

Tips for the Scientific Programmer

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ors and major contributors

The result of a collaborative effort and extensively relies on the estimates rest of various organizations to spenty share and collaborate. The creat including the probability without the subgoint provided by several put representations during GBM's second eaching programme (D14 2014, No Text Seen possible without the extension support of all GBM Society aff. These key contributions are profoundly ackno professions can be found at picture presented and the mark. A m





This talk is about "Middle Performance Computing"

- profiling is invaluable for finding bottlenecks like slow operations in inner loops, but I do that 1-2 times per year
- what it is really essential is instrumenting your code
- what makes the difference is using the right library and the right architecture / data structure



Input/output formats

- I learned the hard way a very essential lesson: *never, EVER change the input formats*
- You cannot. Really, you can not.
- Even if it is impossible to get right the input format at the beginning 🙁
- There is more freedom with the output formats
- Where you can really work is on the internal formats



Inputs formats we are using

- INI (good, but TOML would have been better)
- XML/NRML/XSD (could have been simpler)
- CSV (should have been used more)
- HDF5 (in rare cases: UCERF3, GMPE tables)
- ZIP (okay)



Output formats we are using

- XML / NRML: we are removing it
- CSV with pre-header: we are using it more and more
- HDF5: used sometimes
- NPZ: by necessity



Outputs from calculation 24329

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Internal formats we are using

- .hdf5
- .toml
- .sqlite

They are good 💼



The choice of the data format has a big performance impact

- XML/CSV exporters
- XML/CSV importers
- clearly the choice of the internal formats is even more important: HDF5 is the way to go



Task distribution

- we are using *multiprocessing/zmq* on a single machine
- and *celery/rabbitmq/zmq* on a cluster



• celery/rabbitmq is not ideal for our use case but it works enough, including the REVOKE functionality







Slow tasks

- slow tasks have been a PITA for years 😕
- a few months ago we had a breakthrough: subtasks
- we made the output receiver able to recognize tuples of the form (callable, arg1, arg2, ...) and to send them as tasks



• task producing subtasks:

```
def task_splitter(sources, arg1, arg2, ...):
blocks = split_in_blocks(sources, maxweight)
for block in blocks[:-1]:
    yield (task_func, block, arg1, arg2, ...)
yield task_func(block[-1], arg1, arg2, ...)
```

- heavy tasks can be split in many light tasks
- the weight of a seismic source is the number of earthquakes it can produce
- it can be *very* different from the duration of the calculation



Calibrating the computation

- we introduced a task splitter able to perform a subset of the calculation and to estimate the expected task duration depending on the weight
- it can split the calculation in subtasks with estimated runtime smaller that an user-given task_duration parameter



Automatic task splitting

- successively, we made the engine smart enough to determine a sensible default for the task_duration, depending on the number of ruptures, sites and levels
- => slow tasks are greatly reduced
- except for non-splittable sources



Solving the data transfer issue

- we switched to using zmq to return the outputs 💼
- we switched to NFS to read the inputs (and it is also useful for sharing the code)
- **important**: do not produce too many tasks, the data transfer will kill you, or the output queue will run out of memory, or both



Memory occupation

- a big problem we had to fight constantly is running out of memory (even with 1280 GB split on 10 machines)
- notice that running out of memory *early* can be a good thing
- it is all about the tradeoff memory/speed
- NB: memory allocation can be the *dominating* factor for performance



How to reduce the required memory

- use as much as possible numpy arrays instead of Python objects
- use a site-by-site algorithm if you really must
- remember that big tasks are still better, if you have enough memory
- we measure the memory with psutil.Process(pid).memory_info()



Saving memory by yielding partial results

```
def big_task(sources, arg1, arg2, ...):
accum = []
for src in sources:
    accum.append(process(src, arg1, arg2, ...)
    if len(accum) > max_size:
        yield accum
        accum.clear() # save memory
if accum:
    yield accum
```

Lesson: a nice parallelization framework really helps



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Questions?

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