

# Chaospy:

## A modular implementation of Polynomial Chaos expansions and Monte Carlo methods

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Supervisors:

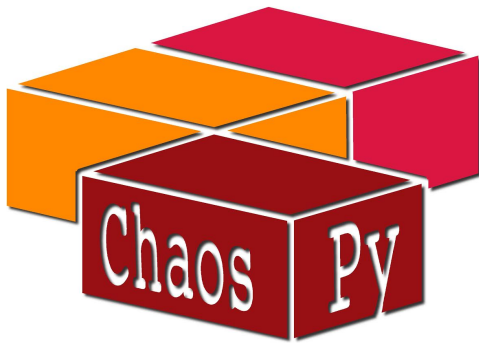
Jonathan Feinberg

Hans Petter Langtangen

Gaute Einevoll

Geir Halmes

University of Oslo, CINPLA



# Chaospy is a Python toolbox for forward model UQ

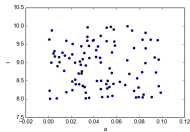


## Properties of Chaospy

# Chaospy is a Python toolbox for forward model UQ



## Properties of Chaospy

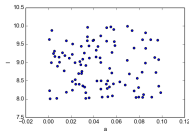


## Monte Carlo methods

# Chaospy is a Python toolbox for forward model UQ



## Properties of Chaospy



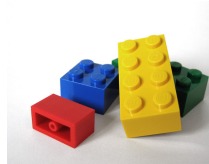
## Monte Carlo methods

$$\sum_{n=0}^N c_n(x) P_n(q)$$

## Polynomial Chaos

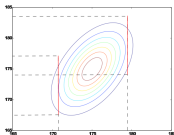
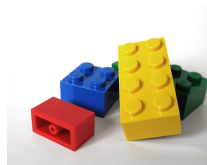
# What is new in Chaospy

**Chaospy is modular and  
therefore very flexible**



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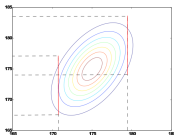
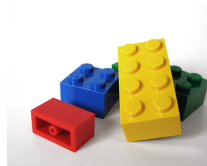
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**Chaospy has support for  
dependent variables**

# What is new in Chaospy

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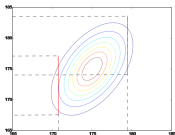
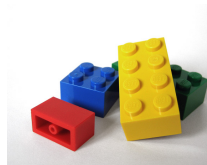


Chaospy has support for dependent variables

**Chaospy has a large collection of methods and distributions**

# What is new in Chaospy

Chaospy is modular and therefore very flexible



Chaospy has support for dependent variables

Chaospy has a large collection of methods and distributions

**It is easy to compare different methods on given a problem**



# Comparing Chaospy with Turns and Dakota

Feature	Dakota	Turns	Chaospy
Distributions	11	26	64
Copulas	1	7	6
Sampling schemes	4	7.5	7
Orthogonal polynomial schemes	4	3	5
Numerical integration strategies	7	0	7
Regression methods	5	4	8
Analytical metrics	6	6	7

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- ▶ Intrusive and non-intrusive polynomial chaos
  - ▶ Pseudo-spectral method
  - ▶ Point collocation/regression

# All Chaospy needs is a Python wrapper around the forward model

```
def solver(*node):  
    # node: tuple of the uncertain stochastic parameters  
  
    model.set_parameters(node)
```



Chaos Py

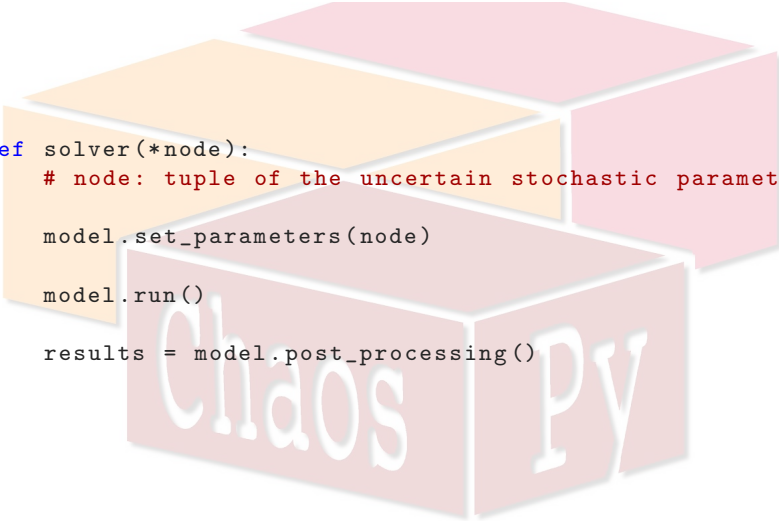


# All Chaospy needs is a Python wrapper around the forward model

```
def solver(*node):  
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    model.run()
```

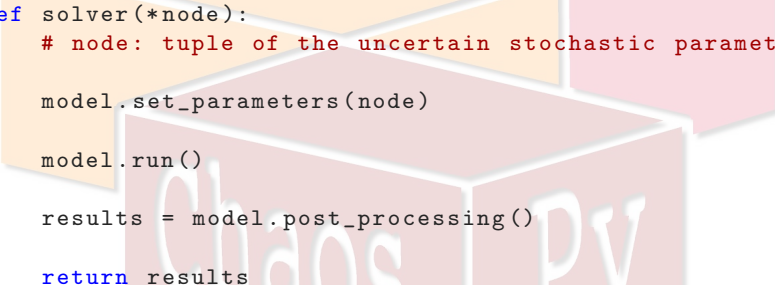
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def solver(*node):  
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    model.run()  
  
    results = model.post_processing()  
  
    return results
```

Chaospy is a completely generic software; for simplicity we use a very simple example problem

$$\frac{du(x)}{dx} = -au(x), \quad u(0) = I.$$

$u$  The quantity of interest.

$x$  Spatial location.

$a, I$  Parameters containing uncertainties.

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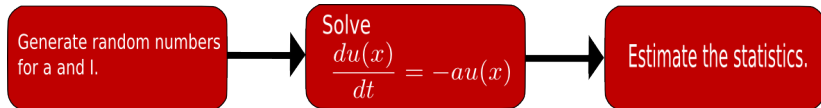
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We want to compute  $E(u)$  and  $\text{Var}(u)$ .

# Monte Carlo integration can be used for any model



# Monte Carlo with Chaospy

```
import chaospy as cp  
import numpy as np
```



Chaos Py



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import chaospy as cp
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dist_a = cp.Uniform(0, 0.1)
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Chaos Py

# Monte Carlo with Chaospy

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import chaospy as cp
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dist_a = cp.Uniform(0, 0.1)
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# Joint distribution
dist = cp.J(dist_a, dist_I)
```



Chaos Py

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dist_a = cp.Uniform(0, 0.1)
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samples = dist.sample(size=1000)
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Chaos Py

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# solver returns u(x), where x is fixed
# solver_u: list of all u(x) for each set of a and I
samples_u = [solver(a, I) for a, I in samples]
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# Monte Carlo with Chaospy

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samples_u = [solver(a, I) for a, I in samples]

E = np.mean(samples_u, 0)
Var = np.var(samples_u, 0)
```

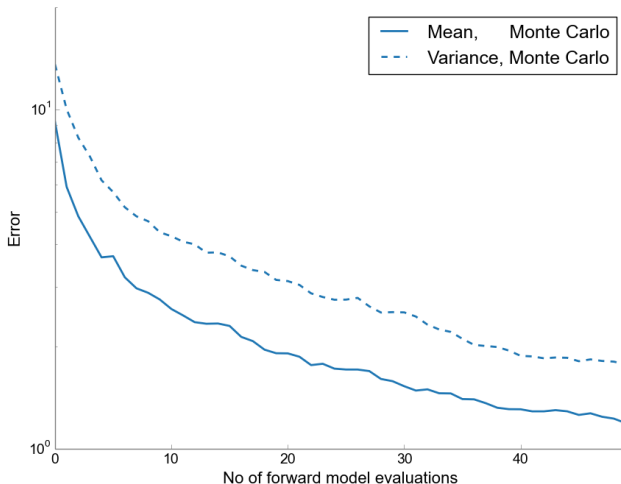
## Convergence of Monte Carlo is slow

$$\varepsilon_E = \int |E(u) - E(\hat{u})| dx \qquad \varepsilon_{Var} = \int |\text{Var}(u) - \text{Var}(\hat{u})| dx$$

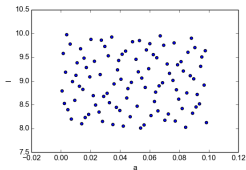
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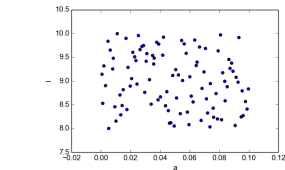
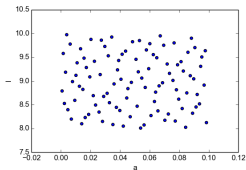


# Chaospy has several variance reduction techniques for sampling a distribution



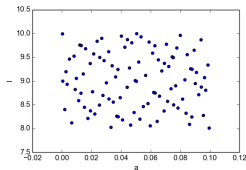
Hammersley sampling:

```
nodes = dist.sample(100, "M")
```



Latin Hypercube sampling:

```
nodes = dist.sample(100, "L")
```



Halton sampling

```
nodes = dist.sample(100, "H")
```

Sobol sampling

```
nodes = dist.sample(100, "S")
```



# The different sampling schemes available in Chaospy compared to Turns and Dakota

	Dakota	Turns	Chaospy
Quasi-Monte Carlo scheme			
Faure sequence	No	Yes	No
Halton sequence	Yes	Yes	Yes
Hammersley sequence	Yes	Yes	Yes
Haselgrove sequence	No	Yes	No
Korobov lattice	No	No	Yes
Niederreiter sequence	No	Yes	No
Sobol sequence	No	Yes	Yes
Other methods			
Antithetic variables	No	No	Yes
Importance sampling	Yes	Yes	Yes
Latin Hypercube sampling	Yes	Limited	Yes

# Quasi-Monte Carlo with Latin Hypercube sampling

```
import chaospy as cp
import numpy as np

dist_a = cp.Uniform(0, 0.1)
dist_I = cp.Uniform(8, 10)
dist = cp.J(dist_a, dist_I)

samples = dist.sample(size=1000)

samples_u = [solver(a, I) for a, I in samples]

E = np.mean(samples_u, 0)
Var = np.var(samples_u, 0)
```

# Quasi-Monte Carlo with Latin Hypercube sampling

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import chaospy as cp
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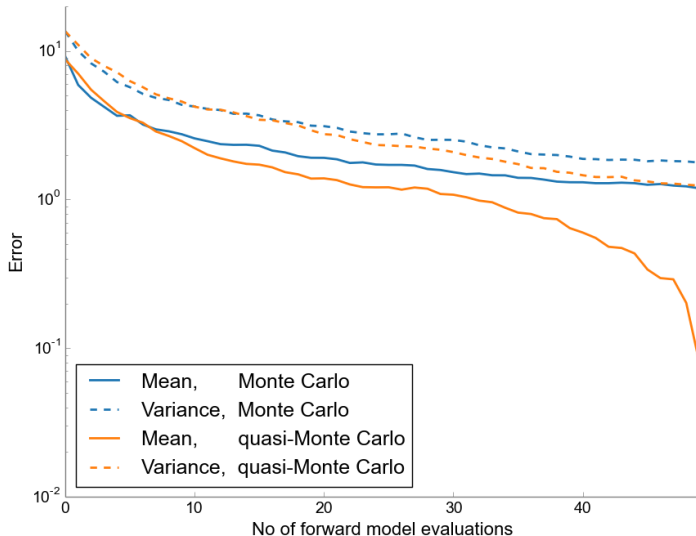
dist_a = cp.Uniform(0, 0.1)
dist_I = cp.Uniform(8, 10)
dist = cp.J(dist_a, dist_I)

samples = dist.sample(size=1000, rule="L")

samples_u = [solver(a, I) for a, I in samples]

E = np.mean(samples_u, 0)
Var = np.var(samples_u, 0)
```

# Convergence of quasi-Monte Carlo is better than Monte Carlo, but still slow



Mapping in probability space; the idea behind Polynomial Chaos (PC) theory is to approximate our forward model with a polynomial

$$u(x; q) \approx \hat{u}_M(x; q) = \sum_{n=0}^N c_n(x) P_n(q)$$

Coefficient      Polynomial

$\hat{u}_M(x; q)$  is the mapping from the uncertain variables  $q$  to the response variable  $u$ ,  $x$  is a set variable.

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$P_n$  are orthogonal polynomials and are generally calculated through the three-term discretized Stiltjes recursion

```
dist = cp.Normal()
```

```
P = cp.orth_ttr(3, dist)
```

Chaos Py

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```
dist = cp.Normal()
P = cp.orth_ttr(3, dist)
print P
[1.0, q0, q0^2-1.0, q0^3-3.0q0]
```

Chaos

Py

# Methods for generating expansions of orthogonal polynomials

Orthogonalization Method	Dakota	Turns	Chaospy
Askey–Wilson scheme	Yes	Yes	Yes
Bertran recursion	No	No	Yes
Cholesky decomposition	No	No	Yes
Discretized Stieltjes	Yes	No	Yes
Modified Chebyshev	Yes	Yes	No
Modified Gram–Schmidt	Yes	Yes	Yes

The pseudo-spectral method, used to calculate  $c_n$ , needs numerical integration, which demands generating quadrature nodes and weights

```
dist = cp.Normal()
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nodes, weights = cp.generate_quadrature(2, dist, rule="G")
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```
dist = cp.Normal()

nodes, weights = cp.generate_quadrature(2, dist, rule="G")

print nodes
[[-1.73205081  0.          1.73205081]]
print weights
[ 0.16666667  0.66666667  0.16666667]
```

# Numerical integration strategies implemented in the three software toolboxes

Node and weight generators	Dakota	Turns	Chaospy
Clenshaw-Curtis quadrature	Yes	No	Yes
Cubature rules	Yes	No	No
Gauss-Legendre quadrature	Yes	No	Yes
Gauss-Patterson quadrature	Yes	No	Yes
Genz-Keister quadrature	Yes	No	Yes
Leja quadrature	No	No	Yes
Monte Carlo integration	Yes	No	Yes
Optimal Gaussian quadrature	Yes	No	Yes

# One slide is enough for the full implementation with the pseudo-spectral method in Chaospy

```
dist_a = cp.Uniform(0, 0.1)
dist_I = cp.Uniform(8, 10)
dist = cp.J(dist_a,dist_I)
```

The logo for Chaospy is composed of three 3D rectangular blocks. Two blocks are light orange and are positioned behind a larger, light pink block. The pink block is in the foreground and has the words "Chaos" and "Py" written on its front face in a white, serif font. The "Chaos" is on the left and "Py" is on the right, separated by a vertical line.

Chaos Py

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The logo for Chaospy, consisting of the words "Chaos" and "Py" in a white, serif font, positioned on the front face of a large, 3D pink cube. The cube is part of a larger arrangement of three cubes: one pink cube in the background, one orange cube to the left, and this pink cube in the foreground. The cubes are slightly offset from each other, creating a sense of depth.

Chaos Py



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samples_u = [solver(*node) for node in nodes.T]
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samples_u = [solver(*node) for node in nodes.T]

u_hat = cp.fit_quadrature(P, nodes, weights, samples_u,
                           rule="Gaussian")
```

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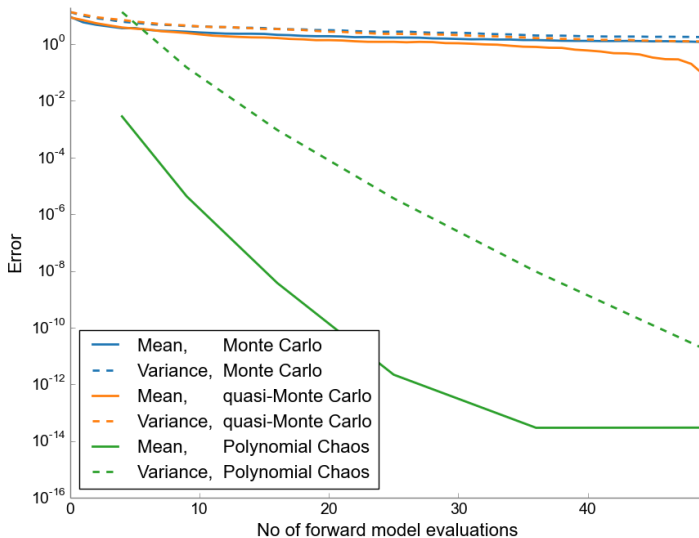
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u_hat = cp.fit_quadrature(P, nodes, weights, samples_u,
                          rule="Gaussian")

mean = cp.E(u_hat, dist)
var = cp.Var(u_hat, dist)
```

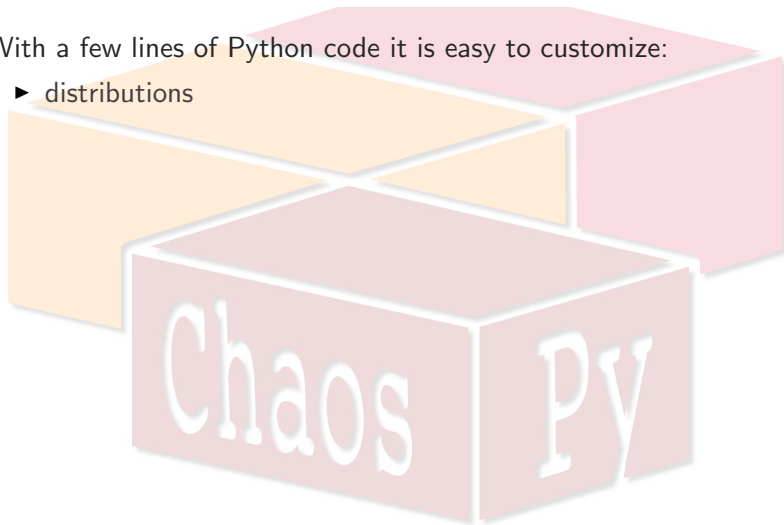
# Convergence of polynomial chaos is much faster than the Monte Carlo methods



# Chaospy is an ideal tool for research in UQ for the statistics expert

With a few lines of Python code it is easy to customize:

- distributions



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Chaos Py

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Chaos

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Chaos

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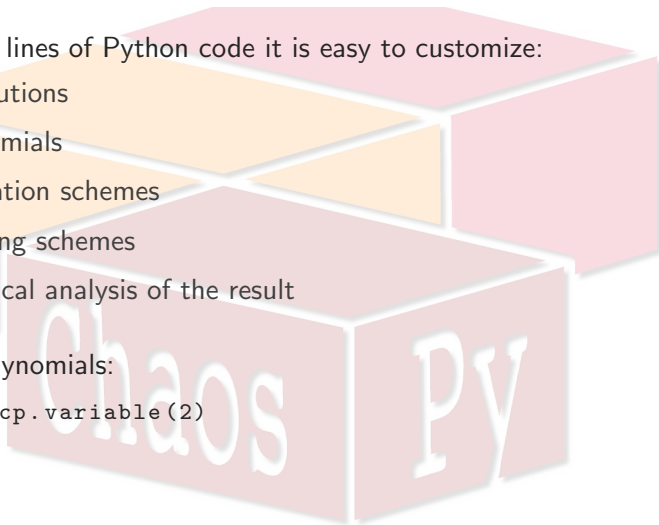
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Custom polynomials:

```
q0, q1 = cp.variable(2)
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Custom polynomials:

```
q0, q1 = cp.variable(2)
phi = cp.Poly([1, q0, q1, q0**2 - 1, q0*q1])
```

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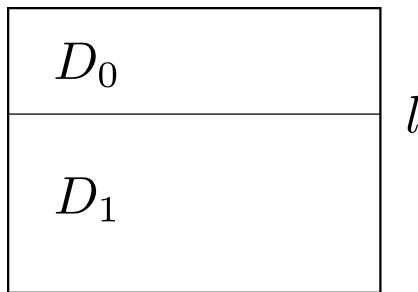
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phi = cp.Poly([1, q0, q1, q0**2 - 1, q0*q1])

print phi
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```

# Chaospy handles Polynomial Chaos expansions with stochastically dependent variables

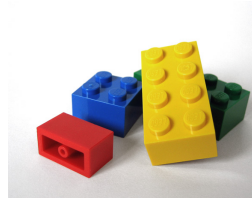
Diffusion in layered media with uncertain boundary,  $l$ , and uncertain diffusion constants,  $D_0$ ,  $D_1$ .



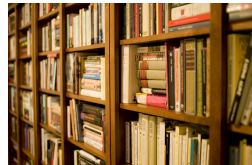
Uncertain  $l$  slows down convergence, but introduction of auxiliary *dependent* variables restores convergence.

# Summary: Chaospy is a Python toolbox for forward model UQ with advanced Monte Carlo methods and Polynomial Chaos expansions

Chaospy is modular, flexible,  
with syntax that resembles  
the mathematics



A vast collection of methods,  
ideal for method comparisons





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## Installation instructions:

<https://github.com/hplgit/chaospy>

## Reference:

Feinberg, J., & Langtangen, H. P. (2015). Chaospy: An open source tool for designing methods of uncertainty quantification. *Journal Of Computational Science*, 11, 46-57

<http://hplgit.github.io/chaospy/doc/pub/chaospy-4screen.pdf>



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## Reference:

Feinberg, J., & Langtangen, H. P. (2015). Chaospy: An open source tool for designing methods of uncertainty quantification. *Journal Of Computational Science*, 11, 46-57

<http://hplgit.github.io/chaospy/doc/pub/chaospy-4screen.pdf>

Questions?

