Large-Scale Spatial Data Science with ExaGeoStat

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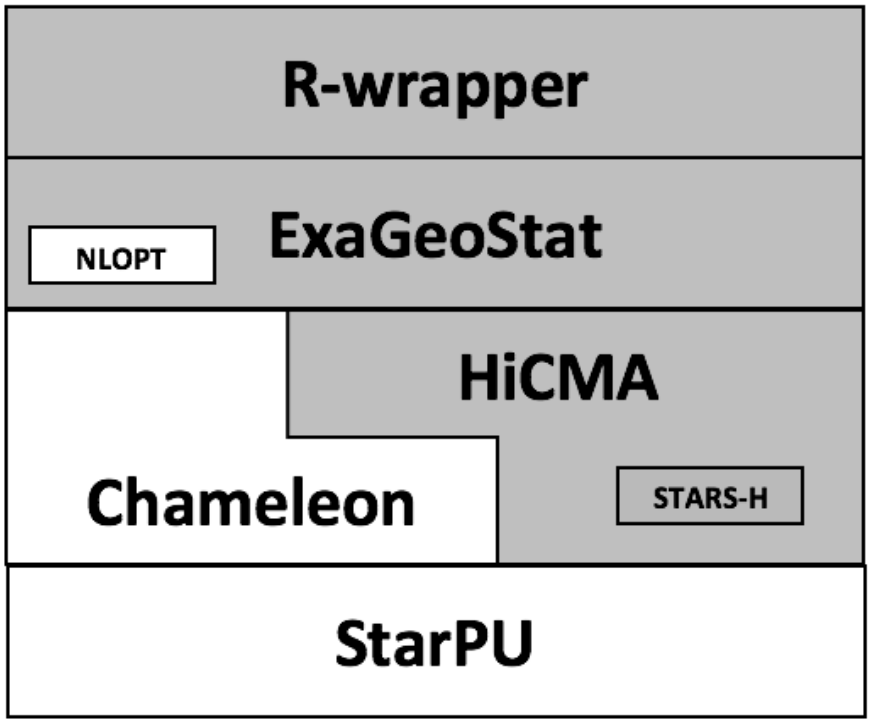
Part III

ExaGeoStatCPP Software in R

ExaGeoStatR

- ExaGeoStatR is a package for large-scale Geostatistics in R that supports parallel computation of the Gaussian maximum likelihood function on shared memory, GPU, and distributed memory systems



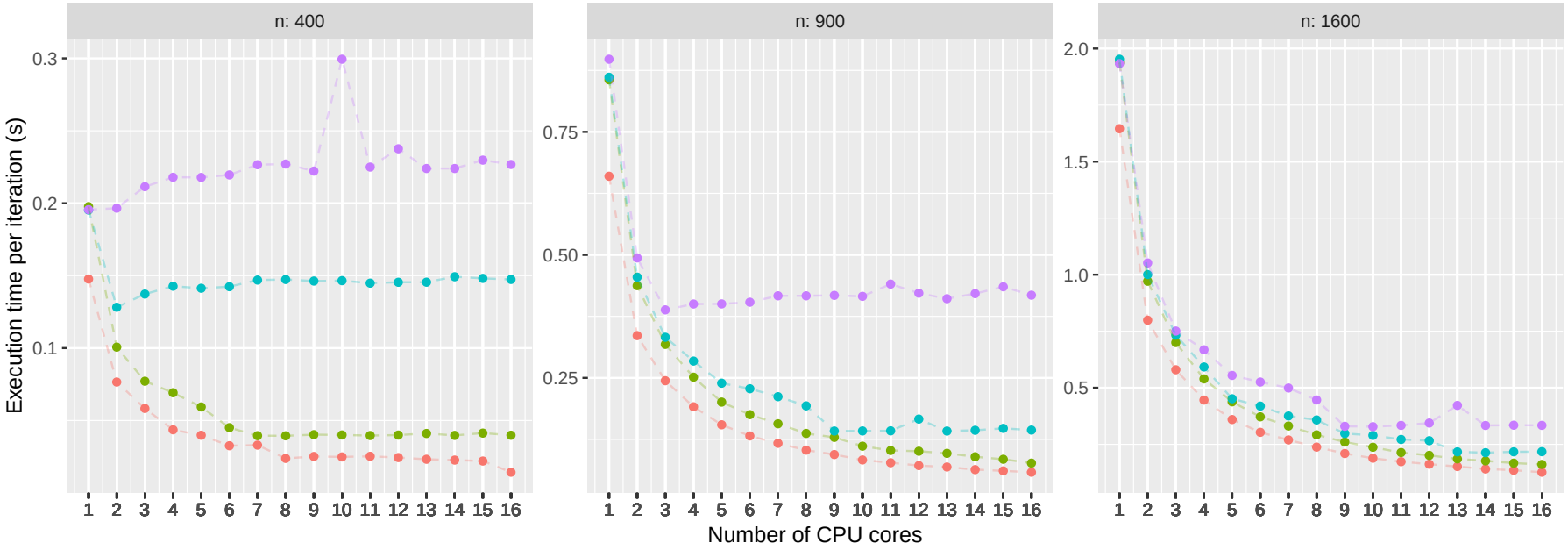
Existing Gaussian Likelihood Calculations in R packages

Package	geoR	fields	ExaGeoStatR
Function name	`likfit`	`MLESpatialProcess`	`exact_mle`
Mean	estimated	estimated	fixed as zero
Variance	estimated	estimated	estimated
Spatial Range	estimated	estimated	estimated
Smoothness	estimated	fixed	estimated
Default optimization method	`Nelder-Mead`	`BFGS`[1]	`BOBYQA`[2]

[1]. BFGS: Broyden-Fletcher-Goldfarb-Shanno. [2]. BOBYQA: bound optimization by quadratic approximation

ExaGeoStatR on Shared-memory System

- 16-core Intel Sandy Bridge Xeon E5-2650 Chip

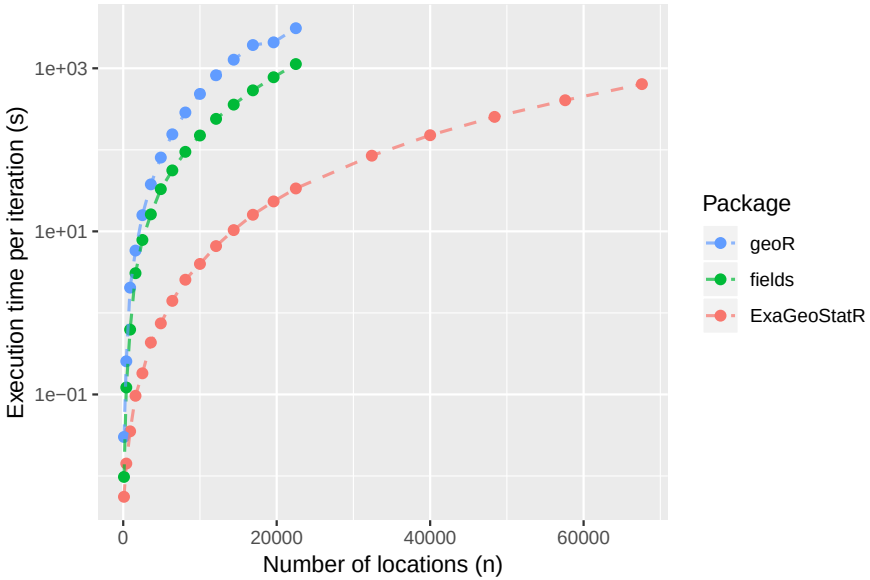


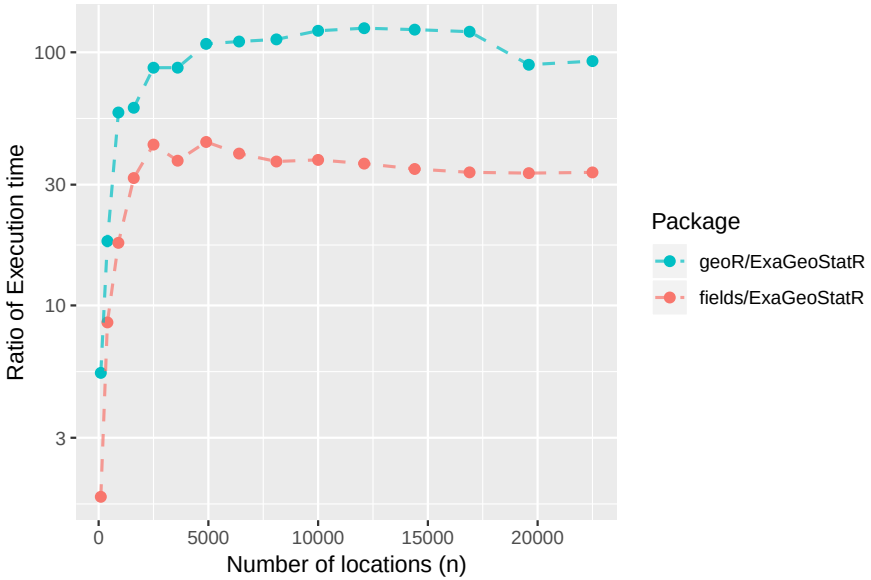
geoR - fields - ExaGeoStatR Comparison (Time)

- Average on 100 samples

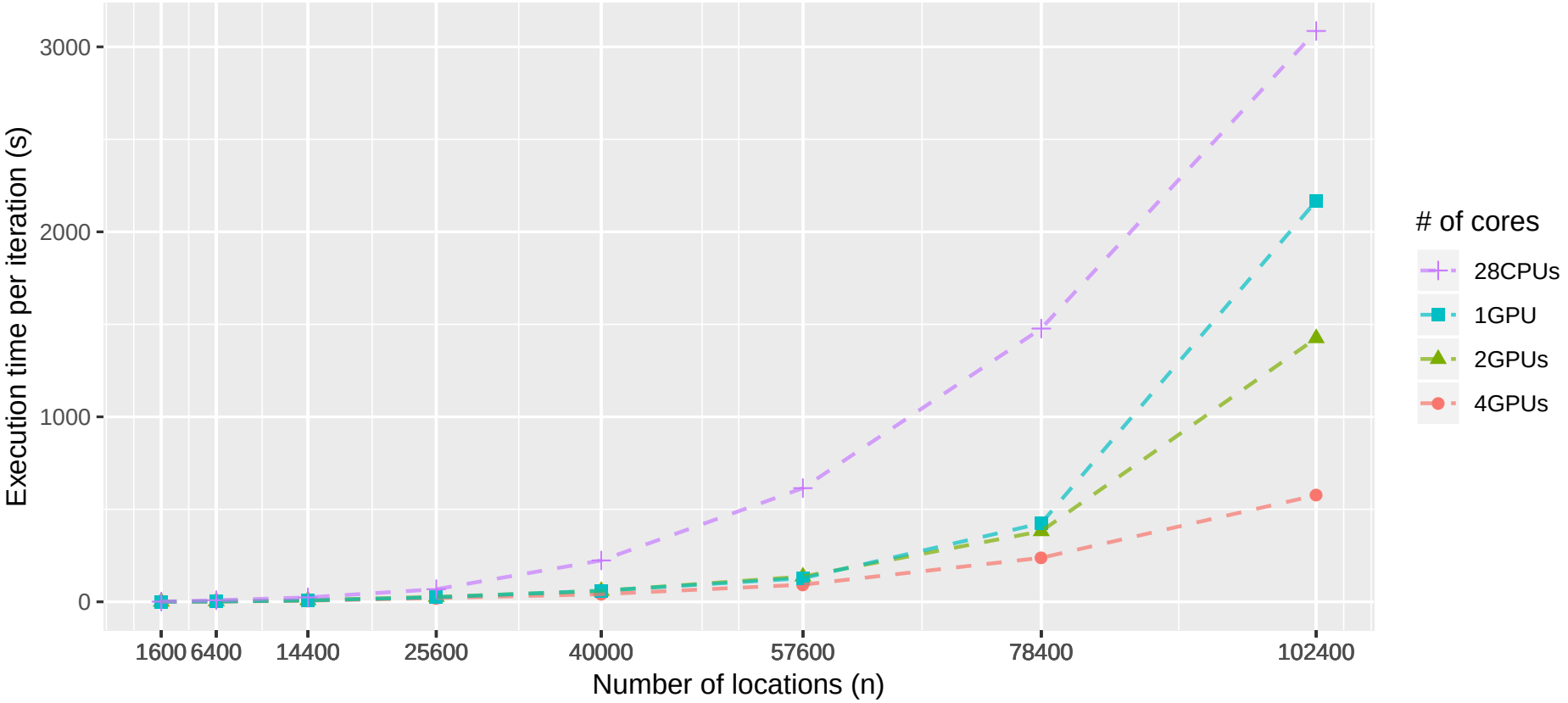
The average execution time per iteration (seconds)									
Package	**geoR**			**fields**			**ExaGeoStatR**		
$\nu=$ \ $\beta=$	0.03	0.1	0.3	0.03	0.1	0.3	0.03	0.1	0.3
0.5	1.39	1.49	1.47	0.75	0.97	0.99	0.10	0.12	0.12
1	1.35	1.49	1.56	0.66	0.90	0.90	0.09	0.13	0.13
2	1.34	1.56	1.57	0.67	0.91	0.93	0.09	0.13	0.13
The average number of iterations to reach the tolerance									
$\nu=$ \ $\beta=$	0.03	0.1	0.3	0.03	0.1	0.3	0.03	0.1	0.3
0.5	160	157	135	73	72	70	231	204	237
1	193	33	23	75	75	80	318	320	275
2	216	25	20	100	70	85	427	436	332

geoR - fields - ExaGeoStatR Comparison (Speedup)

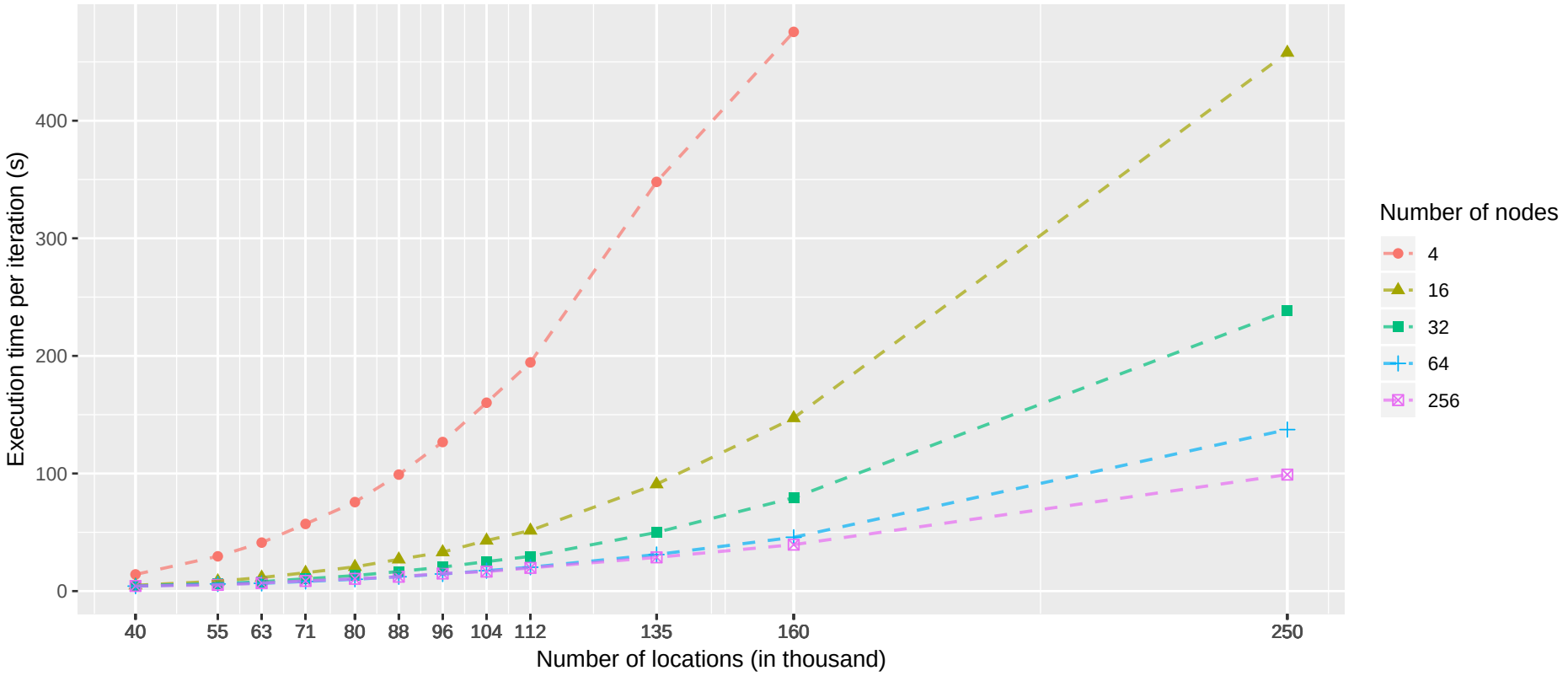




ExaGeoStatR Performance on Heterogeneous System (CPU/GPU)



ExaGeoStatR Performance on Distributed-Memory System (Shaheen-II)



Example (1)

```
### Example 1: Generate and model 2D spatial data using matern covariance without the nugget
# True parameter Theta=c(1,0.032579,1,0)
library("ExaGeoStatCPP")
ncores <- 39
ngpus <- 0
dts <- 360
lts <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)



problem_size <- 10e3

config <- configurations_init(n=problem_size, kernel="univariate_matern_stationary", computation=computation, tile_size=c(dts,lts),
                              iTheta=c(1,0.032579,1), lb_ub=list(c(0.01,0.01,0.01),c(5,5,5)), mle_itr=1000, tol=9, prediction=c(0,0,0,0,0))

data_source <- new(Data, problem_size, "2D")

exageostat_data <- simulate_data(hardware=hardware, config=config, data=data_source)



model_data(hardware=hardware, config=config, data=exageostat_data)
```

Example (2)

```
### Example 2: Generate and model 3D spatial data using matern covariance without the nugget
library("ExaGeoStatCPP")
ncores <- 39
ngpus <- 0
dts <- 360
lts <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)



problem_size <- 10e3

config <- configurations_init(n=problem_size, kernel="univariate_matern_stationary", computation=computation, tile_size=c(dts,lts),
                              iTheta=c(1,0.032579,1), lb_ub=list(c(0.01,0.01,0.01),c(5,5,5)), mle_itr=1000, tol=9, prediction=c(0,0,0,0,0))

data_source <- new(Data, problem_size, "3D")

exageostat_data <- simulate_data(hardware=hardware, config=config, data=data_source)



model_data(hardware=hardware, config=config, data=exageostat_data)
```

Example (3)

```
### Example 3: Generate and model 2D spatial data using matern covariance with the nugget
library("ExaGeoStatCPP")
ncores <- 39
ngpus <- 0
dts <- 360
lts <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)



problem_size <- 10e3

config <- configurations_init(n=problem_size, kernel="UnivariateMaternNuggetsStationary", computation=computation, tile_size=c(dts,lts),
                              iTheta=c(1,0.032579,1, 0.2), lb_ub=list(c(0.01,0.01,0.01,0.01),c(5,5,5,1)), mle_itr=1000, tol=9, prediction=c(0,0,0,0,0))

data_source <- new(Data, problem_size, "2D")

exageostat_data <- simulate_data(hardware=hardware, config=config, data=data_source)



model_data(hardware=hardware, config=config, data=exageostat_data)
```

Example (4)

```
### Example 4: Generate 2D spatial data using matern covariance with the nugget but model it without nugget
library("ExaGeoStatCPP")
ncores <- 39
ngpus <- 0
dts <- 360
lts <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)



problem_size <- 10e3

config <- configurations_init(n=problem_size, kernel="UnivariateMaternNuggetsStationary", computation=computation, tile_size=c(dts,lts),
                              iTheta=c(1,0.032579,1, 0.2), lb_ub=list(c(0.01,0.01,0.01,0.01),c(5,5,5,1)), mle_itr=1000, tol=9, prediction=c(0,0,0,0,0))

data_source <- new(Data, problem_size, "2D")

exageostat_data <- simulate_data(hardware=hardware, config=config, data=data_source)



config <- configurations_init(n=problem_size, kernel="univariate_matern_stationary", computation=computation, tile_size=c(dts,lts),
                             iTheta=c(1,0.032579,1), lb_ub=list(c(0.01,0.01,0.01),c(5,5,5)), mle_itr=1000, tol=9, prediction=c(0,0,0,0,0))

model_data(hardware=hardware, config=config, data=exageostat_data)
```

Example (5)

```
#!/bin/bash
#SBATCH --job-name=job_name
#SBATCH --output=output_file.txt
#SBATCH --partition=XXXX
#SBATCH --nodes=4
#SBATCH --ntasks=4
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=31
#SBATCH --time 00:30:00

srun Rscript Rtest.r
```

Example (6)

```
### Example 6: Play with ncores to show the advantage of increasing the number of cores in performance
library("ExaGeoStatCPP")
# ncores <- 39
ncores <- 19
# ncores <- 9
ngpus <- 0
dts <- 360
lts <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)


problem_size <- 30e3

config <- configurations_init(n=problem_size, kernel="univariate_matern_stationary", computation=computation, tile_size=c(dts,lts),
                              iTheta=c(1,0.032579,1), lb_ub=list(c(0.01,0.01,0.01),c(5,5,5)), mle_itr=5, tol=9, prediction=c(0,0,0,0,0))

data_source <- new(Data, problem_size, "2D")

exageostat_data <- simulate_data(hardware=hardware, config=config, data=data_source)


model_data(hardware=hardware, config=config, data=exageostat_data)
```

Example (7)

```
### Example 7: Play with matrix size to show the scalability
library("ExaGeoStatCPP")
ncores <- 39
ngpus <- 0
dts <- 360
lts <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)


# problem_size <- 30e3
problem_size <- 10e3

config <- configurations_init(n=problem_size, kernel="univariate_matern_stationary", computation=computation, tile_size=c(dts,lts),
                              iTheta=c(1,0.032579,1), lb_ub=list(c(0.01,0.01,0.01),c(5,5,5)), mle_itr=5, tol=9, prediction=c(0,0,0,0,0))

data_source <- new(Data, problem_size, "2D")

exageostat_data <- simulate_data(hardware=hardware, config=config, data=data_source)


model_data(hardware=hardware, config=config, data=exageostat_data)
~
```

Example (8)

```
### Example 8: Use GPU
library("ExaGeoStatCPP")
ncores <- 39
ngpus <-2
dts <- 960
lts <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)


problem_size <- 50e3

config <- configurations_init(n=problem_size,cores_gpus=c(ncores, ngpus), kernel="univariate_matern_stationary", computation=computation, tile_size=c(dts,lts),
                              iTheta=c(1,0.032579,1), lb_ub=list(c(0.01,0.01,0.01),c(5,5,5)), mle_itr=5, tol=9, prediction=c(0,0,0,0,0))

data_source <- new(Data, problem_size, "2D")

exageostat_data <- simulate_data(hardware=hardware, config=config, data=data_source)


model_data(hardware=hardware, config=config, data=exageostat_data)
~
```

Thank You!

Questions?