Supercomputing with R part 2

Agent-based model of all neighbourhoods in the Netherlands

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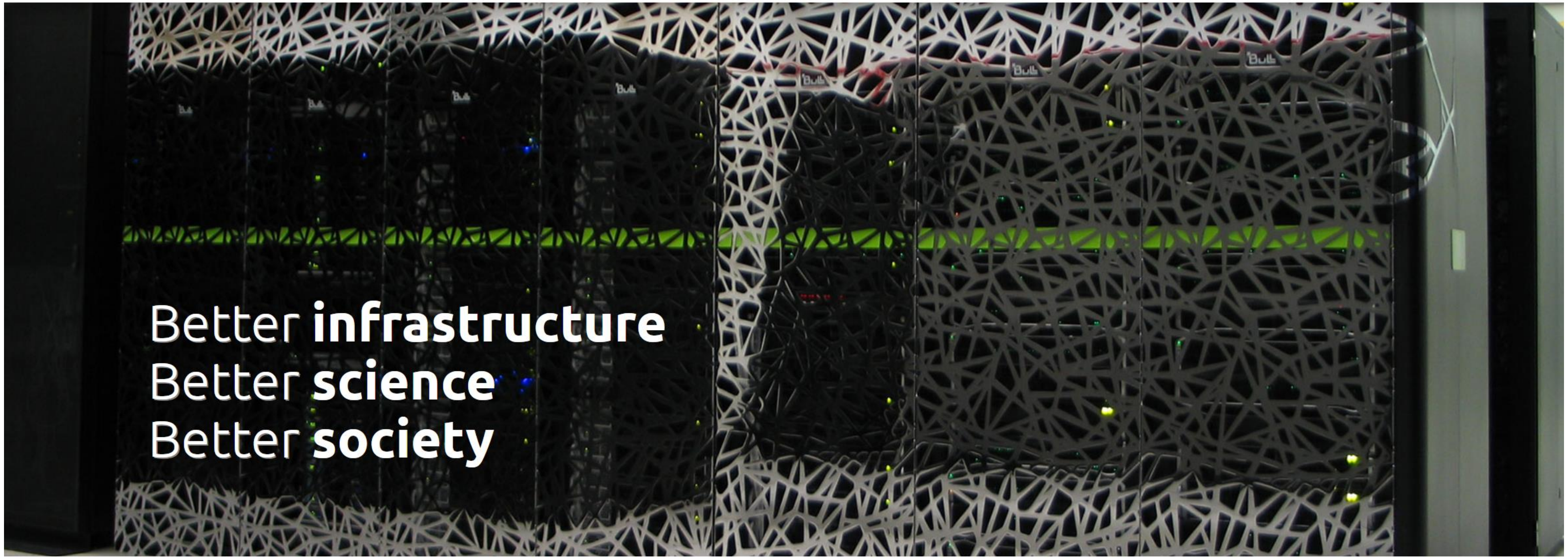
About me

Background

- PhD in **Statistics** (UU)
  Structural Equation Models, high-dimensional data, regularization & penalization, algorithms & optimization
- Assistant professor at **Methodology & Statistics**, UU
  Human Data Science group, teaching Data Science master courses
- Team lead for the **ODISSEI Social Data Science (SoDa) team**
  Advancing data- & computation-intensive research in social science



Using the ODISSEI Secure Supercomputer

In the ODISSEI Secure Supercomputer (OSSC), researchers can perform analyses of highly-sensitive data – such as CBS Microdata – in SURF's high performance computing environment Cartesius. The ODISSEI Secure Supercomputer (OSSC) consists of an enclave of Statistics Netherlands within the domain of SURF. This virtual IT environment offers a high performance computing environment that meets the requirements of Statistics Netherlands in legal, technical and security requirements.

About me

Relevant experience

- Experience with **parallel programming, supercomputing, large simulations**
  statistics, social sciences, a bit of neuroscience (structural MRI), and a bit of bioinformatics (microarrays, epigenetics)
- Native in **R**, capable in **Python**
  dabbled in C++, C#, web languages, Julia, and more
- Many research **consultations**
- Strongly advocating for **open science**
  Make everything available all the time!
- **Almost no experience with agent-based models!!!**

About you

Write down in one short sentence why you are here / what you hope to learn

This afternoon

How to structure R projects for running analyses on a SURF supercomputer

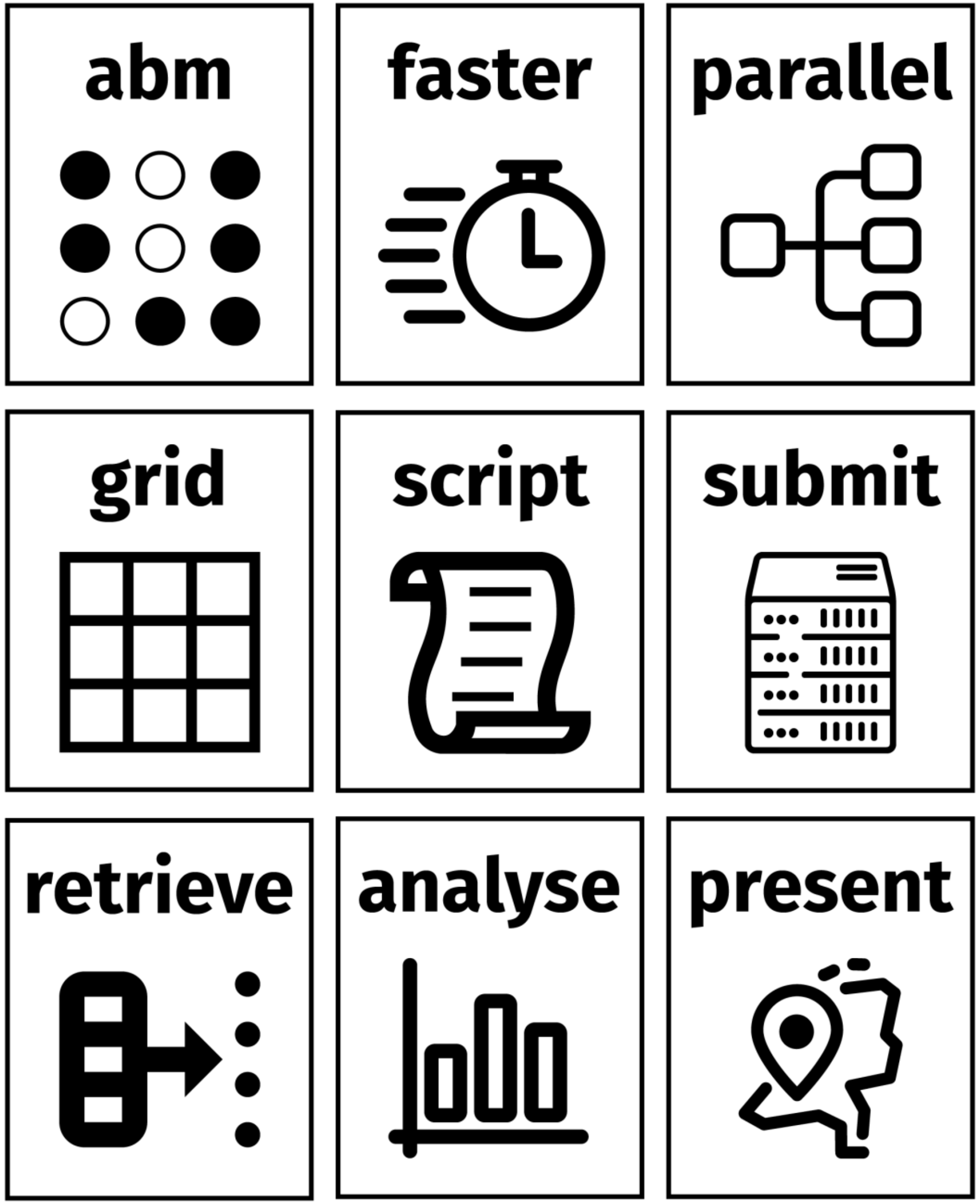
This afternoon

Time	Title
13:00	Lecture: computational limits in social science
13:45	Hands-on: a parallel agent-based model in R
14:30	Break
14:45	Lecture: supercomputing with R
15:30	Hands-on: submitting an R array job
16:00	Break
16:15	Lecture: combining & analysing the results
16:30	Conclusion & Q&A

Hands-on 1

Hands-on 2

Lecture 3



Computational limits in social science

Experimental research in soc. sci.

- Come up with research question
- Design experiment
- Run experiment
- Analyze results (perform statistical test)
- Make inferences about found effect

Observational research in soc. sci.

- Come up with research question
- Collect data
- Create statistical model
- Make inferences about model (pay attention to assumptions)

Computational research in soc. sci.?

- Come up with research question
- Create generative / computational model
- Generate data from computational model
- (compare computational model data with real data)
- Make conclusions about computational model (pay attention to assumptions)

Psych trend: theory construction

*A **formal model** captures the principles of the explanatory theory in a set of equations or rules (as **implemented in a computer program or simulation**).*

*The theorist can then examine whether the theory, as implemented in the formal model, does in fact **generate the phenomena** as a matter of course, either **in a simulation** study or through analytic derivations.*

Borsboom et al. (2021), *Theory Construction Methodology: A Practical Framework for Building Theories in Psychology* doi.org/10.1177/1745691620969647

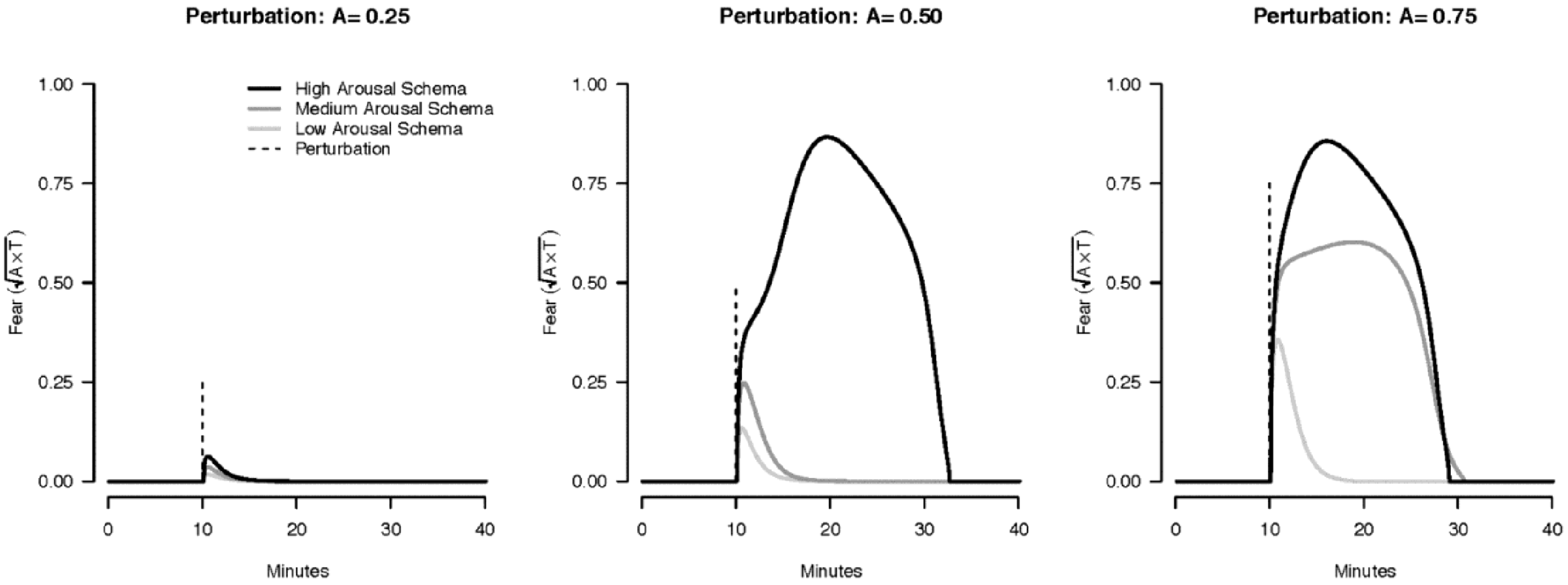
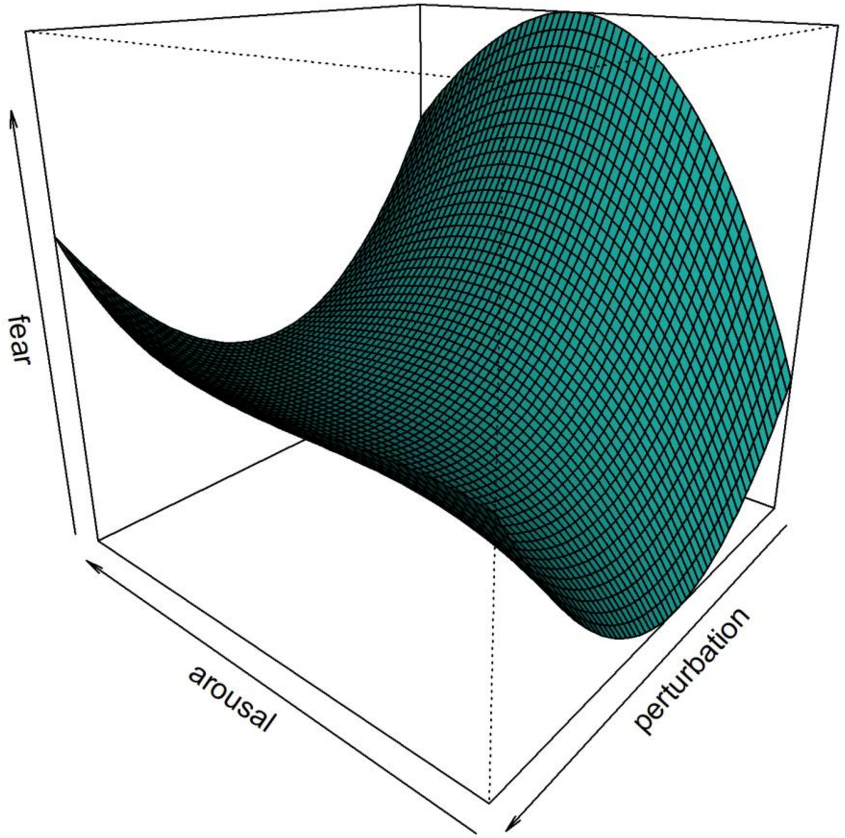


Figure 4. Individual Differences in Vulnerability to Panic Attacks. We simulated perturbations to arousal of varying strength (inducing arousal of .25, .50, and .75) in three conditions: low, medium, and high arousal schema (*S*=.25, .50, and .75, respectively). To

Robinaugh et al. (2019), A Computational Model of Panic Disorder 10.31234/osf.io/km37w

With more parameter settings?



(this is not real, just for illustration)

Agent-based models

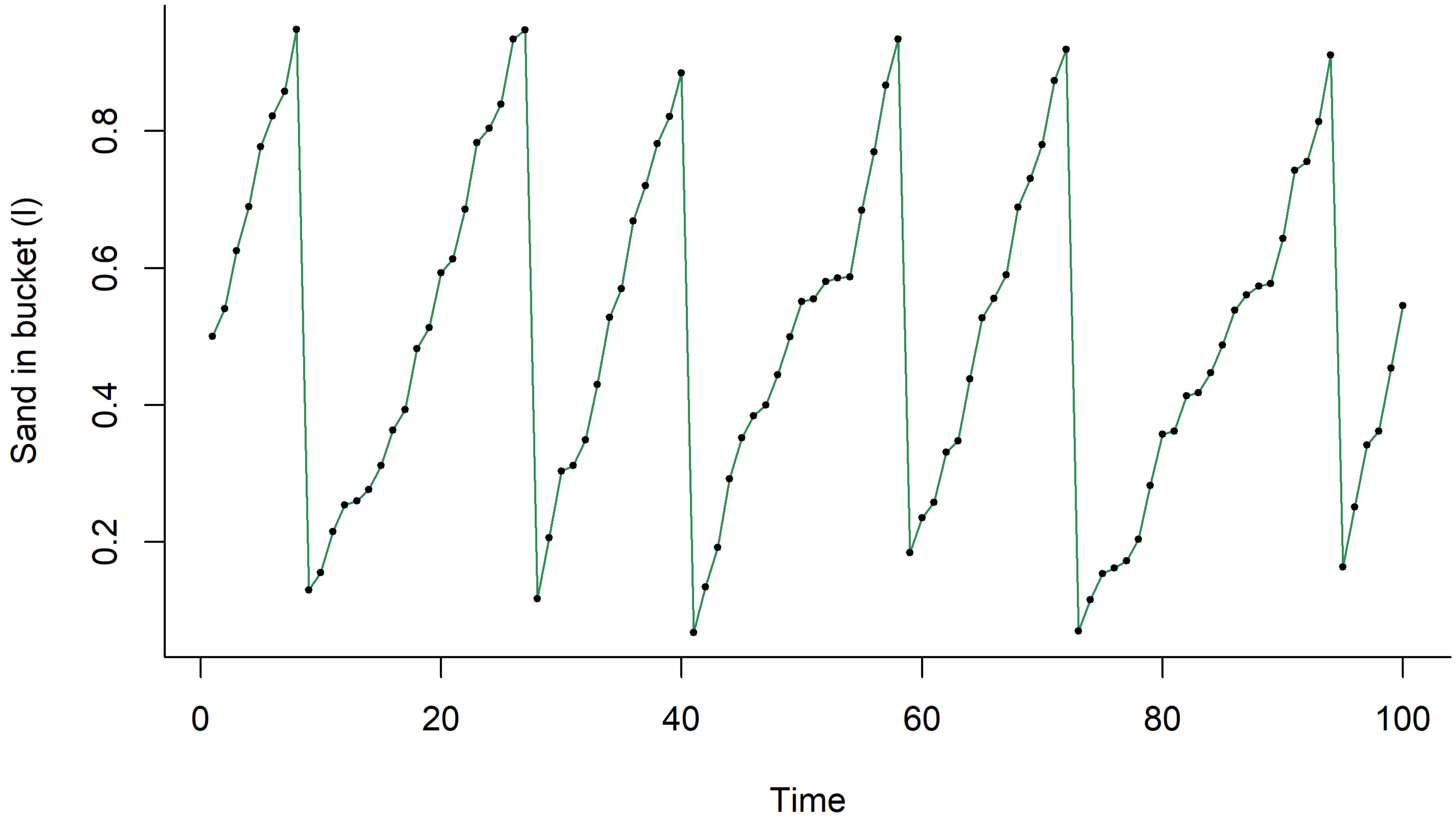
- Used in economics, sociology, ecology, finance, spatial planning, social psychology, and more
- Create **agents** who interact in an **environment**
- Each agent has **rules** based on theory
- Simulating the system means applying these rules repeatedly
- Then you can investigate the system

Agent-based models

Agent-based models

```
child_a ← function(sand) sand + runif(1, 0, 0.1)
child_b ← function(sand) if (sand > 0.95) runif(1, 0.05, 0.2) else sand

sand_vec ← numeric(100)
sand_vec[1] ← 0.5
for (i in 2:100) {
  sand_vec[i] ← child_a(sand_vec[i-1])
  sand_vec[i] ← child_b(sand_vec[i])
}
plot(sand_vec, type = "l")
```

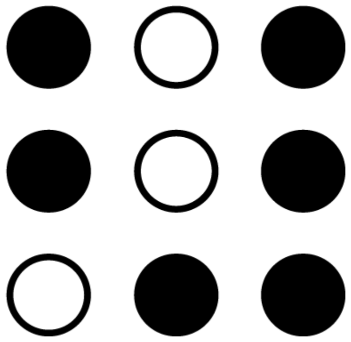
Agent-based models



Interim conclusion

1. Computational methods used by social scientists to formalize & investigate theories
2. Simulation from computational models to inspect phenomena following from model
3. Do this for different parameter settings
4. (2) and (3) may take a long time -> computational limits reached!

abm



Schelling’s model of segregation

Schelling segregation model

- Famous example of ABM in social behaviour

- What are the causes of de facto segregation in society?
- Theoretical / formal model of population dynamics
- Implemented as an agent-based model
- Conclusions drawn based on phenomena resulting from this model

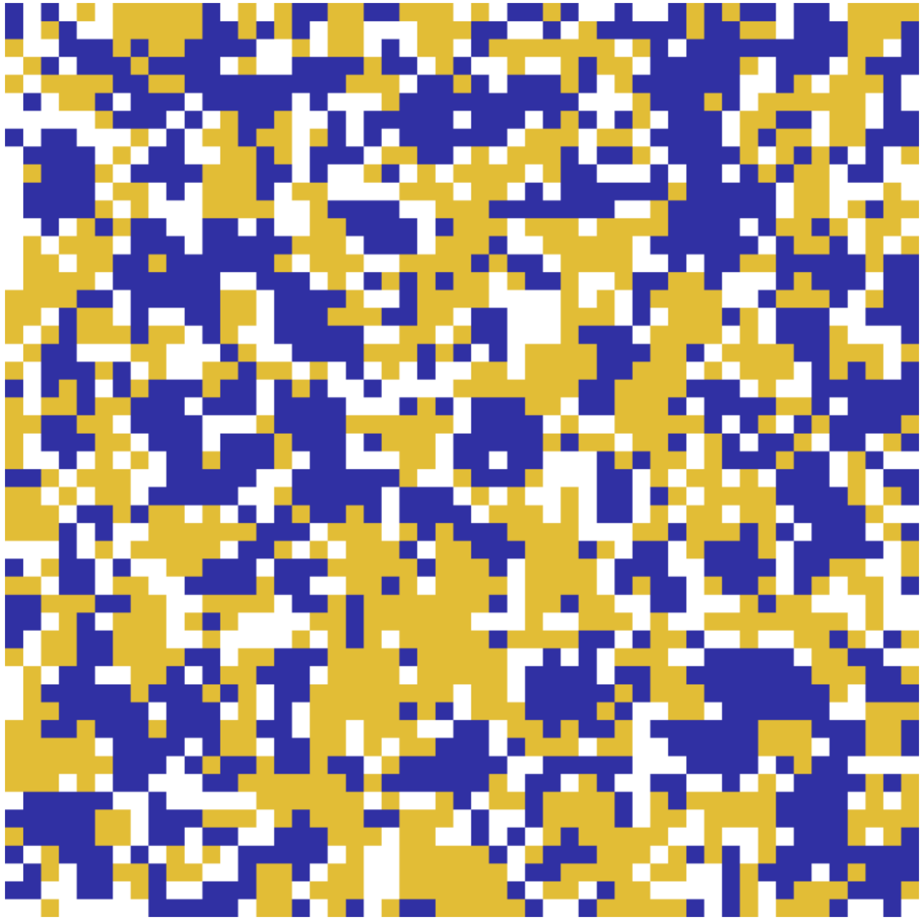
Schelling segregation model

- Environment: two-dimensional grid
- Agents belong to one of two groups
- Agents want to live close to others like themselves
  - Agents have preference ($\boldsymbol{B_a}$) for the proportion of neighbours like them ($\boldsymbol{B}$)
- If B < B_a, then move to random free location on grid
- Else stay

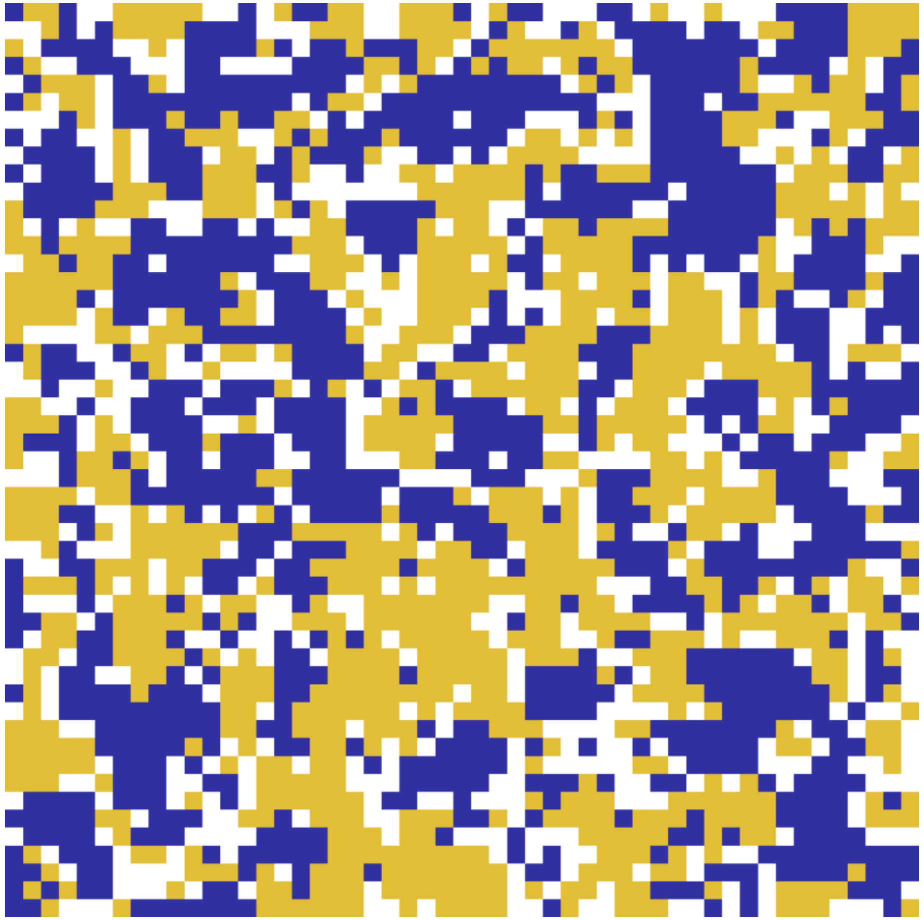
Schelling segregation model

```r
# in-group preference
Ba ← 0.5

# initialize population
pop ← init_population(c(0.5, 0.5))

# occupation matrix
M ← matrix(data = pop, nrow = N)

# happiness matrix
H ← matrix(data = FALSE, nrow = N, ncol = N)

# run for 50 iterations
for (i in 1:50) {
  H ← compute_happiness(M, Ba)
  M ← move_agents(M, H)
}
```

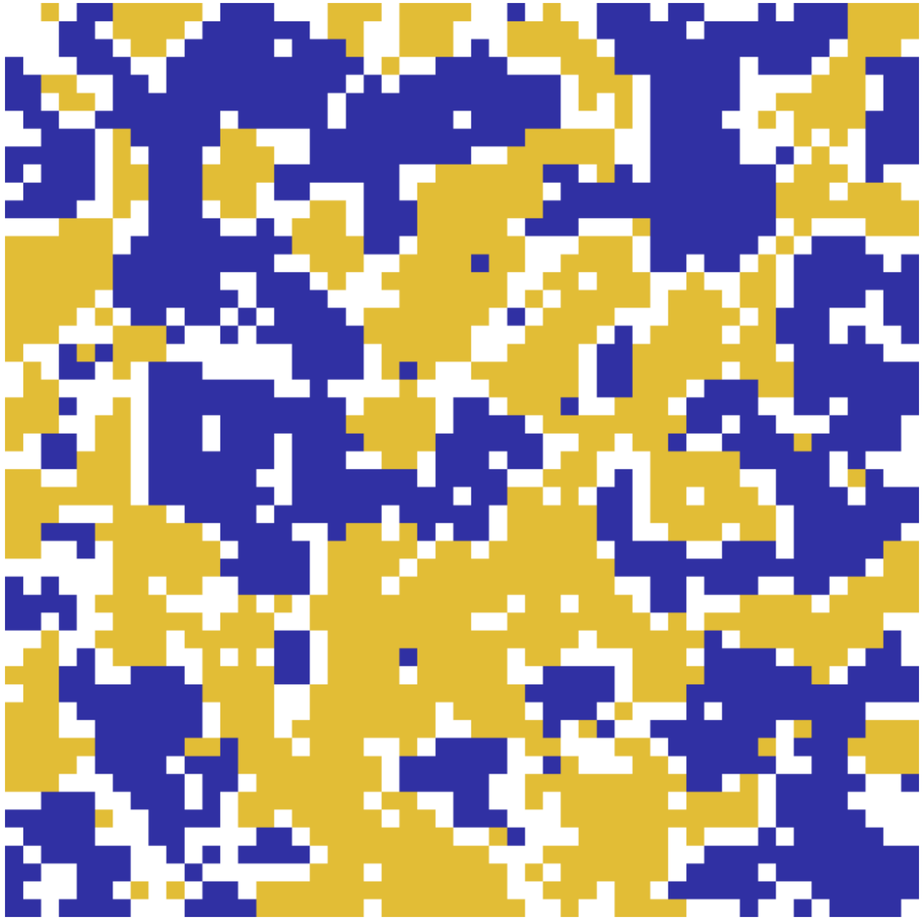
Schelling segregation model



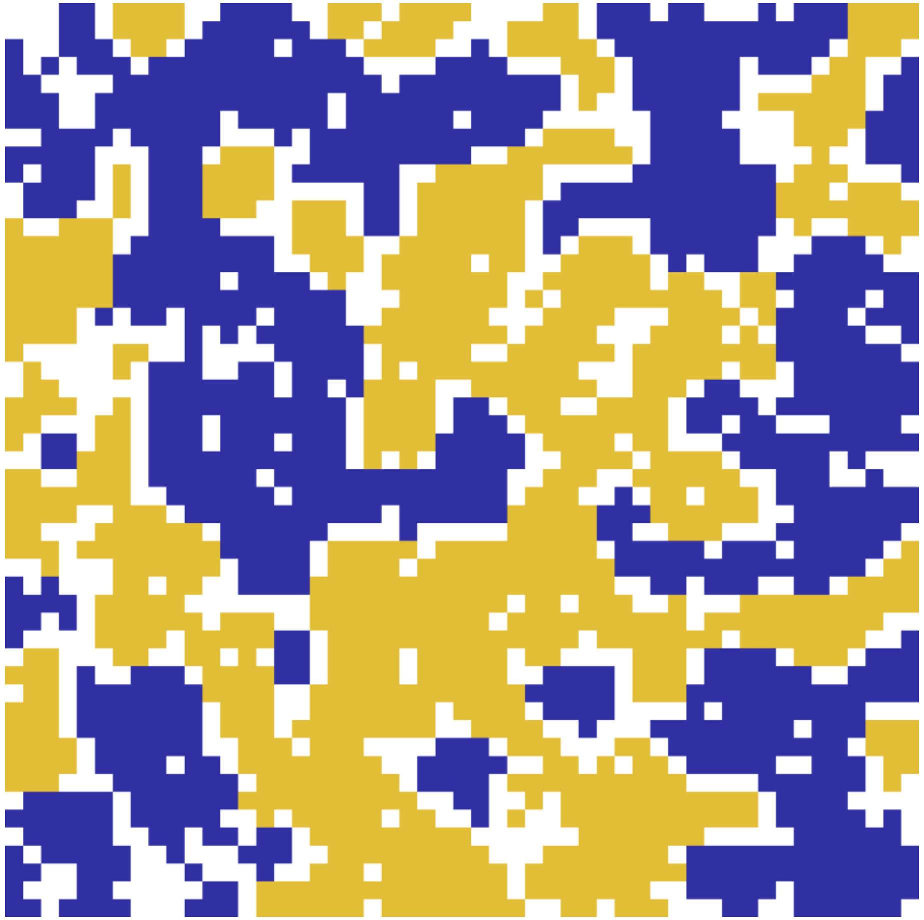
Schelling segregation model



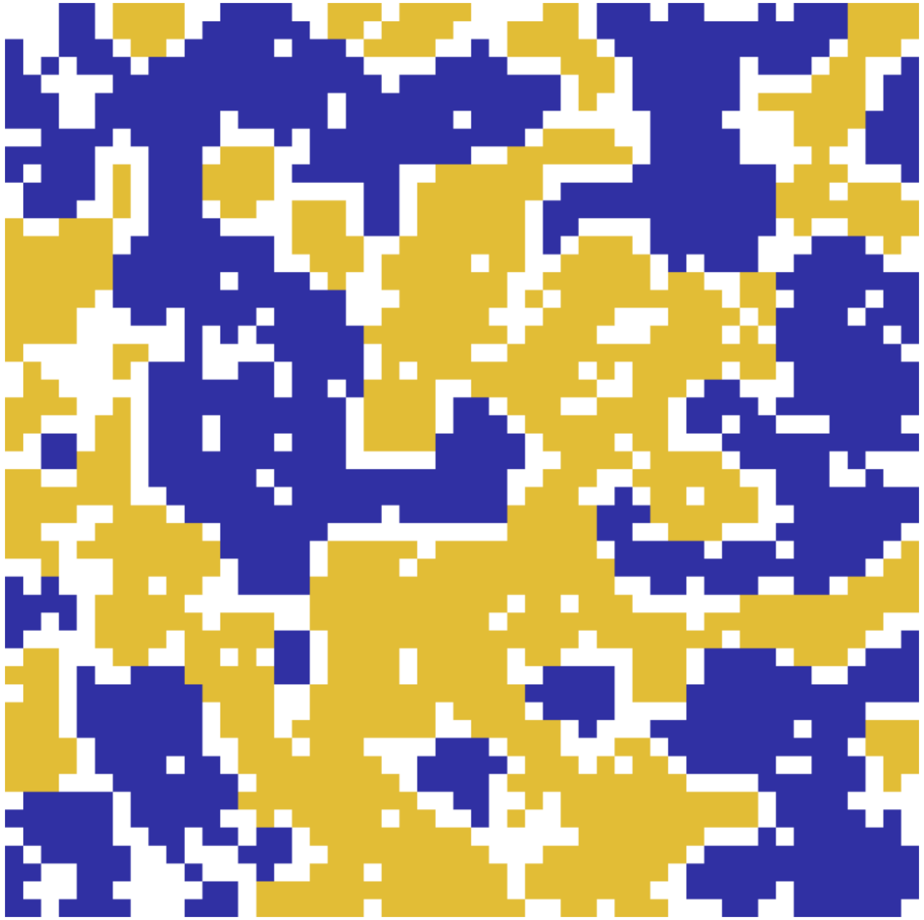
Schelling segregation model



Schelling segregation model



Schelling segregation model



Schelling segregation model

- Micro behaviour: happy or unhappy with current location -> move or stay
- Macro phenomenon: how does the distribution of agents over the grid look?

Schelling segregation model

- Schelling's finding: for groups of equal size with $B_a \gtrsim 0.33$, the system is likely to end in a **segregated** state
- Below that, the system will stay in a **mixed** / random state

Conclusion

Even if there is only a mild in-group preference, the world might still end up very segregated!

(keep assumptions in mind ☺)

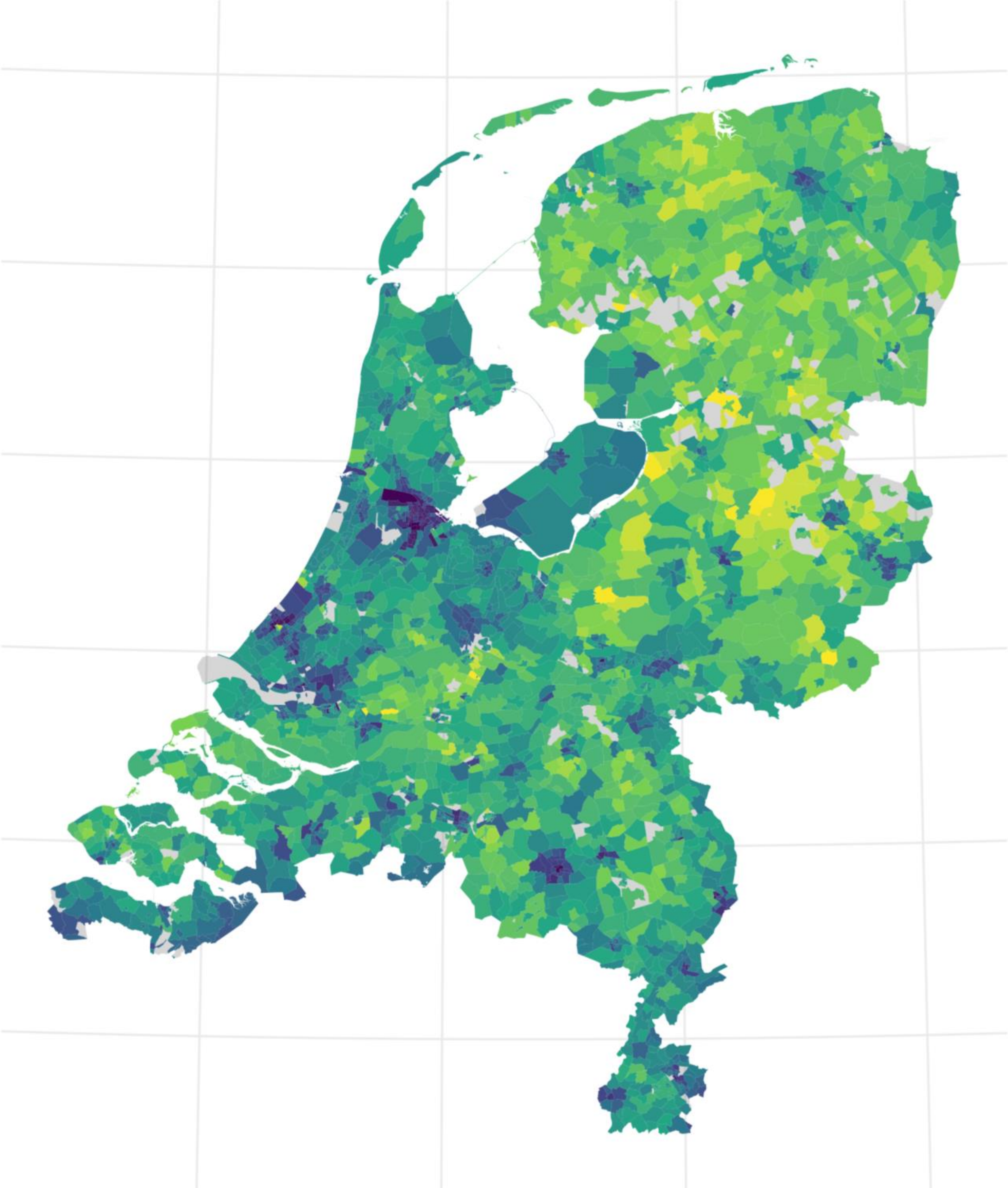
Schelling segregation model

- Note: **randomness** in initialization & in movement to different locations
- At which B_a will the system segregate?
- Need to run this model many times for different B_a and compute expectation (average over the iterations)
- Monte carlo **simulation**

Schelling segregation model

Some more parameters you may want to vary:

- Number of distinct populations
- Relative population sizes
- Number of free spots in the grid
- Neighbour preference
- Radius for looking at neighbours
- Other extensions...

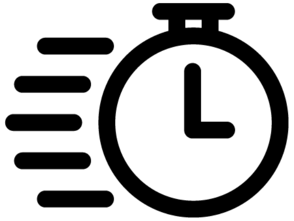


This will take a long time

Speeding up the ABM

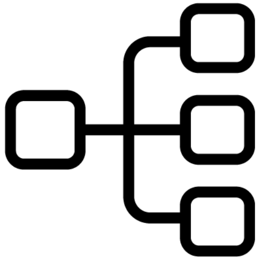
Two options

faster



Write faster, optimized code

parallel



Run multiple ABMs at the same time

Two options

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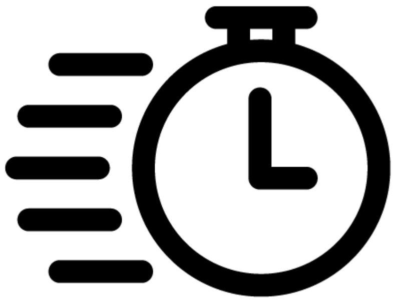


Speeding up slow code

- There isn't one solution for all types of code
- Speeding up slow code takes time
- Investigate smarter algorithms for your problem!
- If you are rewriting your R code, use vectorized & matrix operations where possible (faster than loops!)
- Use benchmarking to check the speed & memory usage of your functions (I like `bench::mark()`)

Speeding up slow code

- Another step: rewrite in C++
- Depending on problem, this may yield great speedup

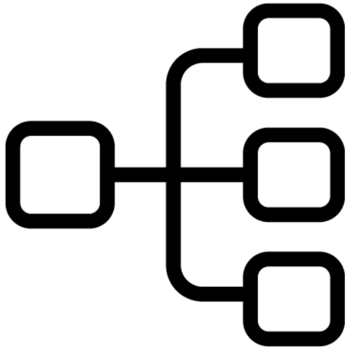
- In R: **Rcpp** package helps with this

```
sourceCpp("my_cpp_function.cpp")
```

An example of Rcpp speedup is in the hands-on later

```
# A tibble: 2 x 13
  expression      min  median `itr/sec` mem_alloc `gc/sec` n_itr  n_gc total_time result
  <bch:expr> <bch:tm> <bch:t>     <dbl> <bch:byt>    <dbl> <int> <dbl>   <bch:tm> <list>
1 r           724.2ms 724.2ms      1.38    4.76MB     5.52     1     4      724ms <NULL>
2 cpp          65.6ms  71.2ms     13.8    41.42MB    11.9      7     6      506ms <NULL>
# … with 3 more variables: memory <list>, time <list>, gc <list>
```

parallel



Parallel programming

- Many problems are of the “embarrassingly parallel” type
  Little to no effort required to separate problem into number of parallel tasks

- ABM itself is **not** embarrassingly parallel: time step 3 requires results from time step 2!
- Running the whole ABM several times to average over uncertainty **is** embarrassingly parallel

Parallel programming

- Computers nowadays can do more than one task at a time: threads
  - Often: 4 or 8 threads
  - Bigger computers have 12, 16 or 32 threads
  - Depending on computer, potential speedup of 32 times! (remember that our Rcpp effort gave ~10 times)

- Parallel programming is built into R (package **parallel**)

```r
library(parallel)

# create a function to run in parallel
my_func ← function(i) sprintf("this is iteration %i", i)

# instantiate 8 workers
clus ← makeCluster(8)

# run the function for iteration 1:100
parSapply(clus, 1:100, my_func)

#>  [1] "this is iteration 1"   "this is iteration 2"   "this is iteration 3"
#>  [4] "this is iteration 4"   "this is iteration 5"   "this is iteration 6"
#>  [7] "this is iteration 7"   "this is iteration 8"   "this is iteration 9"
#> [10] "this is iteration 10"  "this is iteration 11"  "this is iteration 12"
#> [13] "this is iteration 13"  "this is iteration 14"  "this is iteration 15"
#> [16] "this is iteration 16"  "this is iteration 17"  "this is iteration 18"
#> [19] "this is iteration 19"  "this is iteration 20"  "this is iteration 21"
#> ...

# stop the workers (we're done with them now)
stopCluster(clus)
```

An example of parallel programming is in the hands-on later

Interim conclusion

1. Today we are working with the Schelling agent-based model
2. Running the abm with different settings takes a long time
3. We can program the abm itself more efficiently
4. We can perform the abm in parallel

Let’s try it out!

Hands-on session 1