ParaCircE, a parallel Gaussian Random Field (GRF) generator

Simon Legrand, Géraldine Pichot

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SIAM GS21

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Gaussian Random Fields

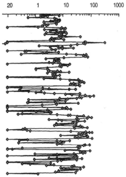
Context

In hydrogeology, permeability/transmissivity are often modeled by **second order stationary fields**, with **lognormal** distributions.

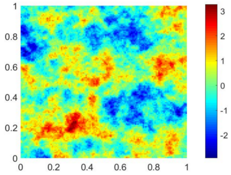
Classical applications are:

- Groundwater ressources management
- Pollution propagation studies
- Waste storage studies in deep geological media

Sand and gravel deposits in Switzerland, Gelhar [1993]



permeability (md)



Matérn isotrope covariance, $L=1$, $n=128^2$, $\lambda=0.125$

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Gaussian Random Fields

1D General algorithm

Let $\Omega \in \mathbb{R}$. To generate $\boldsymbol{y}$, a Gaussian vector, with zero mean and covariance matrix $\boldsymbol{R}$, defined on a $N+1$ points regular grid of Ω:

1. Factorize $\boldsymbol{R} = \boldsymbol{B}\boldsymbol{B}^{\boldsymbol{T}}$
2. Generate $\boldsymbol{\theta} = (\theta_0, ..., \theta_N)^T$, a realization of standard normal variables.
3. One realization is obtained with $\boldsymbol{y} = \boldsymbol{B}\boldsymbol{\theta}$

Among existing methods

- Cholesky factorization, efficient on small problems, but $O(N^3)$
- Karhunen Loève series expansion, expensive when $\lambda << L$
- H-Matrices [Feischl et al., 2018], suited for unstructured meshes
- **Circulant Embedding** [Dietrich et al., 1993], [Graham et al., 2018], with exact correlation structure, suited for large regular grids.

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1D Circulant Embedding algorithm

1. Sample the covariance function to get the vector $\boldsymbol{a} = (c_0, ..., c_N, c_{N-1}, ..., c_1) \in \mathbb{R}^{2N}$, first row of a circulant matrix $\boldsymbol{A}$.
2. If N is large enough, $\boldsymbol{A}$ is SPD, we compute its eigenvalues with FFT, otherwise increase N (padding). $\boldsymbol{s} = \boldsymbol{F}\boldsymbol{a}$ and set $\boldsymbol{D} = Diag(\boldsymbol{s})$
3. Generate realizations of standard normal vectors of size $2N$ $\theta = \theta^{re} + i\theta^{im}$
4. Apply iFFT to compute $\boldsymbol{C}^*\theta$, with $\boldsymbol{C}^* = \frac{1}{\sqrt{2N}}\boldsymbol{F}^*\boldsymbol{D}^{\frac{1}{2}}$
5. Retrieve **two** GRF $\boldsymbol{Y}_1 = (\boldsymbol{C}^*\theta)^{re}(0:N), \quad \boldsymbol{Y}_2 = (\boldsymbol{C}^*\theta)^{im}(0:N)$

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Features

- **Matérn** family of covariance (example in 2D)

$$\rho_{2D}(\mathbf{x}, \nu, \boldsymbol{\lambda}) = \kappa(\frac{\sqrt{\lambda_2^2\, x^2 + \lambda_1^2\, y^2}}{\lambda_1\, \lambda_2}, \nu),$$

with

$$\kappa(r, \nu) = \frac{2^{1-\nu}}{\Gamma(\nu)}(\sqrt{2\nu}\, r)^{\nu} K_{\nu}(\sqrt{2\nu}\, r),$$

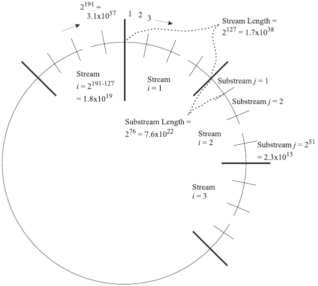
  - $\boldsymbol{x} = (x, y)$
  - Γ the gamma function
  - K_ν the modified Bessel function of the second kind
  - λ_i the correlation length along direction i
  - $\nu > 0$ a smoothness parameter.

- **Parallel** (MPI)
  One direction parallelism (FFTW). The reproducibility is guaranteed whatever the number of processes (RngStream).

Features

- **Independance** and **reproducibility** thanks to the RngStream library [L'Ecuyer et al., 2002]

2^{191}-periodic set of pseudo random numbers, divided into **Streams** and **Substreams**.



- **Accelerated** minimum domain size computation

  If padding is required, save computational resources by approximating the required domain size to get positive eigenvalues [Graham et al., 2018, Legrand et al., 2021].

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Technical overview

- C++17/MPI headers (templated) library
  $\rightarrow$ Static dimension 2D/3D
  $\rightarrow$ Variable numerical precision (double/long double)
- Dependencies
  - MPI
  - FFTW_MPI [Frigo et al., 2005]
  - RngStream [L'Ecuyer et al., 2002]
- Installation with **CMake**
  $\rightarrow$ Portability
  $\rightarrow$ Easy dependencies management

Contents

ParaCircE API

Data structure instantiation

- Domain

```
DiscretDomain2D<double> d{
  {{lx_min, lx_max, nx}, {ly_min, ly_max, ny}}
};
```

- Correlation function

```
auto f = create_function2D<double>(correl_type,
                                    lcx, lcy);
```

- Field generator

```
auto generator = GRF(MPI_COMM_WORLD, d, f);
```

Field generation

```
auto field = generator.generate(nx_local);
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ParaCircE API

For **Monte-Carlo** use, change stream/substream of the pseudo RNG RngStream.
$//generator.set\_state(stream, substream);$

Field generation

```
...
for (size_t i=0; i<nb_mc; i++)
{
  generator.set_state(0, i);
  auto field = generator.generate(nx_local);
  ...
}
```

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Tests environment

- Instrumentation performed with Score-P/Scalasca tools
- Compilation options: *-O3*
- Execution on Inria Paris CLEPS cluster
  - Xeon 5218, 2.4GHz
  - 192Go RAM 2667MHz
  - 100Gb/s Inifiniband network
- 1 core/MPI process
- **Exclusive** access to the nodes
- No hyperthreading

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Strong scaling

- **Fixed** size problem (2048*512*512)
- **Increasing number** of processes

Maximum acceleration given by Amdhal law:

$$A(N) = \frac{1}{s + \frac{p}{N}}$$

N: Number of tasks
s: sequential time fraction = 0.014
p: parallel time fraction = 0.986
Total time $\approx$ 41min

Results

- Scales like FFTW

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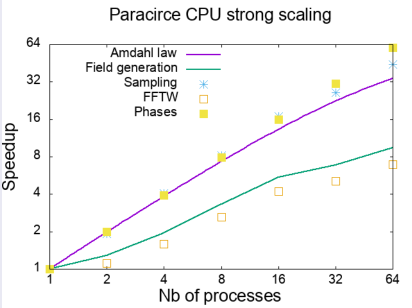

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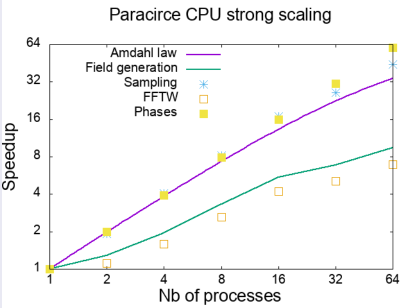

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Memory scaling

- The goal of ParaCircE is to generate **large** fields.
- Main constraint: **Memory occupation** (**R**esident **S**et **S**ize)

Circulant Embedding algorithm implies **symmetrizing** the domain.
In dimension d:

$$RSS \approx complexSize * (\mathbf{2}N)^d$$

For $N = 512, d = 3$, with a complex size of 128 bits:

$$RSS \approx 16 * 8 * 512^3 \approx 16GB$$

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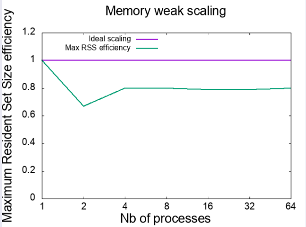
Memory weak scaling

- Both problem size and number of tasks increase
- **Constant workload** per task, $\approx 512^3$ samples

Results

Nb_proc	Time(min)	Max RSS(GB)	RSS Efficiency
1	7.8	15.9	1.00
2	11.2	23.9	0.67
4	16.8	20.0	0.80
8	23.2	20.0	0.80
16	31.0	20.1	0.79
32	41.4	20.1	0.79
64	70.3	20.0	0.80



Relatively **low** execution time

- $\sim$**134 millions** elements: 1 proc $\rightarrow$ **7min48s**
- $\sim$**8.6 billions** elements: 64 proc $\rightarrow$ **1h10min** (would require 1TB in sequential)

Constant memory scaling!

Conclusion

- **Easy** to install and use
- **Fast** even for very large cases
- **Accelerated** method for automated padding computation

Perspectives

- Periodic field generation
- Multithread
- What do you need?

Gitlab repository: https://gitlab.inria.fr/slegrand/paracirce

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For Further Reading I

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For Further Reading II

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