, gdbgui (both using **gdb**), ...

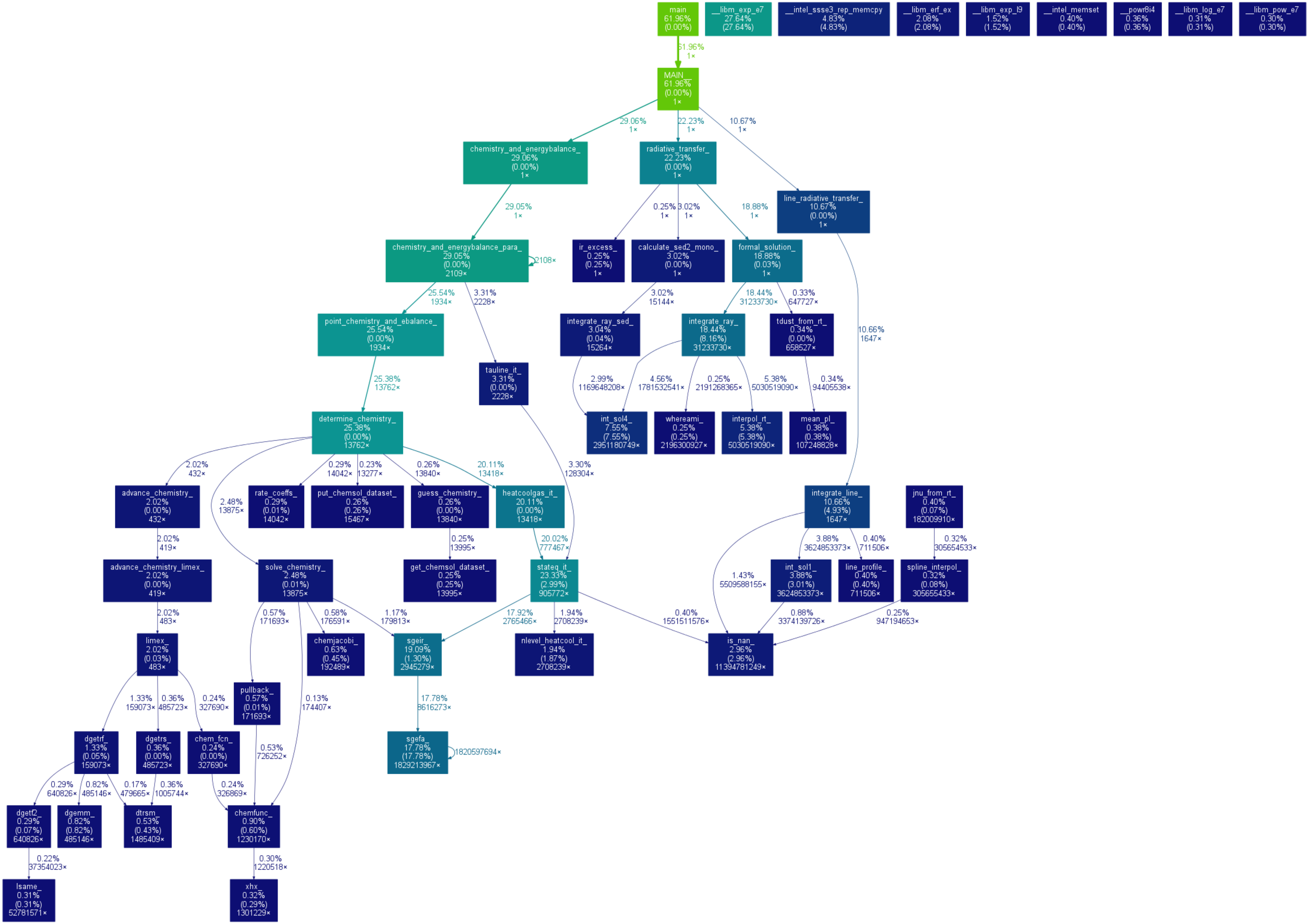
Profiling

- good for: **(1) identify the time-consuming parts of your code,**
  (2) better understand (!) and accelerate your code
- ***most frequent issues***:
  - — inefficient algorithm
  - — inefficient memory layout
  - — inefficient parallelisation
- use profiling ***compiler flags*** (for gprof):
  gfortran: -g -O0 -p
  ifort: -g -O0 -p
- try: (1) UNIX **time** command
  (2) ***self-made in code***, using **CPU_TIME**() and **SYSTEM_CLOCK**()
  (3) **gprof** myprogram → call and time statistics of subroutines/functions
  (4) **gprof** -l myprogram → call and time statistics of code lines
  (5) **gprof** myprogram | **gprof2dot.py** | **dot** -Tpng -o gprof.png
  → graphical output of (3)
- ***graphical*** profiler analysis: **vtune**
- how to improve performance?
  - — can you use ***external packages*** (LAPACK, FFTW, ODE-solver, …)?
  - — think about ***memory re-organisation***, e.g. array(fast,slow,slower)

Self-made profiling

```
implicit none
real*8 :: t0,t1,ut0,ut1
integer :: count, count_rate,count_max

call cpu_time(t0)
call SYSTEM_CLOCK(count, count_rate, count_max)
ut0 = DBLE(count)/DBLE(count_rate)
...
call cpu_time(t1)
call SYSTEM_CLOCK(count, count_rate, count_max)
ut1 = DBLE(count)/DBLE(count_rate)
print*,"total usertime[sec] = ",ut1-ut0
print*,"total CPU time[sec] = ",t1-t0
```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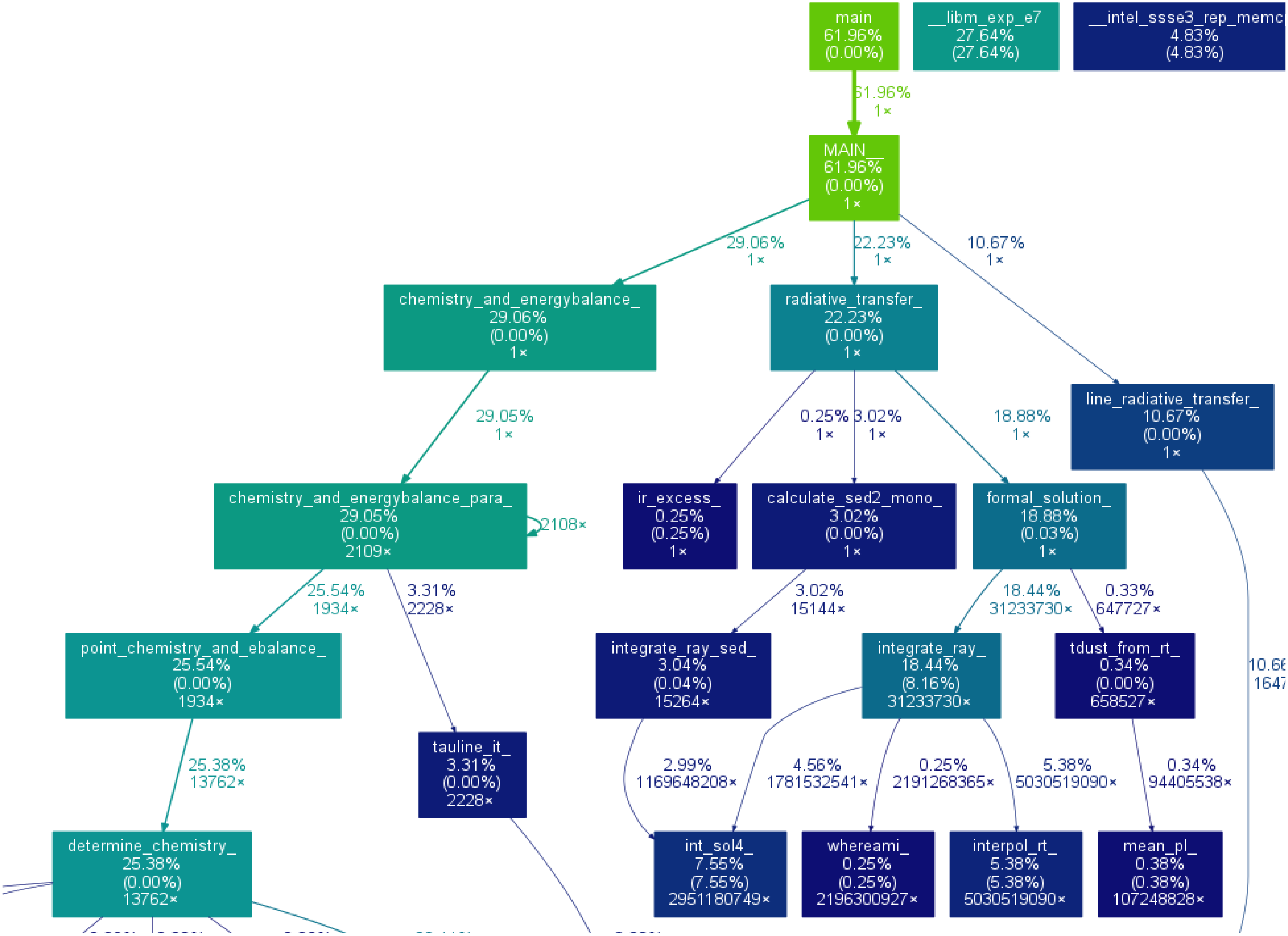
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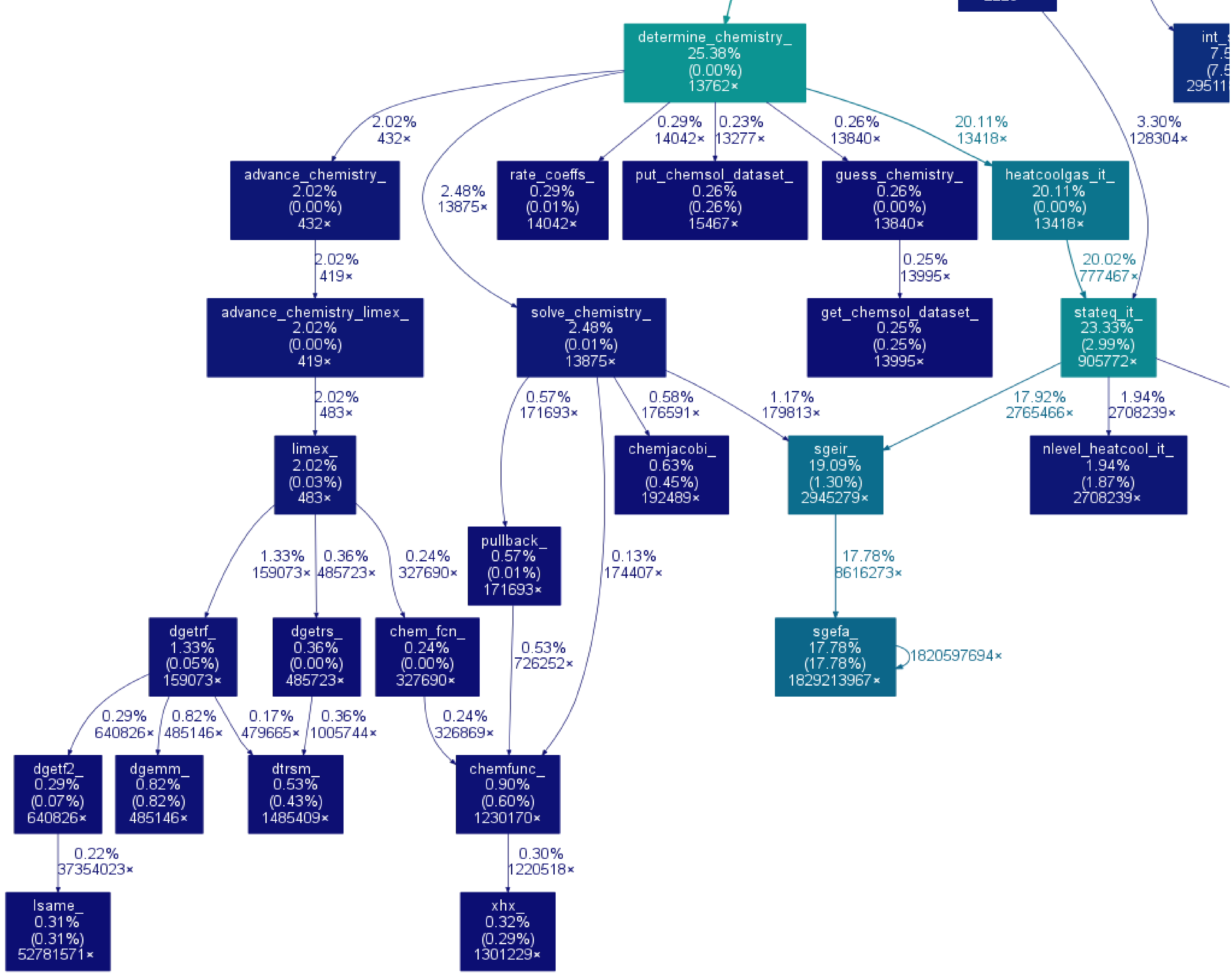
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