OpenTURNS release highlights

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UserDay #13, 5 June 2020, online event

Overview

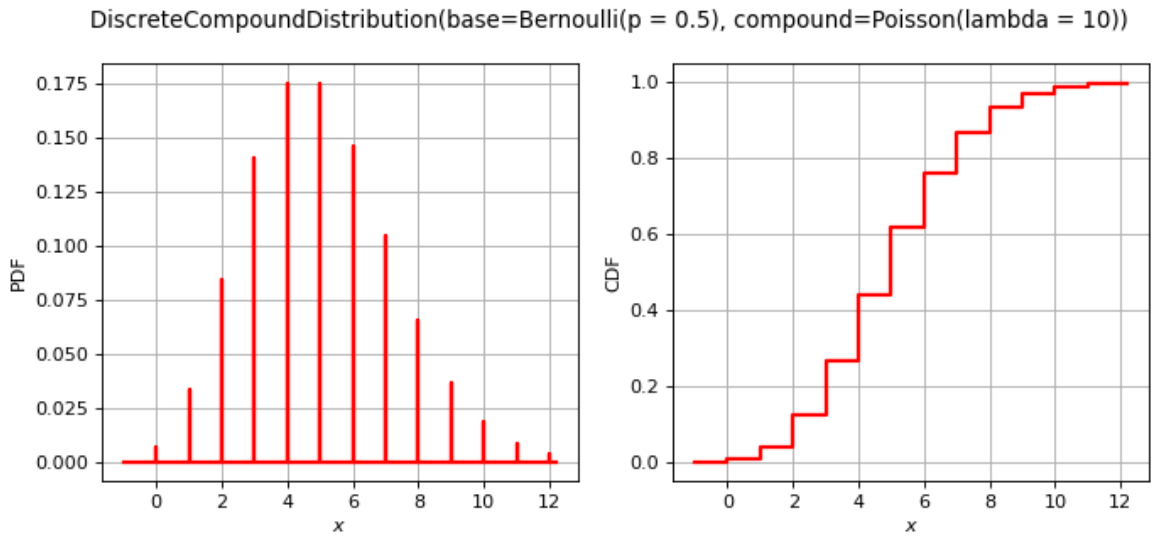
New features since last year in releases:

- v1.14: 2019-11-13
- v1.15: 2020-05-25

Contents

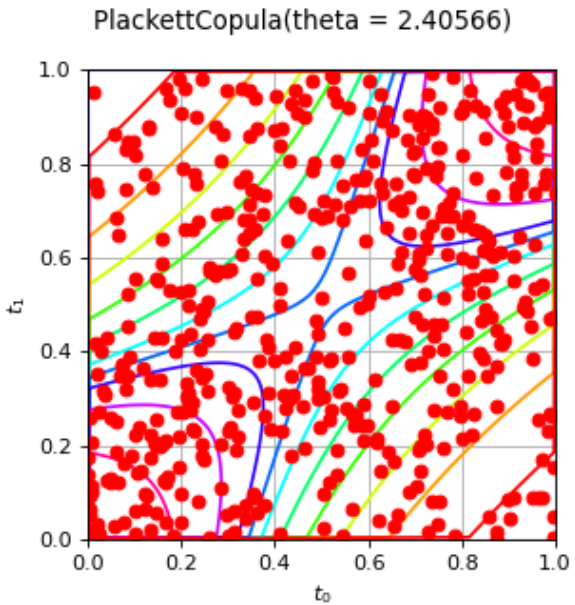
New distributions

- SquaredNormal
- DiscreteCompoundDistribution
- WeibullMax
- Pareto
- MixedHistogramUserDefined



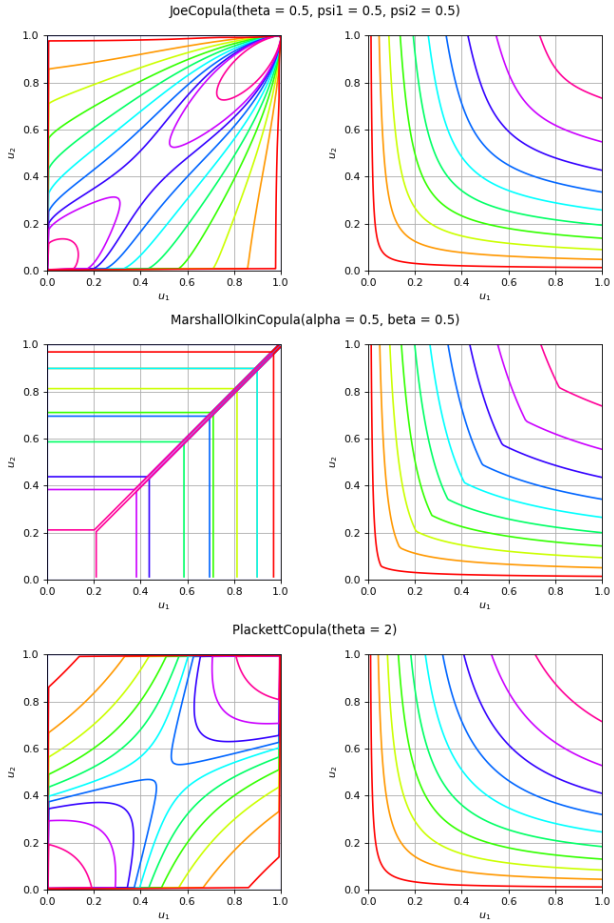
New estimators

- ParetoFactory
- GeneralizedExtremeValueFactory
- PlackettCopulaFactory
- LeastSquaresDistributionFactory (generic service)



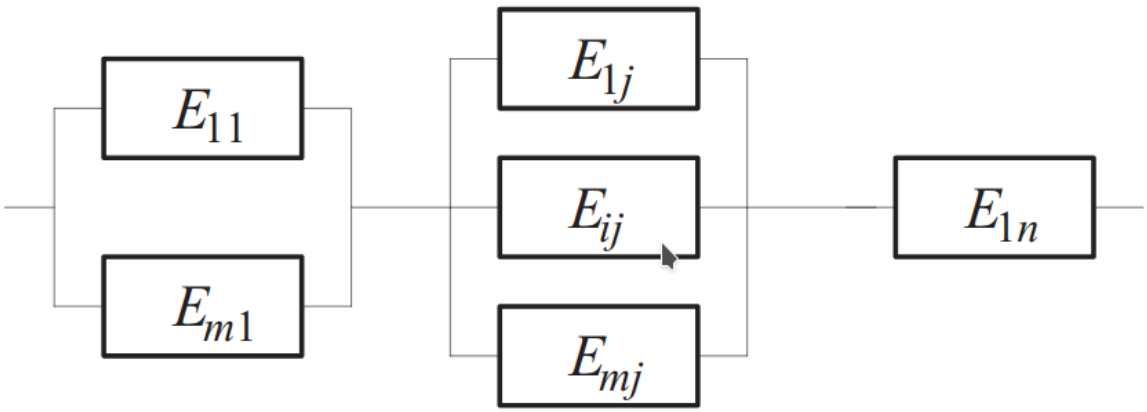
New copulas

- JoeCopula (EV)
- MarshallOlkinCopula
- PlackettCopula



System events

- IntersectionEvent: $E_{sys} = \bigcap_{i=1}^{N} E_i$
- UnionEvent: $E_{sys} = \bigcup_{i=1}^{N} E_i$
- MultiFORM:
  $P(\bigcup_{i=1}^{N} E_i) = 1 - \Phi_k(\underline{\beta}; \underline{\underline{\rho}})$
- SystemFORM:
  $P(\bigcup_{i=1}^{N} E_i) = 1 - \Phi_k(\underline{\beta}; \underline{\underline{\rho}})$
  $P(\bigcap_{i=1}^{N} E_i) = \Phi_k(-\underline{\beta}; \underline{\underline{\rho}})$
  $P(E_{sys}) = P(\bigcup_{i=1}^{N} E_i) =$
  $\sum_{i=1}^{N} P(E_i) - \sum_{i<j} P(E_i \cap E_j) + \cdots + (-1)^N P(E_1 \cap E_2 \cap \cdots \cap E_N)$



System events

- Modelisation

```
X = ot.RandomVector(ot.Normal(dim))
f1 = ot.SymbolicFunction(['x1', 'x2'], ['(x1+2*x2)^2'])
f2 = ot.SymbolicFunction(['x1', 'x2'], ['(x2+3*x1)^2'])
v1 = ot.CompositeRandomVector(f1, X)
v2 = ot.CompositeRandomVector(f2, X)
e1 = ot.ThresholdEvent(v1, ot.Greater(), 5.0)
e2 = ot.ThresholdEvent(v2, ot.Greater(), 5.0)

# define union/intersection
e3 = ot.IntersectionEvent([e1, e2])
e4 = ot.UnionEvent([e1, e2])
e5 = ot.UnionEvent([e3, e4])

# sample system events
e3.getSample(10)
algo = ot.SubsetSampling(e4)
```

System events

- Algorithms

```
# System-FORM
e5 = ot.IntersectionEvent([e1, e2])
e6 = ot.IntersectionEvent([e3, e4])
e7 = ot.UnionEvent([e5, e6])
solver = ot.AbdoRackwitz()
starting_pt = [0.1] * dim
algo = ot.SystemFORM(e7, event, starting_pt)
algo.run()
result = algo.getResult()
pf = result.getEventProbability()
```

Discretization of covariance models on large meshes I

There are many contexts in which the discretization of a covariance model over a large mesh is mandatory:

- to sample a Gaussian process on a large mesh
- to build a Kriging meta-model from a large dataset
- to build the Karhunen-Loeve decomposition of a known covariance model on a large mesh
- ...

The resulting matrices are dense and large, so the first limit is the $\mathcal{O}(N^2)$ memory need ($\sim$ 30000 nodes for covariance model of dimension 3 with 64GB of memory).
Using HMAT, the memory footprint is reduced to $\mathcal{O}(N \log N)$, allowing for much larger meshes (tested on a 900720 nodes mesh with for a covariance model of dimension 3 with 64GB of memory).

Discretization of covariance models on large meshes II

Then, the factorization times, which is $\mathcal{O}(N^3)$ with a dense solver (LAPACK) becomes the limiting factor. With HMAT, it drops to $\mathcal{O}(N \log^2 N)$.

These were the motivation for the introduction of HMAT within OpenTURNS 1.4, nearly 6 years ago... and it didn't worked as expected!

- The regularization procedure developed for LAPACK was not adapted to HMAT, resulting into many (many many) factorizations;
- No compression procedure proposed by the hmat-oss library was adapted to covariance operators.

Discretization of covariance models on large meshes III

These points have been solved in two steps, thanks to Romain Poncet's contributions:

1. OpenTURNS 1.14: the ability to change the regularization factor without recompressing the matrix, and the automatic computation of a reasonable regularization factor (in OpenTURNS 1.14);
2. OpenTURNS 1.15: The development of the ACA-random compression procedure in hmat-oss and its interface in OpenTURNS.

AND IT WORKS! Here we compare LAPACK (with OpenBLAS, 4 cores) and hmat-oss (1 core).

Sampling of a Gaussian process I

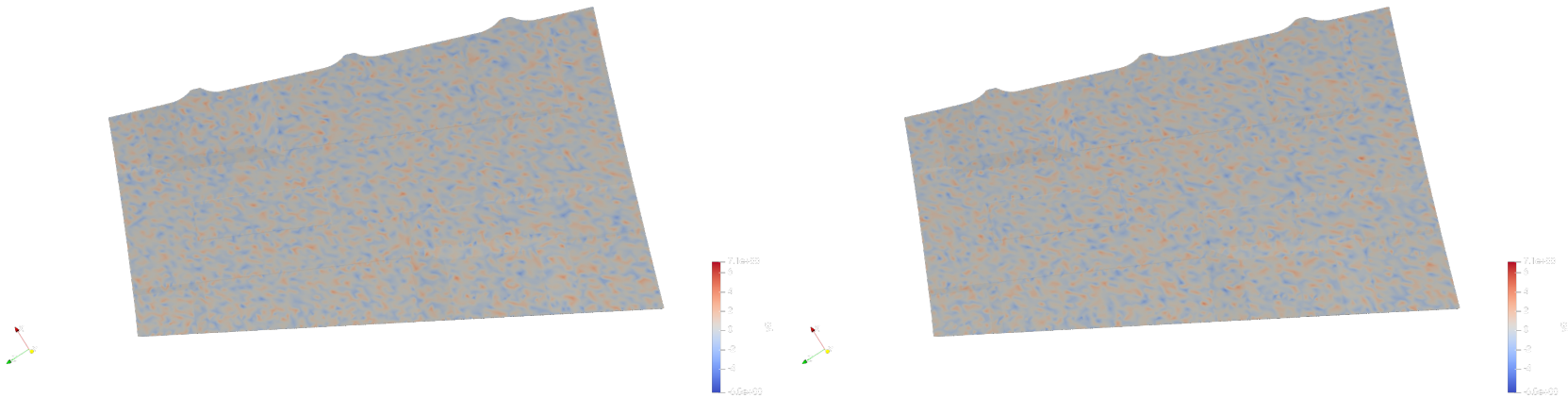


Figure: Matèrn model, 18292 nodes, LAPACK (left, 188 s), HMAT (right, 90 s)

Sampling of a Gaussian process II

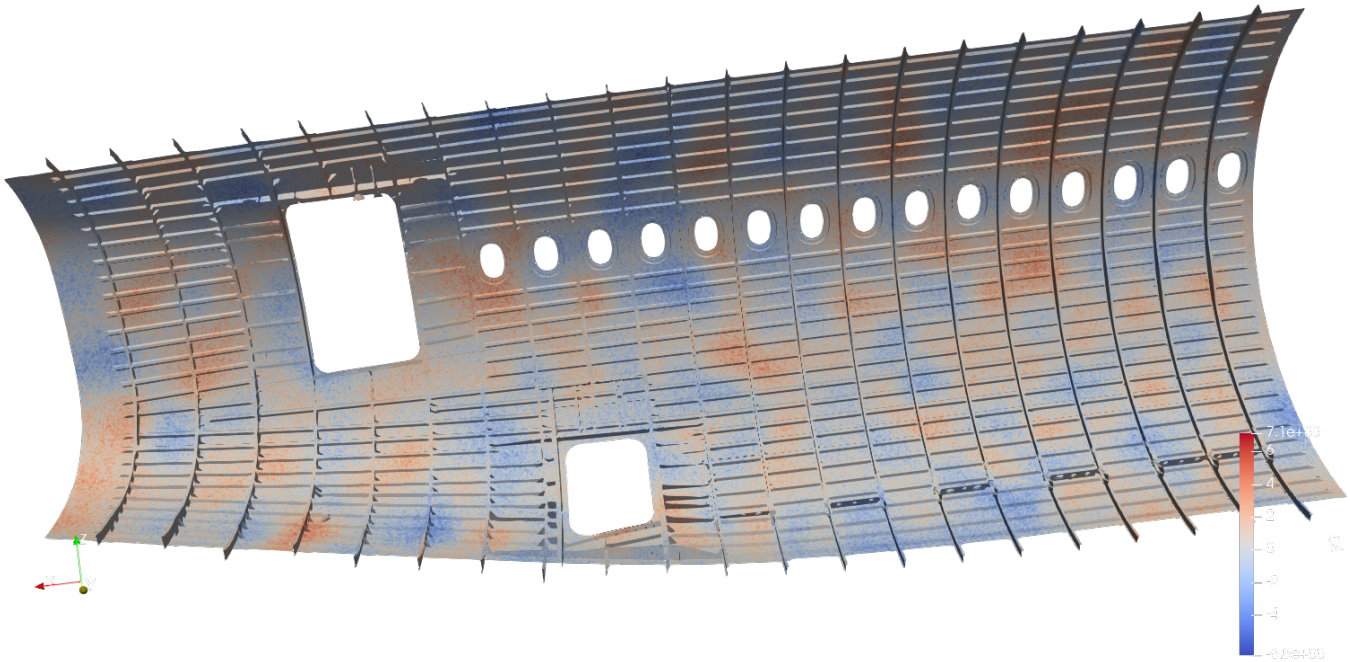


Figure: SquaredExponential model, 900720 nodes, HMAT (610 s)

Sampling of a Gaussian process III

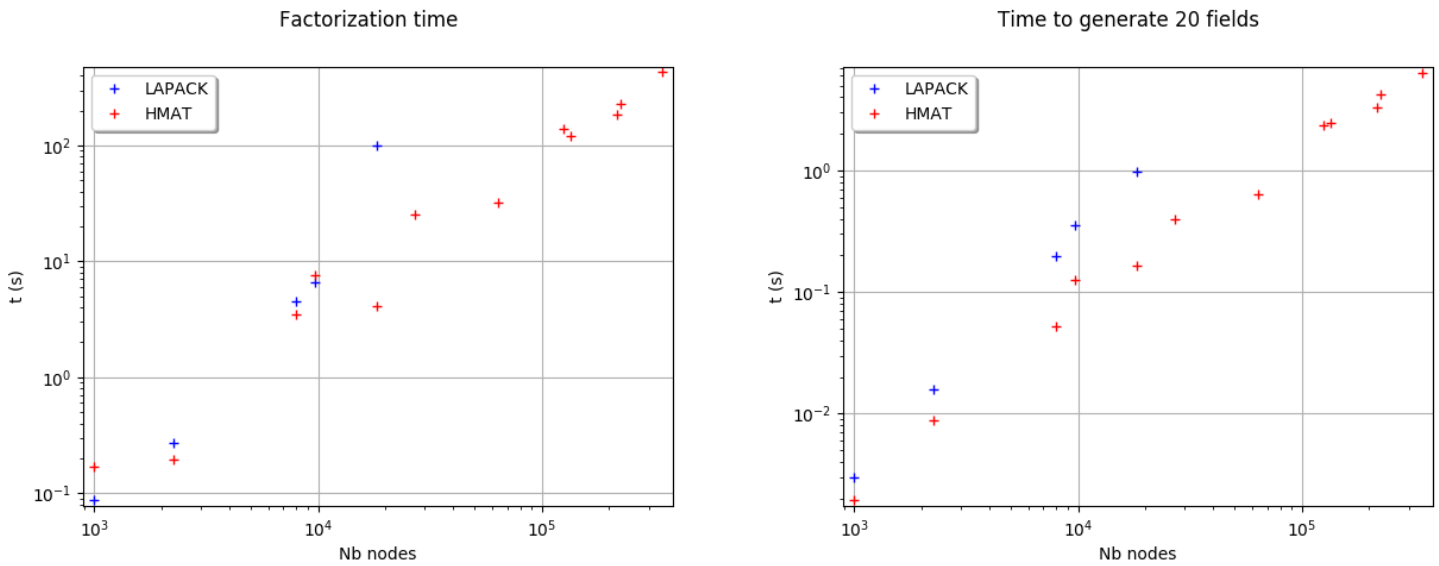


Figure: Factorization time (left) and sampling time (right), lower is better

Karhunen-Loeve decomposition I

The Karhunen-Loeve decomposition of a covariance model on a mesh results in the eigen decomposition of a dense matrix $M = CG$ where G is a sparse matrix, the Gram matrix of the P_1 basis over the mesh, and C a dense, positive symmetric definite matrix, the discretization of the covariance model on the mesh.

- A naive approach is to compute M and to decompose it, which was the only option up to OpenTURNS 1.14.
- Using an iterative algorithm for the eigen decomposition, the product $z = Mx$ for a given vector v can be done using two products $y = Gx$ and $z = Cy$, both allowing for optimizations.

Karhunen-Loeve decomposition II

We rely on the Spectra library (https://github.com/yixuan/Spectra) for the iterative algorithm, we use a compressed sparse column compression scheme for G and an hmat compression for C (no regularization/factorization step here).

Bonus: using Spectra, one can select the maximum number of modes to be computed. Here we choose to compute 20 modes.

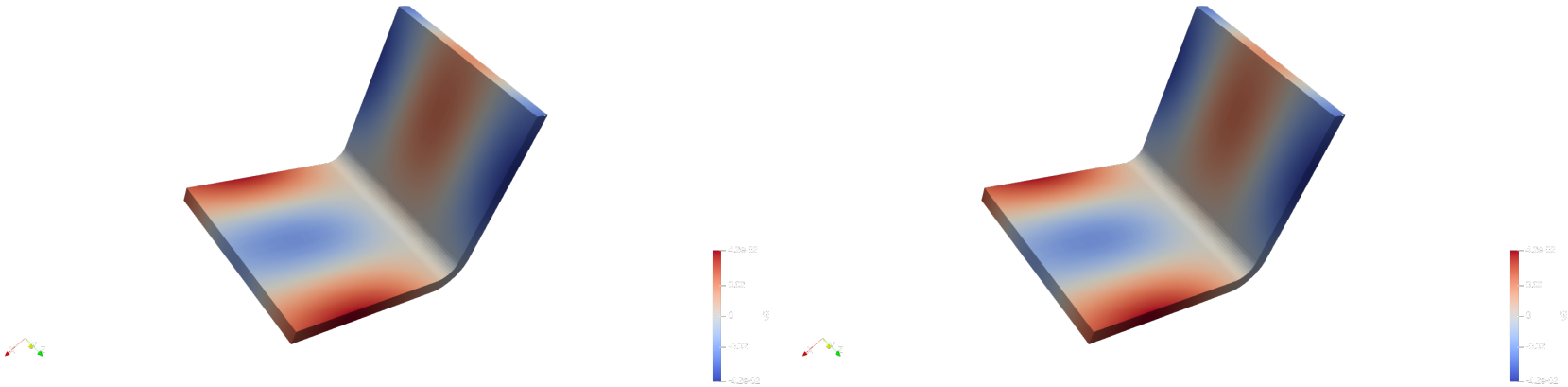


Figure: SquaredExponential model, 2268 nodes, mode 11, LAPACK (left, 15.3 s), HMAT (right, 0.1 s)

Karhunen-Loeve decomposition III

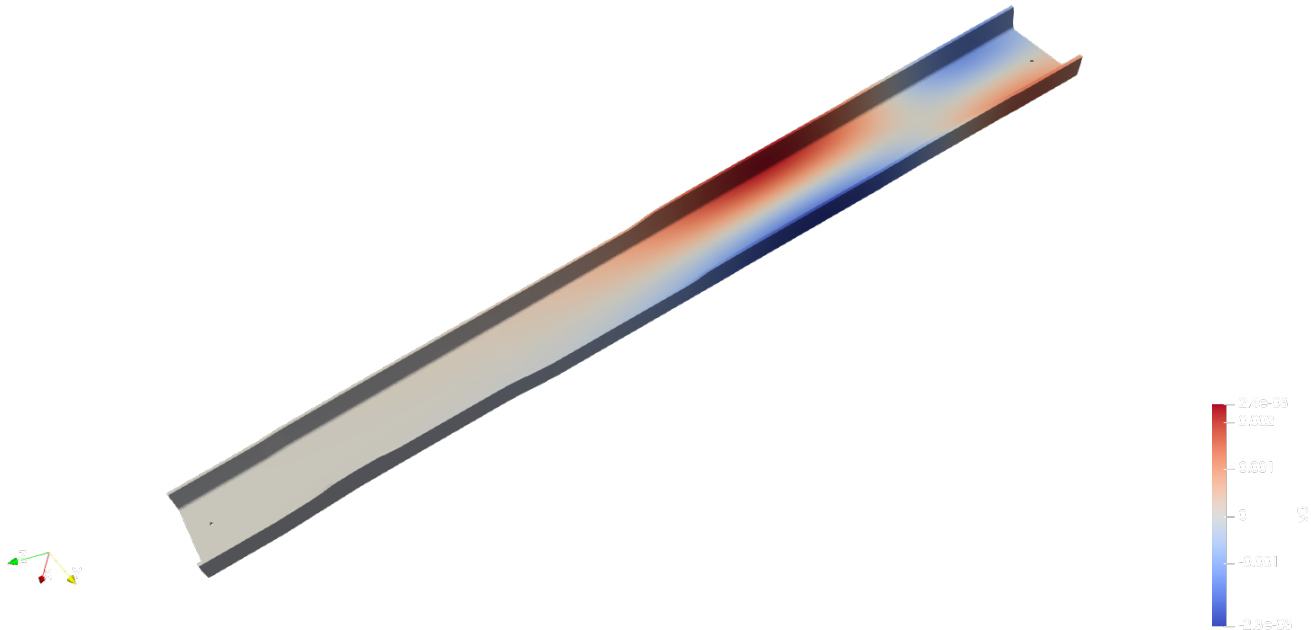


Figure: SquaredExponential model, 224515 nodes, HMAT (30.1 s)

Karhunen-Loeve decomposition IV

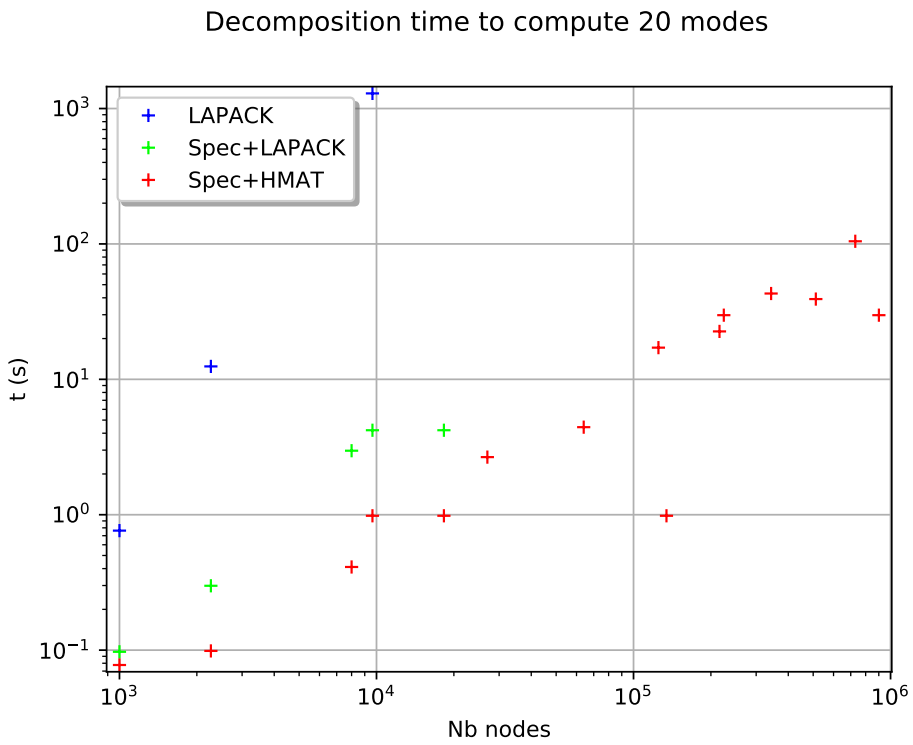
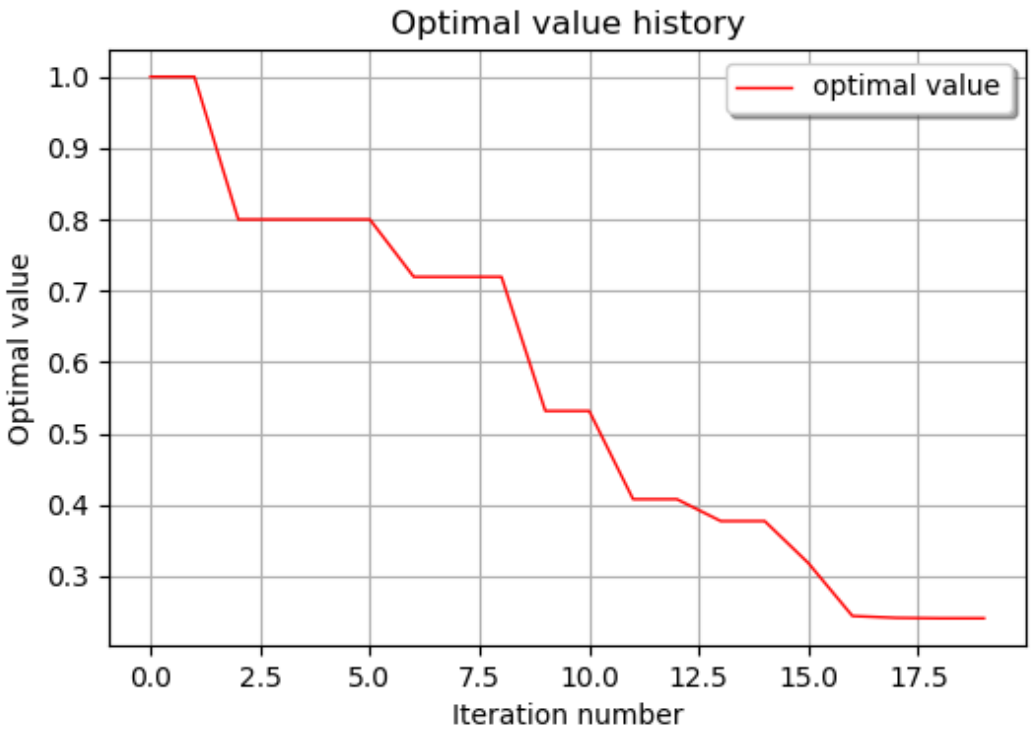


Figure: Decomposition time using LAPACK, Spectra/LAPACK and Spectra/HMAT

Optimization solvers

- Dlib (continuous, general-purpose: CG, BFGS, LBFGS, Newton, GLOBAL, LSQ, TrustRegion)
- Ipopt (continous, large dimension)
- Bonmin (mixed, large dimension: NLP BB, Outer-approx decomp, Quesada and Grossmann's BC, Hybrid outer-approx BC, Iterated feasibility pump)



Performance improvements

- TBB/OpenBLAS parallel regions conflict: huge penalty
- TBB-enabled Windows binaries
- KernelMixture.computePDF x10 speed
- Speed-up Tensor metamodel evaluation: x2
- ODE solvers speedup
- Memory leaks in Python/SWIG layer

Python layer improvements

- Sample improvements

```
x = ot.Sample([[42.0]*3]*8)

# by description marginal accessors
x.getMarginal(['v1', 'v2'])

# get points #2, #5, #6
x[[2, 5, 6]]

# __contains__ operator
[42]*3 in x
=> True
```

Other improvements

- Documentation: added examples
- Bugfixes (and reports), lots of them!
- Gitter chat
- New version of otagrum module

END

Thank you for your attention!
Any questions?