Native distributed and MPI parallelism in the high-level language Julia for quantum Monte Carlo

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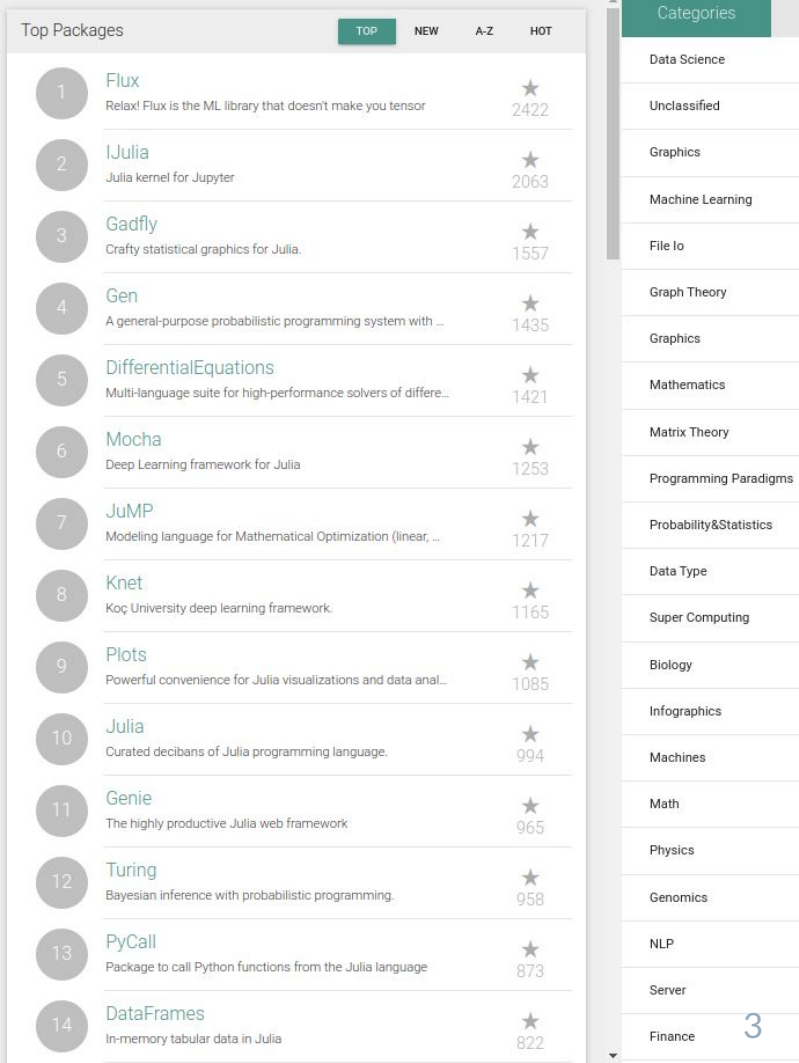
Outline

1. Julia on HPC
2. Paradigms of parallelism
3. Monte Carlo algorithm
4. Profiling the parallel Julia code on NeSI (NeSI consultancy project)

julia: the high level programming language

Key features:

- It's new: released in 2012; v1.0 in 2018
- High level language: fewer lines of code
- High performance: just-in-time (JIT) compiler
- 4225 (today) packages available in Julia =>
- Rapidly growing community
- Open source (it is free!)
- **Designed for parallel computing**



Parallel computing with julia

Options:

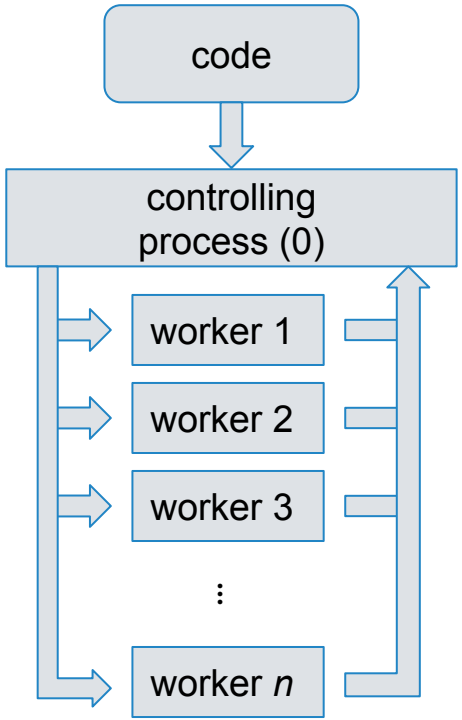
- **Distributed Computing (built-in with Distributed.jl, Julia standard library)**
  (distributed memory, works across nodes)

- Multi-Threading (built-in with @threads macro, available in Julia v1.3 or higher)
  (shared memory, works only within a single node)

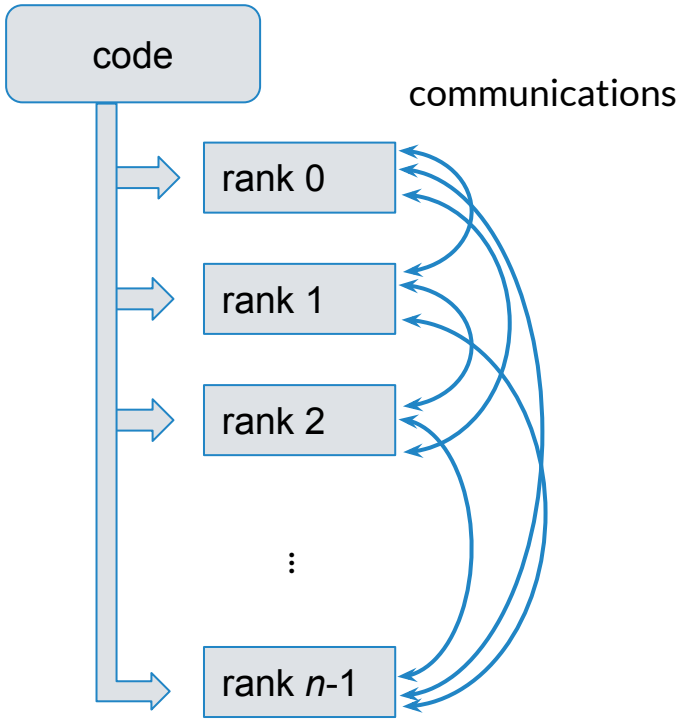
- **Message Passing Interface (with MPI.jl wrapper of external C MPI library)**
  (distributed memory, works across nodes with fast hardware communication)

Paradigms: Distributed vs MPI (for n processors)

Distributed.jl (built-in Julia package):



MPI.jl (with external MPI library):



Running Julia on HPC

- Julia is available as a module on NeSI's Mahuika & Maui, alternatively you can use the binary version

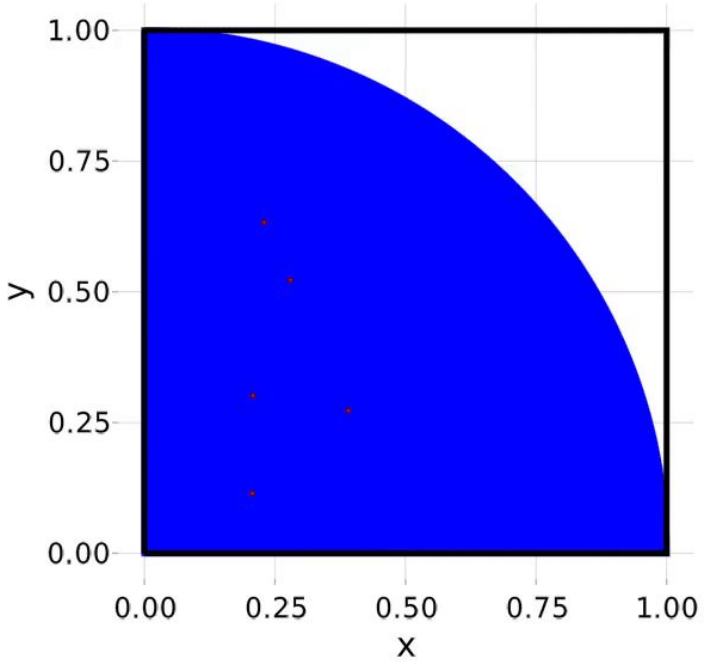
- For Distributed, use `--ntasks=1` and `--cpus-per-task=n` for slurm, and use `julia -p n <your_julia_code>.jl` to run your code

- For MPI, use `--ntasks=n` and `--cpus-per-task=1` in slurm, and use `srun julia <your_julia_code>.jl` to run your code

  A MPI module may also need to be loaded depends on the Julia build

Monte Carlo methods

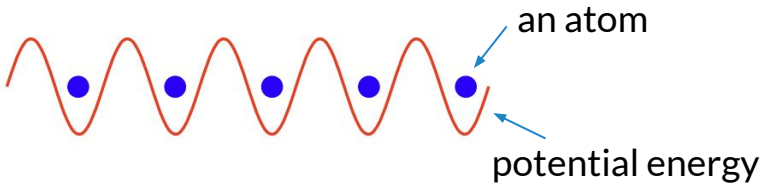
Estimating the value of π with random numbers:



$$\text{value of } \pi = 4\frac{(\text{area the } \blacktriangle)}{(\text{area the } \square)} \approx 4\frac{(\#\text{ of dots inside the } \blacktriangle)}{(\text{total } \#\text{ of dots})}$$

Monte Carlo sampling becomes very efficient for high-dimensional problems

Ultracold atom physics: experimentalists "put" particles into washboard-like potential:



The wave function:

$$\Psi = \sum_i c_i |D_i\rangle$$

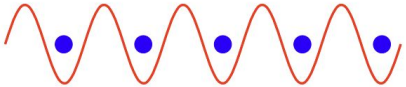
a coefficient

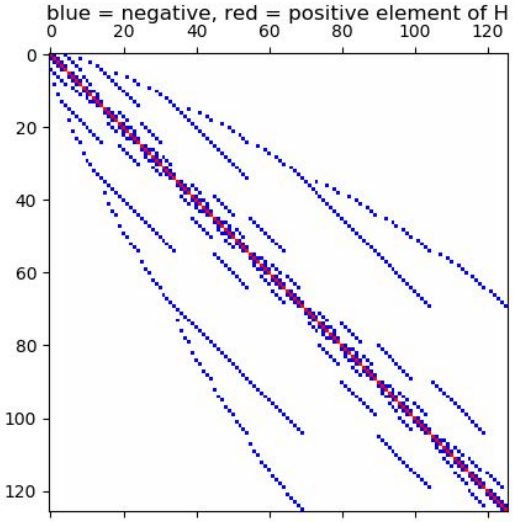
a configuration

Monte Carlo methods

Solve it as a (sparse) matrix eigenvalue problem

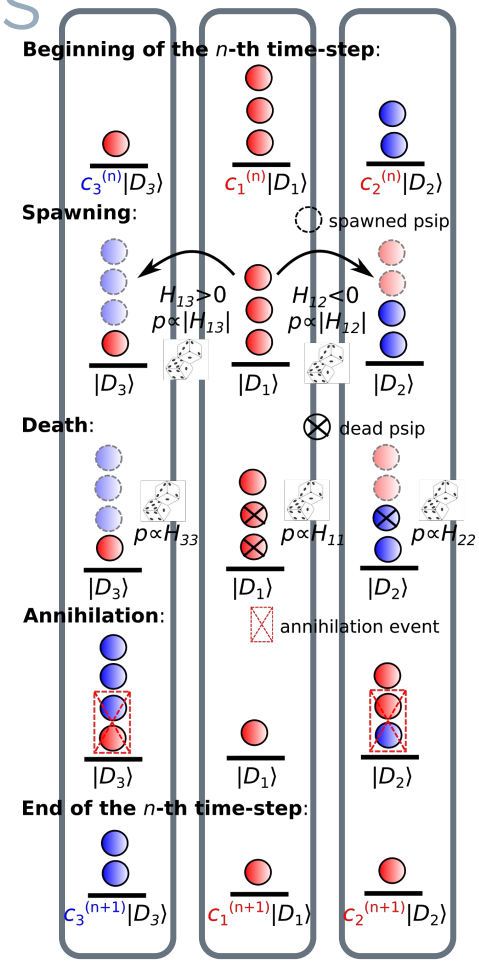
Schrödinger equation $\mathbf{H}\Psi = E\Psi$





Matrix dimension can get very large >> 10^{100} !!!

Full Configuration Interaction quantum Monte Carlo (FCIQMC) walker dynamics:



The wave function:

$$\Psi = \sum_i c_i |D_i\rangle$$

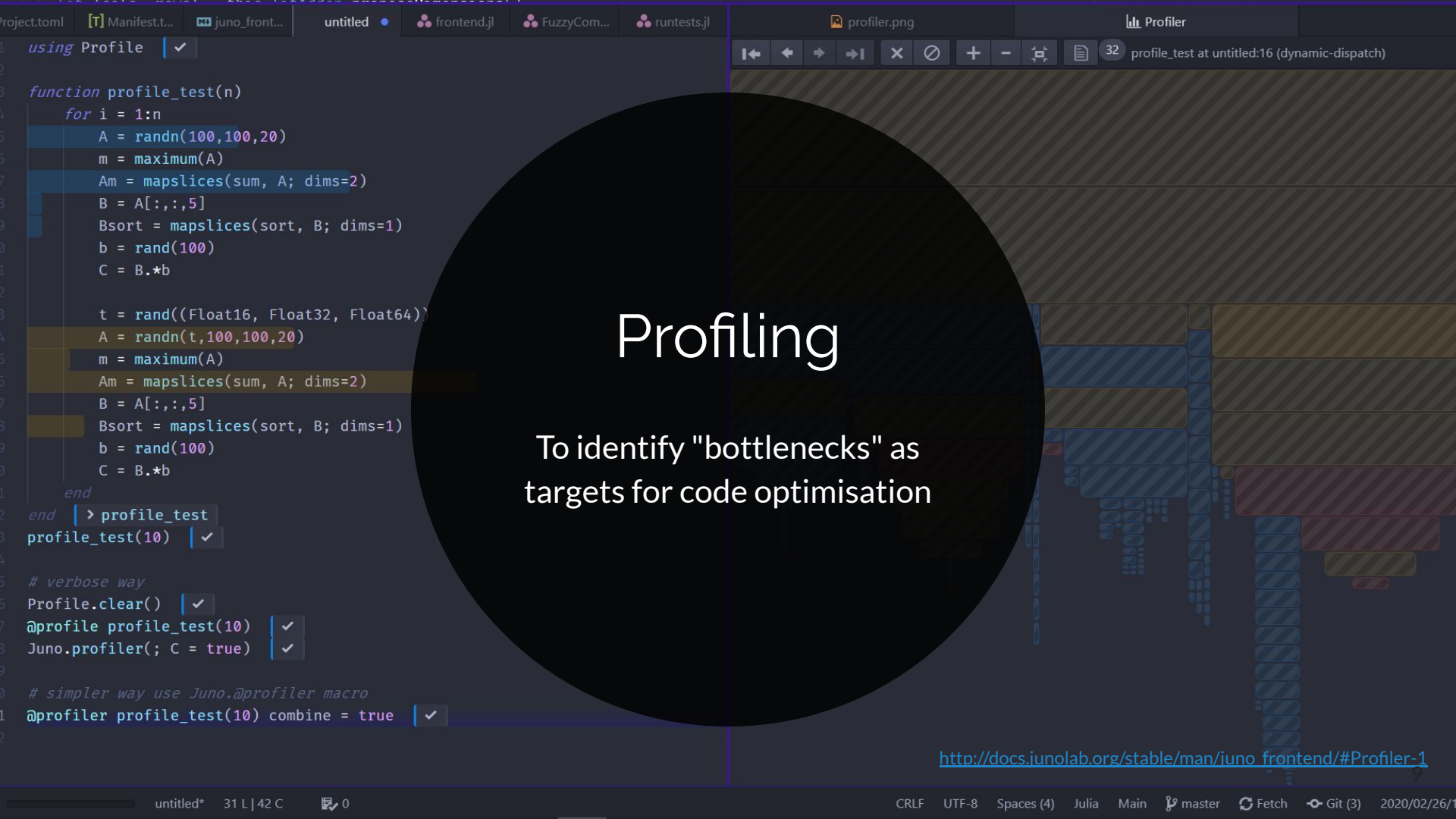
an integer

a bit "address" 01011011100...

Typically 10^6 to 10^9 walkers are used

Need parallelism and HPC!

$\|D_i\rangle$	: configuration
c_i	: coefficient
●	: (+ve) walker
●	: (-ve) walker


Project.toml
Manifest.t...
juno_front...
untitled
frontend.jl
FuzzyCom...
runtests.jl
using Profile
function profile_test(n)
for i = 1:n
A = randn(100,100,20)
m = maximum(A)
Am = mapslices(sum, A; dims=2)
B = A[:,:,5]
Bsort = mapslices(sort, B; dims=1)
b = rand(100)
C = B.*b
t = rand((Float16, Float32, Float64))
A = randn(t,100,100,20)
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B = A[:,:,5]
Bsort = mapslices(sort, B; dims=1)
b = rand(100)
C = B.*b
end
end
profile_test
profile_test(10)
# verbose way
Profile.clear()
@profile profile_test(10)
Juno.profiler(; C = true)
# simpler way use Juno.@profiler macro
@profiler profile_test(10) combine = true
profiler.png
Profiler
32
profile_test at untitled:16 (dynamic-dispatch)
Profiling
To identify "bottlenecks" as targets for code optimisation
http://docs.junolab.org/stable/man/juno_frontend/#Profiler-1
untitled*
31 L | 42 C
0
CRLF
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Spaces (4)
Julia
Main
master
Fetch
Git (3)
2020/02/26/1

Project.toml | Manifest.t... | juno_front... | untitled | frontend.jl | FuzzyCom... | runtests.jl

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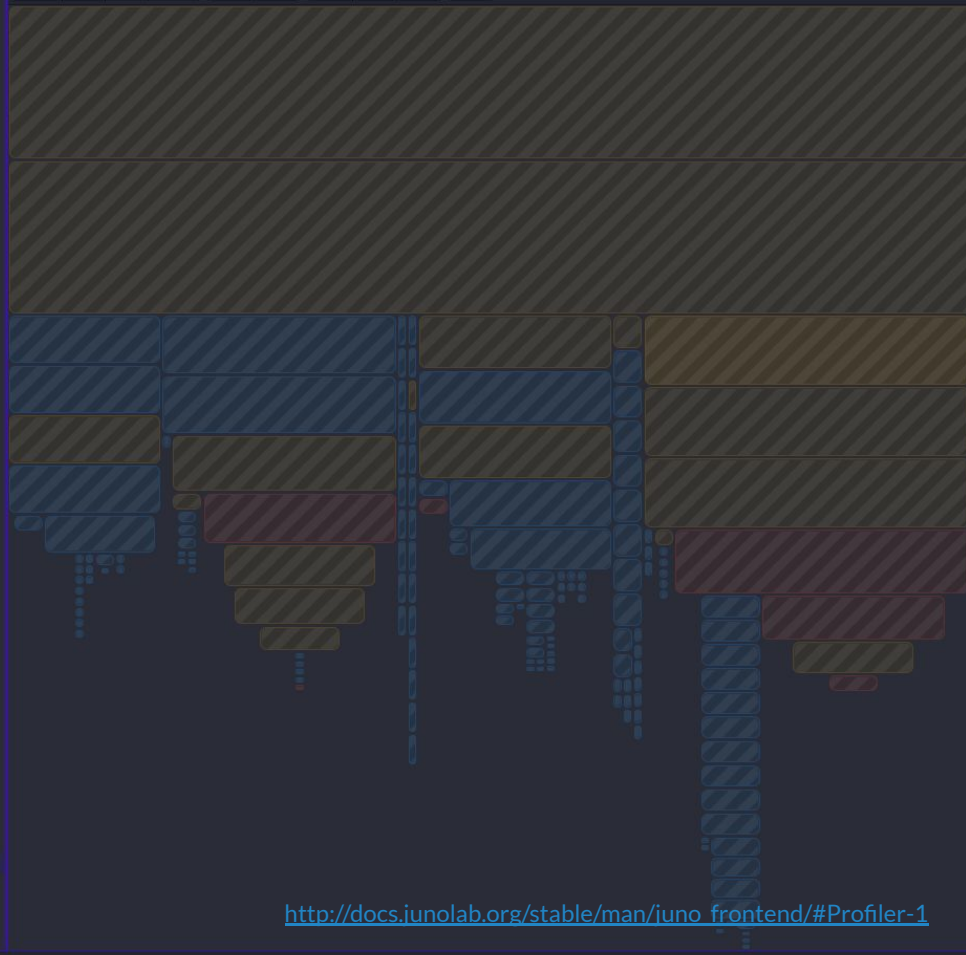
profiler.png | Profiler

32 profile_test at untitled:16 (dynamic-dispatch)



http://docs.junolab.org/stable/man/juno_frontend/#Profiler-1

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Profiling parallel Julia code (NeSI consultancy project)

With Chris Scott, Alexander Pletzer and Wolfgang Hayek

Challenges:

- Julia is new - limited guidance
- Some commercial tools do not support Julia yet
- Combined with parallelisation makes it harder for Julia native profiler
- Collect and visualise data on HPC (NeSI)

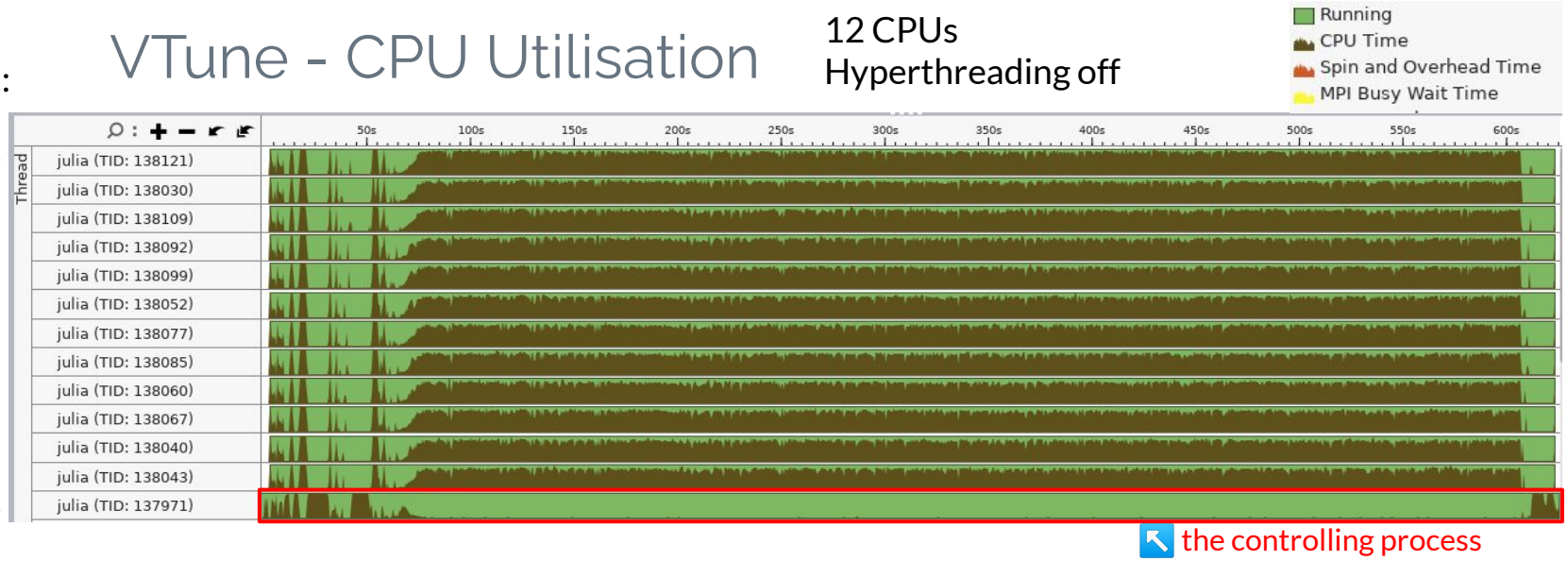
Outcomes:

- Slurm profiling - limited insight
- Intel® VTune™ Profiler works well for Julia with parallelism
- VTune's GUI is informative and fairly easy to navigate
- Need a special build for Julia to use VTune (won't work with binary version) - available now (v1.2; v1.4)

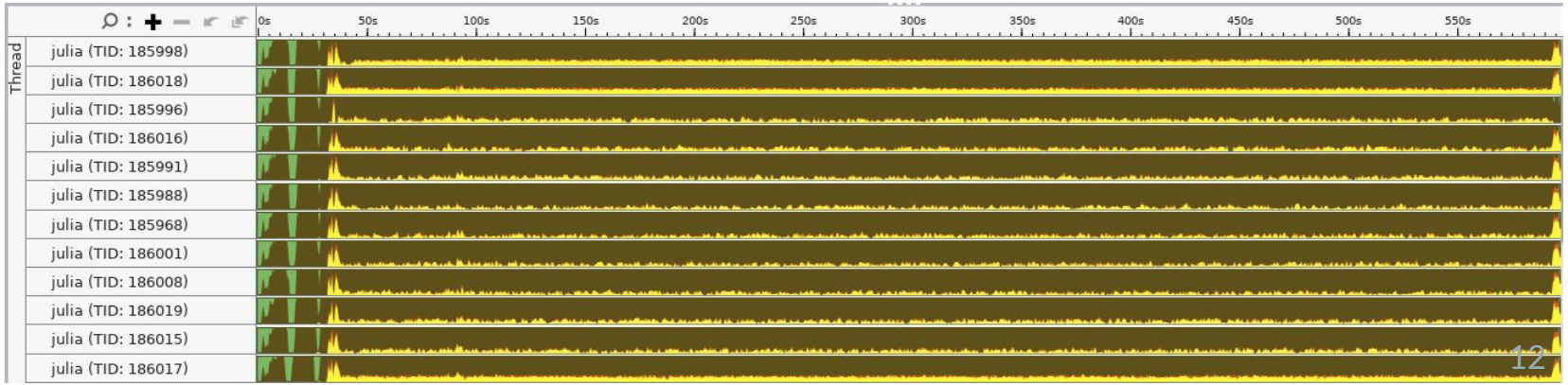
VTune - CPU Utilisation

Distributed.jl :

12 CPUs
Hyperthreading off



MPI.jl :



What's learned

Distributed:

- Small scale computation (small number of walkers)
- Single node (slower across nodes)
- Good for serial file IO
- Pure Julia code and no hardware dependency

MPI:

- Large scale (large number of walker with balanced load)
- Multiple nodes (fast InfiniBand interconnection)
- File IO in parallel (HDF5)
- Coding: more low-level thinking required

Profiling + NeSI consultancy:

- Optimised code (20x faster)
- *https://github.com/joachimbrand/Rimu.jl*
- *https://www.nesi.org.nz/services/consultancy*

Summary

- Julia is modern and powerful
- Multiple parallelisms available
- Many new things to explore
- NeSI consultancy is very helpful

Acknowledgement

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Chris Scott, Alexander Pletzer and Wolfgang Hayek

Thank you!