Managing task-parallel computations with jobber

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DER FORSCHUNG | DER LEHRE | DER BILDUNG

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`https://thomas.orgis.org/jobber`

teaser

- university compute cluster with very diverse user base
- many inexperienced users with serial or at most node-local parallel computations
- enabling them to fill cluster node allocations sensibly
- prerequisite: learning to phrase the set of tasks as shell script lines as universally applicable skill
- no need for details on the batch system, re-use personal setup on different sites

teaser example

- medical parameter study with statistics over generated data sets of certain size (one crucial parameter) and combinations of analysis methods
- researcher knows R and the science at hand, but not much else regarding computer use
- a bit of help to pass parameters into the existing R script from shell wrapper

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(Researcher was rather happy about that and did not hesitate to try the larger data set sizes after all.)

teaser batch script

```
#!/bin/bash
#SBATCH --job-name=someRstuff
#SBATCH --partition=std
#SBATCH --nodes=1
#SBATCH --tasks-per-node=1
#SBATCH --time=06:00:00
#SBATCH --export=NONE
. /sw/batch/init.sh

module switch env env/2020Q3-gcc-openmpi
module load R/4.0.2
module load jobber/r1254

# Simplest case. Could run multiple jobs of differing runtime
# sequentially or in parallel here (with or without srun).
jobber task.list 1

if jobber task.list more; then
  sbatch $0
fi
```

teaser job chain control

- stop execution of job chain:
  `jobber task.list stop`
- enable executon again:
  `jobber task.list start`
- make things more parallel:
  `for n in $(seq 1 $N); do sbatch batch.sh; done`
- check progress:
  `jobber task.list done failed todo`

but first ...

Why was this inevitable?

once upon a time, a physics student

- Data analysis for student lab experiments via office spreadsheet software?

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- Data analysis for student lab experiments via office spreadsheet software?
- Write Perl scripts for common computations on measurements in text files (Text::NumericData on CPAN) and for automated plotting using scriptable tools.

taking the routine out of routine

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- Working in an experimental physics group where routine measurements were routinely analysed in the same ways using recurring mouse click patterns in glorified office spreadsheet software?
- Locate the scripting mechanism in that software, but in the end ...
- ... write more of the text data scripts and configurations for analysis pipes with a GUI for the colleagues to do the routine analyses on a batch of measurements.

counting with your fingers

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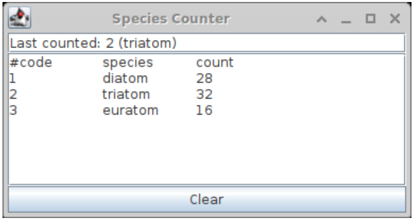
- Working alongside biologists who look at dead things through microscopes, counting different types of dead things, manually writing down counts in spreadsheets software?
- Write a trivial Java GUI that counts key presses for a massive productivity boost

counting with your fingers



```
Last counted: 2 (triatom)
#code       species     count
1           diatom      28
2           triatom     32
3           euratom     16
```

(a useful Java program, 2009 vintage)

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- Write shell-based replacement using Makefiles and a file hierarchy to handle dependencies of simulations.
  (**Bonus:** Does not crash all the time!)

a pattern

Organize things differently for fun and profit!

solving my own problems

- **simple big problem:** high-resolution simulation run that can be split into consecutive pieces on the time axis

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- parallelize with OpenMP and/or MPI, just one chain of jobs or a single big one if HPC site permits it (we rather don't;-)

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- **lots** of **little problems** amounting to a big one: a parameter study with varying resolutions and dynamics, a pile of model runs with varying runtimes
- lots of trial and error with job parameters, re-running failed computations

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- Keeping track in spreadsheets? No!
- Domain-specific, fat, hungy & fragile GUI? No!
- Got something that nicely works as a simple shell tool? Well ...

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- **xargs:** similar, good for ad-hoc parallelism

jobber features

- organize a list of tasks, posed as **lines of shell script**
- **syncronize** access while picking tasks
- record and **manage state** of each task, to know what to re-run
- **pack** multiple small/short tasks to **better fill job time slots and allocated compute resources**
- work on the same tasks in **batch system** or just a random **personal computer**, possibly going back and forth
- easy **job chains** via **generic** batch script

generic batch script

```
#!/bin/bash
#SBATCH --job-name=manytasks
# we got 16-core nodes, not shared
#SBATCH --nodes=1
#SBATCH --time=12:00:00

# cluster-specific init stuff
# maybe load some modules

# Pack  many single-processor-jobs into our time slot,
# until time runs out.
jobber --parallel=16 --time=$((11*3600)) task.list all

# Continue work in next batch job.
if jobber task.list more; then
  sbatch $0
fi
```

(pretty generic)

one way (for HPC people)

- master-worker program using OpenMP on a node
- some number of OMP threads
- `#pragma omp critical` section around a function that determines the next piece of work to do, if any
- actual work with custom code, or maybe using `system()`

another way (for HPC people)

- proper master-worker program using MPI
- central process distributing tasks
- `MPI_Recv()` and `MPI_Send()` on both sides
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Who writes real programs these days?

jobber implementation

- **no central server process** for management (serverless;-)
- safe operations on a single database **file with POSIX rename semantics**, also on network file systems
- **flush and sync**, see Stewart Smith: „Eat My Data - How everybody gets file I/O wrong“ (`https://www.slideshare.net/nan1nan1/eat-my-data`, `https://www.youtube.com/watch?v=LMe7hf2G1po`)
- behaves **like a database** with server backend, but still just **plain files** for data and control
- limitation: transaction rate low, but no issue for sensible tasks needing **more than a few seconds** each

one thing left to do

```
#!/bin.sh
LANG=C; set -ex

test -e jobber ||
wget https://thomas.orgis.org/jobber/jobber

test -e jobber.sig ||
wget https://thomas.orgis.org/jobber/jobber.sig

#gpg --search-key thomas@orgis.org
gpg --verify jobber.sig

chmod +x jobber
mkdir -p man1
./jobber -h=-100 | pod2man > man1/jobber.1
./jobber -h=-100 | pod2text > jobber.txt
```