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GENFIELD: A parallel software for the generation of stationary Gaussian random fields

Géraldine Pichot, Simon Legrand, Jocelyne Erhel, Mestapha Oumouni

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Introduction

Context

In hydro-geology, natural permeability fields are classically modeled by a **second-order stationary field** which has a lognormal distribution, with an isotropic exponential covariance function. In this poster, we expose an algorithm to generate Gaussian random fields based on the **Circulant Embedding method** and its implementation in **C++/MPI**.

Useful in different applications

- sustainable management of groundwater resources
- pollution propagation studies
- feasibility studies of waste storage in deep geological media

General algorithm in 1D

Let $\Omega = [0, 1]$. We discretize Ω over a regular grid composed of $N + 1$ elements.

To generate a realization of the random vector Y of normal variables with zero mean and autocovariance matrix R , we use the following algorithm:

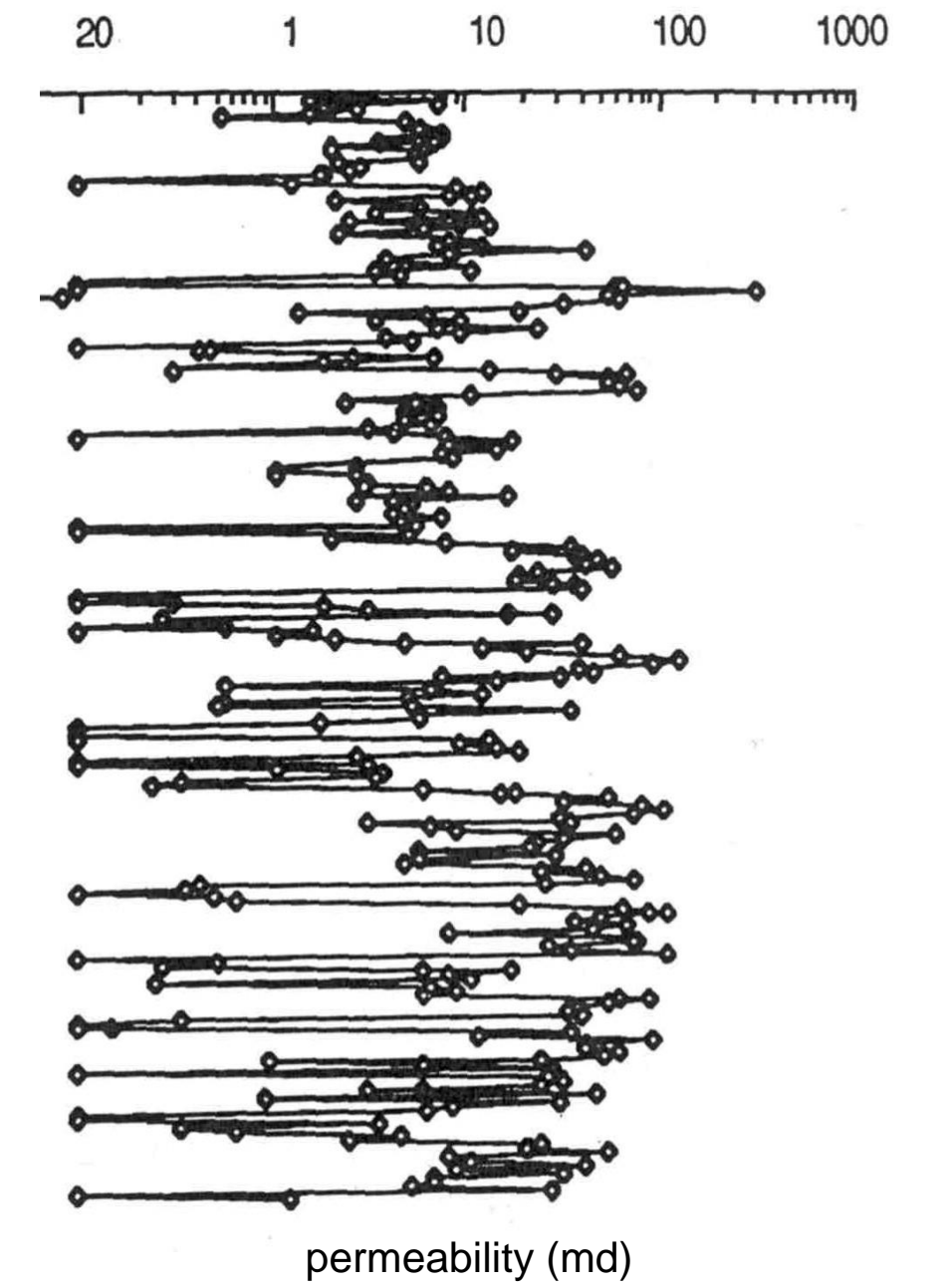
1. Factorize $R = BB^T$
2. Generate a vector $\theta = (\theta_0, \dots, \theta_N)^T$ as a realization of uncorrelated random normal variables with zero mean.
3. One realization is obtained by $Y = B\theta$.

The usual method to decompose R is Cholesky. Its cost is in $O(N^3)$ and becomes too prohibitive for large problems.

The **circulant embedding method** is a very interesting alternative as it relies on the Discrete Fourier Transform. This latter has an efficient $O(N \log N)$ implementation in the **FFTW library**



Sand and gravel deposits in Switzerland, Gelhar [1993]



Circulant embedding method in 1D

Algorithm when no padding is required (i.e. when all eigenvalues are positive in step 2.):

1. Sample the autocovariance function to get circulant vector $a \in \mathbb{R}^{2N}$.
2. Compute the vector of eigenvalues $s = Fa$ with FFT and set $D = \text{Diag}(s)$.
3. Generate two realizations of standard normal random vectors of size $2N$, θ^{re} and θ^{im} :

$$\theta = \theta^{re} + i\theta^{im},$$

4. Apply iFFT to compute $C^*\theta$ with $C^* = \frac{1}{\sqrt{2N}} F^* D^{\frac{1}{2}}$
5. Take

$$Y_1 = (C^*\theta)^{re}(0 : N) \text{ and } Y_2 = (C^*\theta)^{im}(0 : N)$$

Our objective is to introduce a new parallel implementation of the circulant embedding method.

C++/MPI Implementation

0. Parameters parsing and padding estimation Boost

1. Covariance function discretization MPI

2. Fast Fourier Transform MPI
FFTW3

3. Gaussian random vectors Boost
Rngstream

4. Inverse Fast Fourier Transform MPI
FFTW3

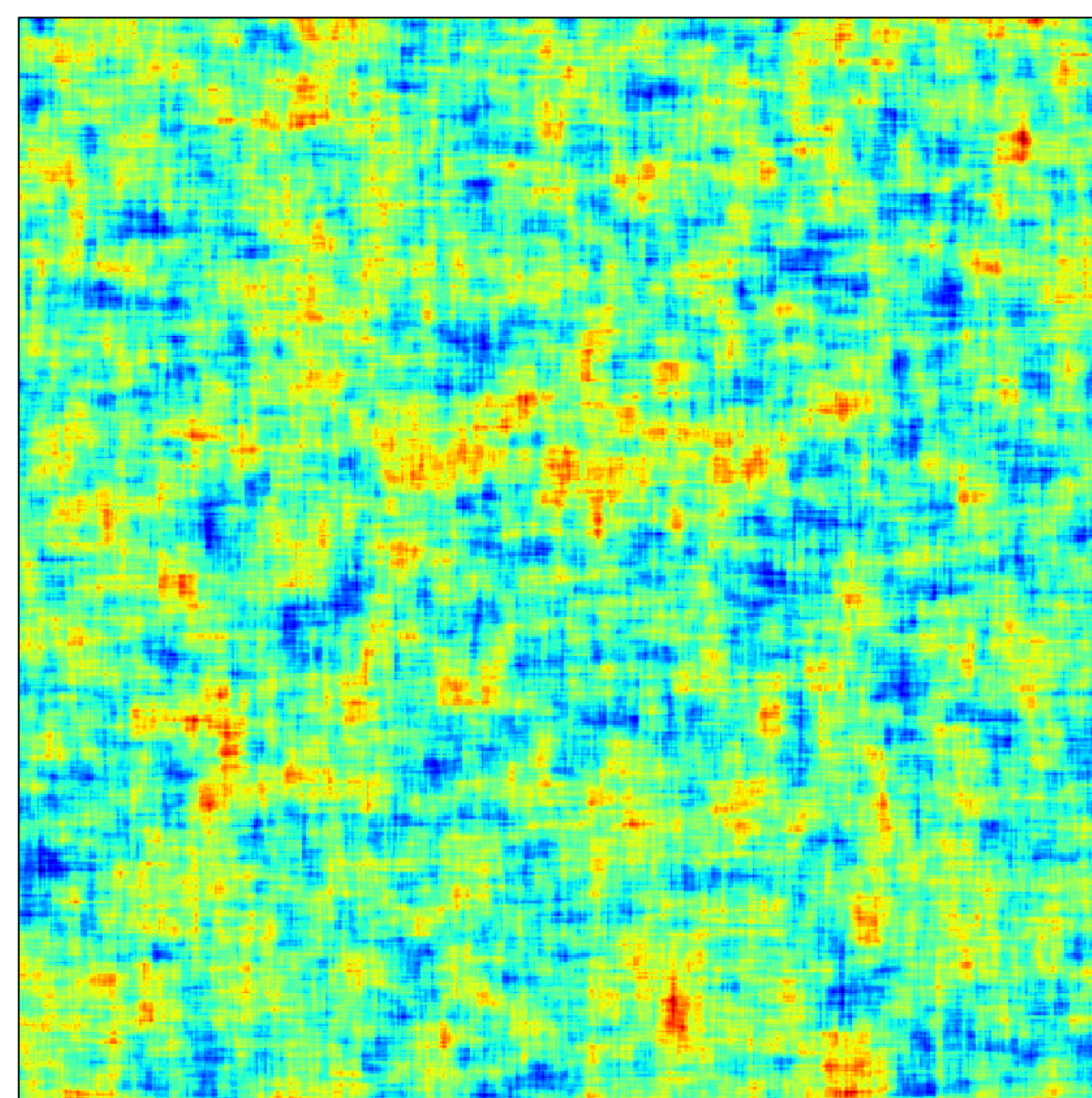
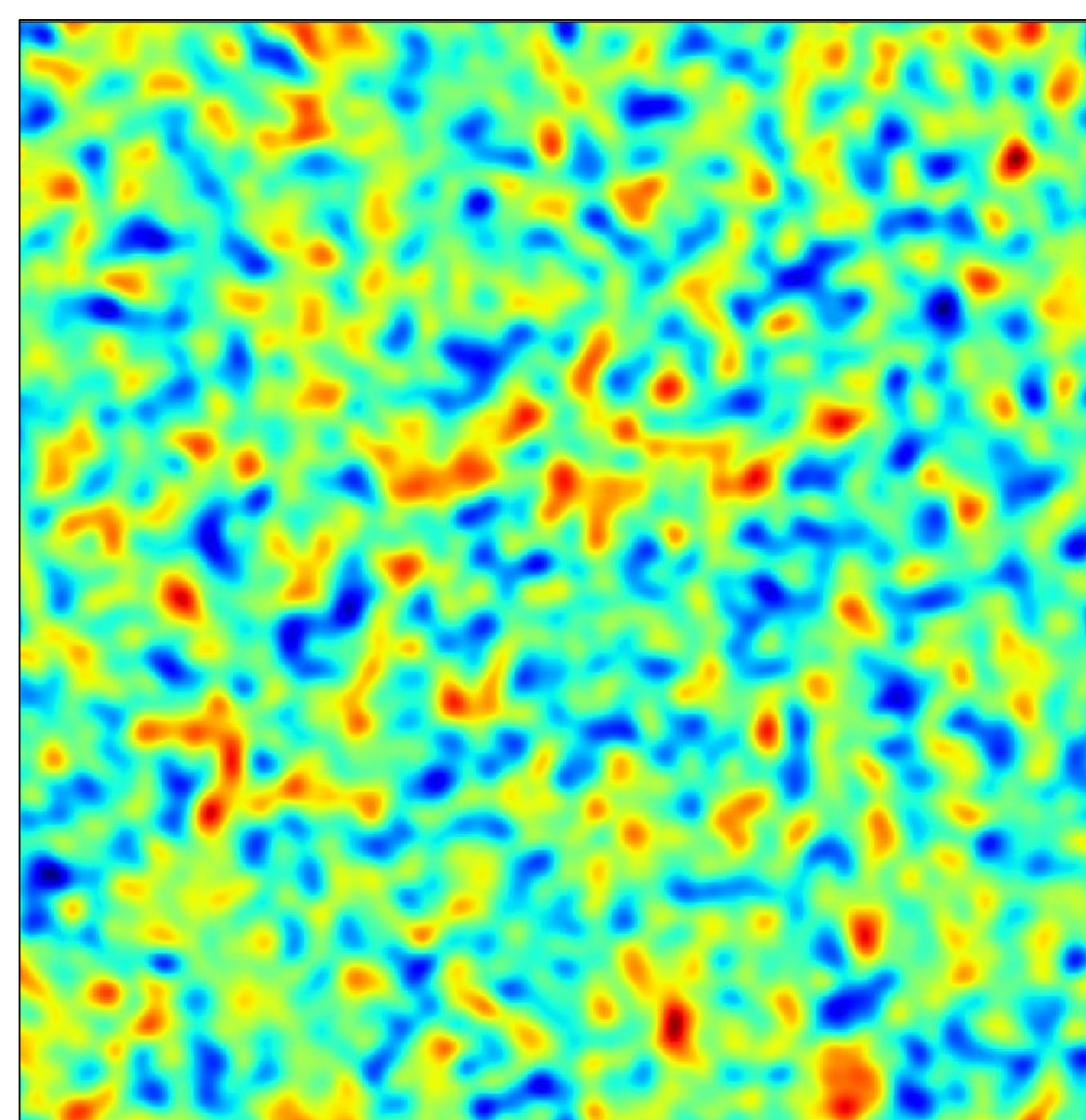
5. Field retrieval MPI

Parallel sections Sequential sections

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Examples of fields in 2D

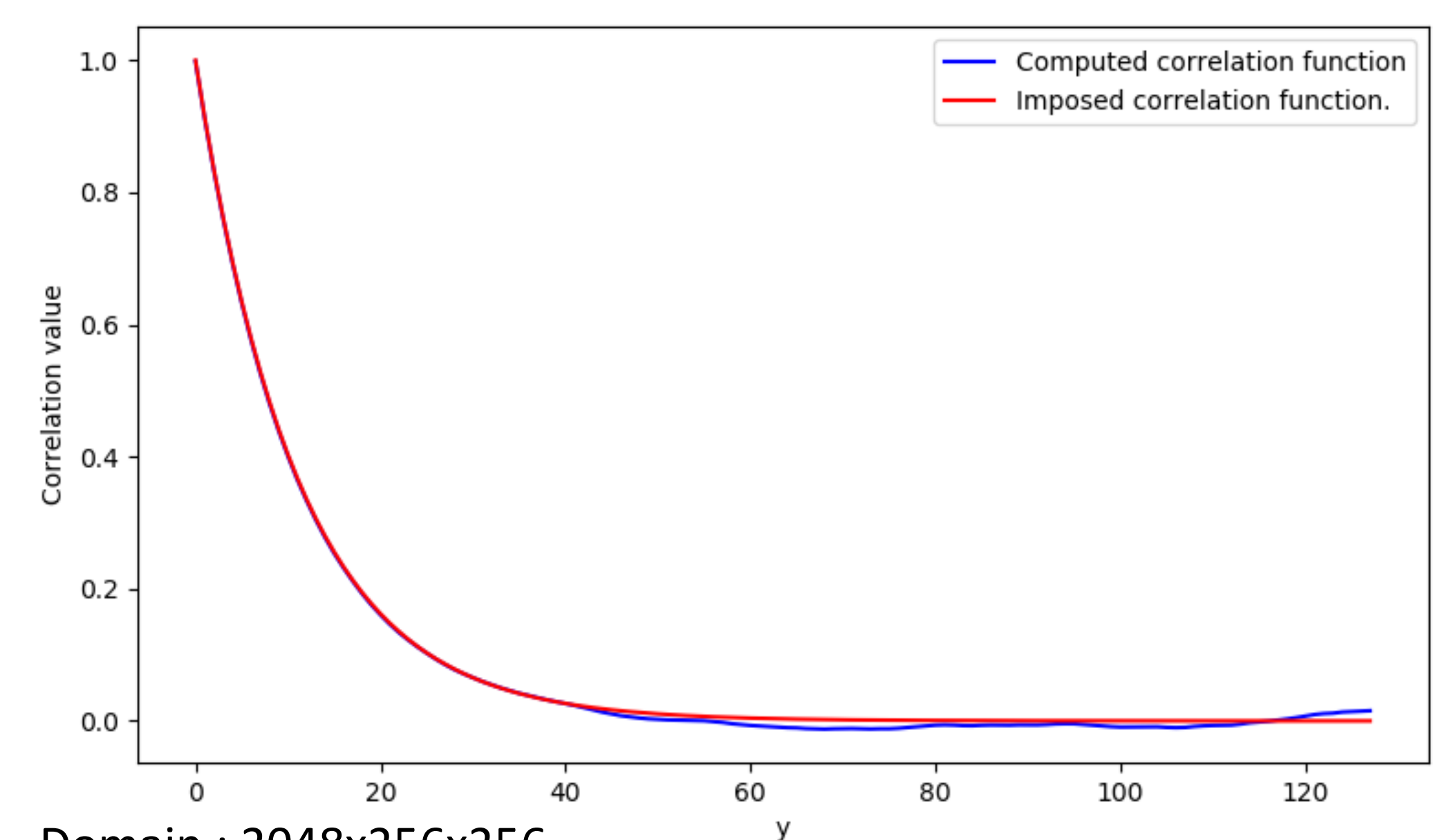
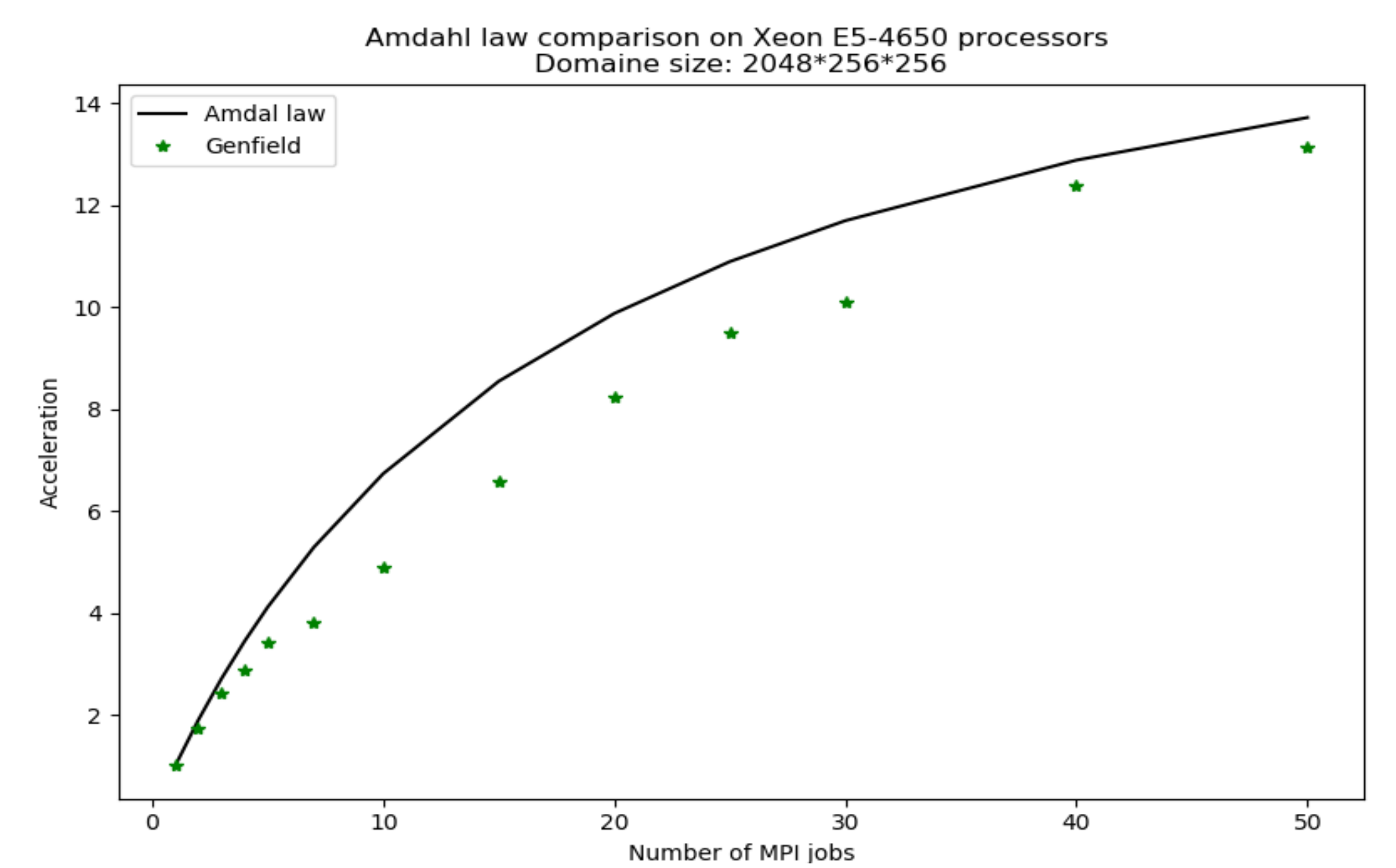


Domain : 256 x 256

Up: Gaussian covariance function

Bottom: Exponential covariance function

Performances in 3D



Up: Speedup curve compared with Amdahl law (5% sequential)

Bottom: comparison between the computed and the imposed covariance function

Acknowledgments. Computer simulations were performed on the ADA cluster at the **Institute for Development and Resources in Intensive Scientific Computing**, France.

Perspectives

- Parallelize the last 5% of the code, i.e. the generation of the gaussian random vectors using the pseudo-random numbers generator Rngstream written by P. L'Ecuyer.
- Extend the inputs/outputs to other formats such as xml, json and hdf5.