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Using Python for scientific computing: Efficient and flexible evaluation of the statistical characteristics of functions with multivariate random inputs[☆]

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ABSTRACT

This paper examines the feasibility of high-level Python based utilities for numerically intensive applications via an example of a multidimensional integration for the evaluation of the statistical characteristics of a random variable. We discuss the approaches to the implementation of mathematically formulated incremental expressions using high-level scripting code and low-level compiled code. Due to the dynamic typing of the Python language, components of the algorithm can be easily coded in a generic way as algorithmic templates. Using the Enthought Development Suite they can be effectively assembled into a flexible computational framework that can be configured to execute the code for arbitrary combinations of integration schemes and versions of instantiated code. The paper describes the development cycle using a simple running example involving averaging of a random two-parametric function that includes discontinuity. This example is also used to compare the performance of the available algorithmic and executional features. The implemented package including further examples and the results of performance studies have been made available via the free repository [1] and CPCP library.

Program summary

Program title: spirrid

Catalogue identifier: AENL_v1_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AENL_v1_0.html

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: Special licence provided by the author

No. of lines in distributed program, including test data, etc.: 10722

No. of bytes in distributed program, including test data, etc.: 157099

Distribution format: tar.gz

Programming language: Python and C.

Computer: PC.

Operating system: LINUX, UNIX, Windows.

Classification: 4.13, 6.2.

External routines: NumPy (http://numpy.scipy.org/), SciPy (http://www.scipy.com)

Nature of problem:
Evaluation of the statistical moments of a function of random variables.

Solution method:
Direct multidimensional integration.

[☆] This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).
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Running time:
Depending on the number of random variables the time needed for the numerical estimation of the mean value of a function with a sufficiently low level of numerical error varies. For orientation, the time needed for two included
examples: examples/fiber_tt_2p/fiber_tt_2p.py with 2 random
variables: few milliseconds
examples/fiber_po_8p/fiber_po_8p.py with 8 random
variables: few seconds

1. Introduction

High-level languages for scientific computing offer application programmers a convenient and efficient tool for the formulation and implementation of mathematical models. Examples of widely used high-level software for the rapid prototyping of scientific applications are Maple, Matlab, Octave, R and S+. These tools provide rich documentation, visualization utilities, symbolic operators and a large number of numerical methods. The suitability of the Matlab toolkit for the prototyping of numerical applications and for teaching courses has been discussed e.g. in [2]. Compared to the low-level programming languages like FORTRAN and C or C++ these high-level tools make development more productive, especially at the early stages of application development. On the other hand, such high-level tools can seldom compete with the performance of applications written in compiled languages. The trade-off between flexibility and efficiency is a daily issue for application programmers in the area of scientific computing. An ideal development environment should provide both high productivity at the early stages of development and, at the same time, an easy way to accelerate code execution once the application has reached a mature state.

A particularly appealing development environment has emerged during the last decade in the area of open source software. The scripting language Python has established a platform for developing and integrating two rich numerical libraries `numpy` and `scipy`. These libraries embody algorithms and methods developed over the past decades in the compiled languages FORTRAN and C++ (http://www.netlib.org). The flexibility of scripting in Python applied to scientific applications has been thoroughly presented in the textbook [3]. As further documented in [4,5], the high flexibility of the scripting language is not necessarily accompanied by a lower efficiency with respect to the compiled code. Indeed, when implementing mathematical expressions in vectorized form using compact array representation [6], the trade-off between flexibility and efficiency is reduced to an acceptable level [7].

Besides the comparison with the compiled low-level languages, the productivity and efficiency of the Python development environment has been compared with Matlab and Octave using several benchmark examples [8,9]. These studies came to the conclusion that the functionality of the Python based environment is comparable with that of commercial tools. However, in the authors' opinion, the Python environment has a decisive advantage in one crucial area: it has an open and extensible object model behind its language so that it can evolve further. The possibility of extending the class definition in the language using metaclasses allows the incorporation of design patterns into the language that further increase the productivity of developers. In particular, the Enthought Tool Suite (http://www.enthought.com) has introduced a refined definition of a class using predefined traits [10]. A class trait corresponds to the usual attribute in an object-oriented language but extends it with information on initialization, validation, notification of changes and visualization. Such an extended attribute specification has been used to incorporate the Model-View-Controller design pattern into the language and provide automatic object visualization and dynamic control of state changes with minimum programming effort. This semantically rich language support allows developers to benefit from automatic generation of the user interface directly from the class view specification, persistence of objects, declaration of state dependencies and effective support for data visualization.

This paper reports on the feasibility of the Python-based environment for the development of scientific applications. The concepts, observations and conclusions made here are relevant for readers interested in three disciplines: estimation of statistical moments, programming of scientific computing applications and simulation of fiber bundles and/or of brittle matrix composites. Throughout this paper, the applied implementation concepts are demonstrated on the estimation of statistical moments of the stress–strain response of a set of parallel fibers. This task corresponds to the estimation of the statistical moments of an "elementary" function with random parameters. An example of such a function describing the stress–strain response of a fiber loaded in tension with two independent, identically distributed random parameters for stiffness and strength is shown in Fig. 1, left. Random realizations of the single fiber's response are displayed in Fig. 1, right. The goal is to efficiently estimate the mean response of a fiber within the bundle, which is plotted as the solid black line in Fig. 1, right.

The implementation of this specific example has been generalized so that it is applicable for the statistical characterization of an arbitrary function with independent random parameters. The implemented framework falls into the domain of multivariate analysis packages, as does `pychem` [11]. We shall demonstrate that when using the aforementioned implementation environment, the abstract nature of the mathematical formulation can be reflected in the code without any additional performance penalty. The particular motivation of the paper is to

- show the rapid prototyping of an application starting with a simple Python script,
- show how to generalize and scale up the script to a configurable algorithmic object that can incorporate several variants of random sampling and options for the speeding up of the code,
- provide a framework for the verification of results and for studies of execution efficiency for all available features of the implementation.

The paper is organized as follows. First, the symbolic specification of the implemented algorithms is presented in Section 2. After that, simple implementations of the algorithm in pure Python on the one hand and using the `numpy` and `scipy` packages on the other hand are constructed in Section 3. Next, the algorithm implementation is generalized to incorporate other types of sampling and languages (Section 4). The introduced variants of the algorithm are then merged in the general interactive framework for multidimensional integration in Section 5 using Enthought traits as a glue. The configurable package allows for a thorough comparison of the efficiency of several versions of the sampling types described in

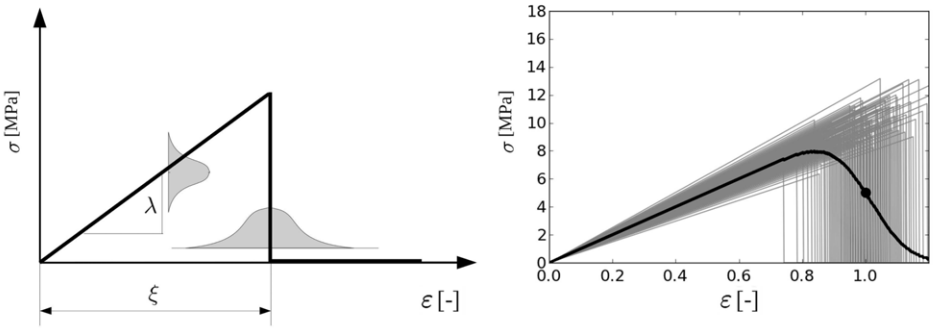


Fig. 1. Left: elementary response described by a function with two random parameters; Right: sample of random responses (gray) and the calculated mean response (black).

Section 8. The execution efficiency is compared for three types of code generated and compiled on the fly for the current response function and its randomization in Section 9. The code segments provided throughout the paper constitute an executable script included in the `spirrid` package that is available for downloading from the online CPCP Library and in the github.com repository [1].

2. Estimation of statistical moments of a function with independent random variables

The goal is to estimate the statistical moments of a random problem Q given as a function of a control variable ε and of random variables $\theta_1 \cdots \theta_m$ constituting the random domain $\boldsymbol{\Theta}$:

$$Q = q\left(\varepsilon; \theta_1, \ldots, \theta_m\right) \tag{1}$$

with $q(\varepsilon; \boldsymbol{\theta})$ further referred to as a response function. The k-th raw statistical moment of such a random problem is given as

$$\mu_k(\varepsilon) = \int_{\boldsymbol{\Theta}} \left[q\left(\varepsilon; \boldsymbol{\theta}\right)\right]^k g(\boldsymbol{\theta})\, d\boldsymbol{\theta}. \tag{2}$$

Since only independent random variables are considered here, the joint probability density function $g(\boldsymbol{\theta})$ (PDF) of the random vector $\boldsymbol{\theta}$ can be replaced with the product of univariate marginal densities

$$\mu_k(\varepsilon) = \int_{\Theta_1} \cdots \int_{\Theta_m} \left[q\left(\varepsilon; \boldsymbol{\theta}\right)\right]^k \times g_1(\theta_1) \cdots g_m(\theta_m)\, d\theta_1 \cdots d\theta_m. \tag{3}$$

The integration is to be performed numerically as a summation of discrete values distributed over the discretized random domain

$$\mu_k(\varepsilon) = \sum_{\Theta_1} \cdots \sum_{\Theta_m} \underbrace{\left[q\left(\varepsilon; \theta_1 \cdots \theta_m\right)\right]^k}_{Q^k} \times \underbrace{\Delta G_1(\theta_1) \cdots \Delta G_m(\theta_m)}_{\Delta G}, \tag{4}$$

where $\Delta G_i(\theta_i)$ denote the weighting factors that depend on the particular type of sampling as specified below. The distribution of the integration points Θ_m within the random domain can be expressed as

$$\Theta_i = [\theta_{ij}, j \in 1 \cdots n_i], \quad i \in 1 \cdots m, \tag{5}$$

where n_i is the number of discretization points for the i-th variable and j counts the discretization point along a variable. There are many ways to cover the random domain by sampling points. In order to demonstrate the expressive power of the language and to discuss the computational efficiency of the possible implementation techniques we shall implement the integral (3) in four different ways:

I. *Equidistant grid of random variables (TGrid)*. The i-th random variable is covered by regularly spaced values θ_{ij}. The probability associated with an integration cell is given as

$$\Delta G_i(\theta_{ij}) = g_i(\theta_{ij}) \Delta\theta_i \tag{6}$$

with $\Delta\theta_i$ denoting the spacing between discretization points.

II. *Non-equidistant grid of random variables*. Sampling points are generated through an equidistant grid of sampling probabilities π_{ij} (PGrid). The transformation of sampling probabilities into the random domain Θ in Eq. (5) is performed for each random variable enumerated as $i = 1 \cdots m$ using the inverse cumulative distributions (also referred to as percent point function):

$$\theta_{ij} = G_i^{-1}\left(\pi_{ij}\right) \tag{7}$$

where the values π_{ij} are obtained as

$$\pi_{ij} = \frac{j - \frac{1}{2}}{n_i}, \quad j \in 1 \cdots n_i. \tag{8}$$

The integration cells rendered through this kind of sampling share the same probability (weight) for each variable:

$$\Delta G_i(\theta_{ij}) = \frac{1}{n_i} \tag{9}$$

and each integration cell has an equal probability in the m-dimensional space of random variables

$$\Delta G(\theta) = \prod_{i=1}^{m} \frac{1}{n_i}. \tag{10}$$

This type of sampling is introduced here as a combination of the grid-type of sampling with the concept of the Monte Carlo type of sampling with constant integration cell probability.

III. *Crude Monte Carlo Sampling (MCS)*. Instead of using a structured grid of π_{ij} as given in Eq. (8) the sampling probabilities are selected randomly from $\pi_{ij} \in \langle 0, 1 \rangle$ and the corresponding sampling points are selected according to Eq. (7). The underlying data structure of Θ_i arrays can be flattened as the number of sampling points $n_i = n_{\mathrm{sim}}$ is equal for all random variables and integration can be done in a single loop as

$$\mu_k(\varepsilon) = \sum_{j=1}^{n_{\mathrm{sim}}} \underbrace{\left[q\left(\varepsilon; \theta_{1j}, \ldots, \theta_{mj}\right)\right]^k}_{Q^k} \cdot \frac{1}{n_{\mathrm{sim}}}. \tag{11}$$

IV. *Latin Hypercube Sampling (LHS)*. An enhanced version of Monte Carlo type sampling which uses stratification of the distribution functions of input random variables to ensure uniform coverage of the sampling probabilities [12–14]. An LHS sample tends to be more uniformly distributed through the unit hypercube of sampling probabilities π_{ij} than a Monte Carlo sample. As a result, the variance of the statistics estimators such as the one in Eq. (11) is usually reduced in comparison with MCS. Indeed, Stein [15] has shown that LHS reduces the variance compared to simple random sampling (crude Monte Carlo). The amount of variance reduction increases with the degree of additivity and monotonicity in the random quantities on which the function q depends.

Similarly as in the case of MCS, the underlying data structure can be flattened and integration can be performed in a single loop as prescribed in Eq. (11). The sampling points in Eq. (7) are obtained through sampling probabilities calculated as:

$$\pi_{ij} = \frac{r_{ij} - \frac{1}{2}}{n_{\mathrm{sim}}}, \quad j = 1 \cdots n_{\mathrm{sim}} \tag{12}$$

with r_{ij} representing an (m, n_{sim}) matrix containing random permutations of a sequence $1, \ldots, n_{\mathrm{sim}}$ on each row. By using this scheme, the *medians* of each stratum are selected as sampling points.

Further improvements of the method can be achieved by selecting probabilistic means in each stratum [16]. We remark that the random ordering of sampling probabilities does not ensure an exact unit correlation matrix of simulated data especially for small sample sizes, see [17]. A possible remedy has been proposed in [16] by employing an algorithm diminishing the undesired correlation of the sample.

In order to make the explanation of the implementation illustrative let us introduce a simple two-parametric response function depicted in Fig. 1 (left) as

$$q(\varepsilon; \lambda, \xi) = \lambda\, \varepsilon \cdot H\,(\xi - \varepsilon)\,. \tag{13}$$

This function defines the stress for a given positive control strain ε of a linear elastic, brittle fiber with the stiffness parameter λ and breaking strain ξ. The symbol $H(x)$ represents the Heaviside function yielding zero for $x < 0$ and one for $x \geq 0$. We deliberately chose a function containing discontinuity in order to study the ability of the integration algorithm to reproduce the smoothness of the average response of an ensemble with a constituent response governed by a non-smooth function. If many fibers act in parallel, as is the case in a crack bridge in a composite, they exhibit imperfections. This means that the material parameters λ and ξ must be considered random. The mean stress–strain behavior of a fiber within a bundle can be obtained using Eq. (4) as

$$\mu_q(\varepsilon) = \sum_{\Theta_\lambda} \sum_{\Theta_\xi} \underbrace{q\,(\varepsilon; \lambda, \xi)}_{Q}\; \underbrace{g_\lambda g_\xi\;\, \Delta\theta_\lambda \Delta\theta_\xi}_{\Delta G}\,. \tag{14}$$

The result of this expression is plotted in Fig. 1 (right, black curve). It demonstrates that the average response of the filament is nonlinear. The described integral exhibits the structure of a strain-based fiber bundle model describing the behavior of yarns and composite materials [18]. The authors have used the procedure for modeling the tensile tests of multi-filament yarns [19].

3. Scripting implementation of an equidistant integration scheme

In order to demonstrate the possible approaches to the implementation of the numerical model, let us construct a short script delivering the result of Eq. (14). In the first step we define the probability distributions of the parameters λ and ξ as normal and generate an equidistant discretization of the random domains Θ_λ and Θ_ξ with 20 values together with the values of marginal densities g_λ and g_ξ.

```
from scipy.stats.distributions import norm                  1
import numpy as np                                          2
# set the mean and standard deviation of la and xi          3
m_la, std_la = 10.0, 1.0                                    4
m_xi, std_xi = 1.0, 0.1                                     5
# construct objects representing normal distributions       6
pdistrib_la = norm(loc=m_la, scale=std_la)                  7
pdistrib_xi = norm(loc=m_xi, scale=std_xi)                  8
# get operators for probability density functions           9
g_la = pdistrib_la.pdf                                      10
g_xi = pdistrib_xi.pdf                                      11
# number of integration points set equal for both variables 12
n_i = 10                                                    13
# generate midpoints of n_i intervals in the range (-1,1)   14
theta_arr = np.linspace(-(1.0 - 1.0 / n_i),                 15
                         1.0 - 1.0 / n_i, n_i)              16
# scale up theta_arr to cover the random domains            17
theta_la = m_la + 4 * std_la * theta_arr                    18
theta_xi = m_xi + 4 * std_xi * theta_arr                    19
# get the size of the integration cells                     20
d_la = (8 * std_la) / n_i                                   21
d_xi = (8 * std_xi) / n_i                                   22
```

Note that the random domain has been covered by an equidistant set of integration points generated in two steps: First, the range $\langle -1, 1 \rangle$ was covered by an array of midpoints of n_i integration intervals at line 15. Second, the range was centered around the mean value and scaled up by four standard deviations at lines 18–19 in order to sufficiently cover the non-zero domain of the normal distribution. The response function itself is implemented consistently with Eq. (13)[1]

```
def Heaviside(x):                                           23
    """Heaviside function."""                               24
    return x >= 0.0                                         25
                                                            26
def q_eq13(eps, la, xi):                                    27
    """Response function of a single fiber."""              28
    return la * eps * Heaviside(xi - eps)                   29
```

Note that the use of the control statements `if` and `else` has been avoided. Instead, a Heaviside function returning Boolean values is used in order to allow arrays as parameters of the response function.[2] This is necessary to permit a vectorized evaluation of the function as shall be explained later on.

A simple implementation of the summation expression in Eq. (14) would consist of three loops: one loop for gathering the response values along the control variable ε and two loops along the random variable domains Θ_λ and Θ_ξ:

```
def mu_q_eq14_loops(eps_arr):                               30
    """Loop-based calculation of mean values."""            31
    mu_q_arr = np.zeros_like(eps_arr)                       32
    for i, eps in enumerate(eps_arr):                       33
        mu_q = 0.0                                          34
        for la in theta_la:                                 35
            for xi in theta_xi:                             36
                dG = g_la(la) * g_xi(xi) * d_la * d_xi      37
                mu_q += q_eq13(eps, la, xi) * dG            38
        mu_q_arr[i] = mu_q                                  39
    return mu_q_arr                                         40
                                                            41
# construct an array of control strains                     42
eps_arr = np.linspace(0, 1.2, 80)                           43
mu_q_arr = mu_q_eq14_loops(eps_arr)                         44
```

[1] Code blocks in Python are introduced by indentation levels.

[2] Another option would be to use masked arrays skipping the array values associated with the `True` value of the logical expression defining the mask. However, as we shall comment in Section 9 this option is connected with significant losses of performance.

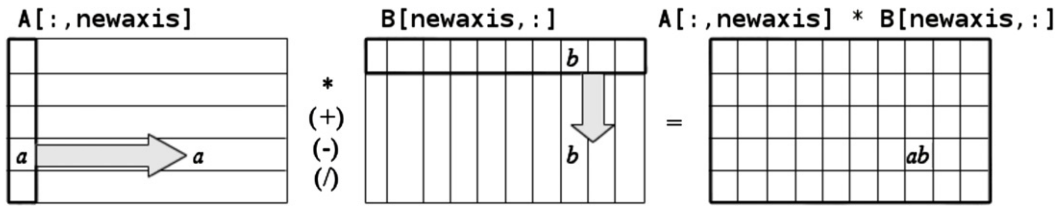


Fig. 2. Broadcasting as a tool to construct a cross product between two arrays.

This implementation is naive and extremely slow and is introduced here solely for illustrative purposes. The above script is about 1000 times slower than the same code written in the C language. It is obvious that in this form Python code cannot compete with FORTRAN or C compiled code.

Efficient and more competitive Python code can be produced using the numerical package numpy. The basic concept behind speeding up the code is to avoid interpreted loops in the implementation by using the array-based operators of numpy. Consistent with Eq. (14), the terms Q and ΔG shall be calculated separately for all combinations of the parameters within the discretized random domain $\boldsymbol{\Theta} = \Theta_\lambda \times \Theta_\xi$ as two-dimensional arrays and, subsequently, the array-based product and summation operators of numpy are to be applied. The array containing the weight factors ΔG can be conveniently evaluated using the vectorized product operator over two numpy arrays:

```
dG_la = g_la(theta_la) * d_la                              45
dG_xi = g_xi(theta_xi) * d_xi                              46
dG_grid = dG_la[:,np.newaxis] * dG_xi[np.newaxis,:]        47
```

In the first two lines, 45–46, the PDF functions g_la and g_xi previously constructed at lines 10–11 are reused. However, now the random variables are represented as the arrays theta_la and theta_xi. The result of the call g_la(theta_la) is an array of PDF values for all values in theta_la. Such a vectorized evaluation is executed completely in the compiled code of the numerical library numpy. The loop over the array elements is not explicitly given in the code. Therefore, this kind of code is often somewhat imprecisely referred to as loopless.

The implicit loops are also used during the computation of the dG_grid at line 47 delivering the two-dimensional array of joint integration weights: $\Delta G_{\lambda\xi}(\theta_\lambda, \theta_\xi) = \Delta G_\lambda(\theta_\lambda) \cdot \Delta G_\xi(\theta_\xi), \;\; \forall \theta_\lambda \in \Theta_\lambda, \forall \theta_\xi \in \Theta_\xi$. Line 47 demonstrates the use of index operators in numpy to construct an outer product of two arrays in order to avoid slow Python loops. The machinery behind the implicit loops uses two concepts:

- A new dimension (np.newaxis) with the length of 1 was added to the one-dimensional arrays dG_la and dG_xi so that they became two-dimensional column (dG_la[:,np.newaxis]) and row (dG_xi[np.newaxis,:]) matrices, respectively. Note that the index operator [:] stands for a slice, i.e. all values along that dimension. Thus, the construct dG_xi[:,np.newaxis] reshapes an array and makes it open for operations with operands possessing the second dimension.
- The orthogonal shape of the arrays dG_la[:,np.newaxis] and dG_xi[np.newaxis,:] is used for "broadcasting" the data across dimensions, a concept illustrated in Fig. 2: If a column matrix A of the shape $(m, 1)$ is multiplied with a row matrix B of the shape $(1, n)$ the resulting matrix will have the shape (m, n). The nonexistent columns of A and nonexistent rows of B are augmented with the values from the first column and row, respectively, so that $a_{(i,2\cdots m)} = a_{(1,j)}$ and $b_{(2\cdots n,j)} = b_{(i,1)}$.

The described technique is applicable in multiple dimensions:

```
dG_grid = dG_t1[:,np.newaxis,np.newaxis] * \
    dG_t2[np.newaxis,:,np.newaxis] * \
    dG_t3[ np.newaxis,np.newaxis,:]
```

It significantly increases the speed of the code compared to pure Python due to the vectorized evaluation of the algorithm and is more than sufficient for the prototyping phase of application development. Further speedup is possible as shall be discussed later in Section 9.

Having constructed the array with probabilistic weights ΔG we may approach the array-based implementation of the response function $q(\varepsilon; \lambda, \xi)$ given in Eq. (13). We remark again that instead of using the control blocks if and else in the listing (lines 27–29) to introduce discontinuity (i.e. to distinguish whether or not the fiber is broken) a simple implementation of the Heaviside function has been used (lines 23–25). In this form, the function parameters la and xi can have both scalar or array values so that a "vectorized" evaluation of the function is possible. The use of if and else would only permit scalar parameters and no array-based, loopless evaluation would be possible.

In analogy to the probabilistic weights ΔG, the values Q of the response function can be obtained in a loopless manner using the broadcasting concept. The expression q(eps, theta_la[:,np.newaxis], theta_xi[np.newaxis,:]) evaluates the response function for all combinations of λ and ξ and stores them in a two-dimensional array. Thus, the expression in Eq. (14) previously implemented using loops at lines 34–39 can be reimplemented in a loopless form in the method

```
def mu_q_eq14(eps):                                   48
    """Loopless calculation of mean value."""         49
    q_grid = q_eq13(eps,                              50
                    theta_la[:,np.newaxis],           51
                    theta_xi[np.newaxis,:])           52
    q_dG_grid = q_grid * dG_grid                      53
    return np.sum(q_dG_grid)                          54
```

Note that q_grid and dG_grid have the same shape (n_i,n_i) so that the variable q_dG_grid calculated at line 53 contains element-by-element products of the response function values and associated probabilistic weights. At line 54, summation over all dimensions is performed to obtain the mean value.

By issuing for example the call mu_q_eq14(1.0) one obtains the mean response for the control variable 1.0, see the circle in Fig. 1, right. In order to get the stress for multiple values of the strain in a single call, the function mu_q_e14 can be vectorized[3] to permit an array as an input parameter:

```
mu_q_eq14_vct = np.vectorize(mu_q_eq14)               55
# eps_arr from line 43 reused here                    56
mu_q_arr = mu_q_eq14_vct(eps_arr)                     57
```

[3] The np.vectorize method performs a repeated evaluation of the supplied function over an array in a Python loop. Due to the lower efficiency of the vectorized operator it should only be used in outer loops of an application. For inner loops, either implicitly vectorized operators of numpy combined with broadcasting, or acceleration packages like cython or weave discussed later should be used.

Finally, plotting can be done using the `matplotlib` package. We shall use the `matlab`-like interface for `matplotlib` called `pylab`:

```
import pylab as p                                                58
p.plot(eps_arr, mu_q_arr)                                        59
p.show()                                                         60
```

This code produces the diagram shown in Fig. 1 (right) with the mean response shown as a black curve. The example demonstrates the prototyping step in the development of a numerical application. The script is limited to a particular response function and predefined randomization pattern.

4. Generalization for other sampling schemes

The abstract nature of the mathematical formulation (Eq. (4)) permits the use of an arbitrary type of the response function $q(\varepsilon;\boldsymbol{\theta})$ and probability distributions $g_i(\theta_i)$. It is desirable to preserve this flexibility of the mathematical model also in its implementation. The script implemented in the previous section uses the equidistant discretization given in Eq. (6). In order to implement the other three discretizations of the random domain mentioned in Section 2 we shall capture the discretization-independent part of the code in a generic algorithmic template. The following code exploits the fact that functions can be treated as variables in Python and defines the integration procedure without specifying the particular type of data structure for the sampling/integration points:

```
def get_mu_q_fn(q, dG, *theta):                                  61
    """Return a method evaluating the mean of q()."""            62
    def mu_q(eps):                                               63
        Q_dG = q(eps, *theta) * dG                               64
        return np.sum(Q_dG)                                      65
    return np.vectorize(mu_q)                                    66
```

The function `get_mu_q` instantiates the generic template for the integral in Eq. (14) and/or Eq. (11) for an arbitrary response function `q` and the list of variables `*theta` and `dG`. The code does not make any assumption about the particular type of input variables and thus it can be used to instantiate the integration procedures for all four sampling schemes introduced in Section 2. In this form, the code captures the algorithmic commonalities of the integration methods and remains open for further specializations:

I. *`TGrid` sampling*. The previously constructed values of the ΔG grid and Θ_i are reused to instantiate the template and calculate the results as

```
# SAMPLING:                                                      67
# ... reuse dG_grid and theta (lines 18, 19 and 45—47)           68
                                                                 69
# INSTANTIATION:                                                 70
mu_q_fn = get_mu_q_fn(q_eq13, dG_grid,                           71
                      theta_la[:,np.newaxis],                    72
                      theta_xi[np.newaxis,:])                    73
                                                                 74
# CALCULATION:                                                   75
mu_q_arr = mu_q_fn(eps_arr)                                      76
```

Note that in contrast with the first implementation (line 52), the broadcasting is now performed outside of the generic integration function at line 73 to keep the integration template open for a flattened sampling data structure.

II. *`PGrid` sampling*. The integration algorithm based on a grid of constant sampling probabilities can be instantiated using the code

```
# SAMPLING:                                                      77
# equidistant sampling probabilities (see Eq. 8)                 78
j_arr = np.arange(1, n_i + 1)                                    79
pi_arr = (j_arr - 0.5) / n_i                                     80
# use ppf (percent point function) to get sampling points        81
# (pdistrib_la and pdistrib_xi was defined at lines 7, 8)        82
theta_la = pdistrib_la.ppf(pi_arr)                               83
theta_xi = pdistrib_xi.ppf(pi_arr)                               84
# get the total number of integration points                     85
# for 2 random variables with equal n_i                          86
n_sim = n_i ** 2                                                 87
                                                                 88
# INSTANTIATION:                                                 89
mu_q_fn = get_mu_q_fn(q_eq13, 1.0 / n_sim,                       90
                      theta_la[:,np.newaxis],                    91
                      theta_xi[np.newaxis,:])                    92
                                                                 93
# CALCULATION:                                                   94
mu_q_arr = mu_q_fn(eps_arr)                                      95
```

Here, broadcasting is used again at line 92 and instead of a grid of weighted parameters (`dG_grid`) only a single value $\Delta G = 1/n_{\mathrm{sim}}$ is used for instantiation.

III. *`MCS` sampling*. The integration template can also be used for the non-regular discretization used in Monte Carlo sampling. For a comparison between grid sampling and the Monte Carlo types of sampling we shall consider an equal number of function evaluations, so that $n_{\mathrm{sim}} = \prod_{i=1}^{m} n_i$, where n_i represents the number of values along each of the m dimensions in the grid discretizations.

```
# SAMPLING:                                                      96
# generate n_sim random realizations                             97
# using pdistrib objects (lines 7, 8)                            98
theta_la_rvs = pdistrib_la.rvs(n_sim)                            99
theta_xi_rvs = pdistrib_xi.rvs(n_sim)                            100
                                                                 101
# INSTANTIATION:                                                 102
mu_q_fn = get_mu_q_fn(q_eq13, 1.0 / n_sim,                       103
                      theta_la_rvs, theta_xi_rvs)                104
                                                                 105
# CALCULATION:                                                   106
mu_q_arr = mu_q_fn(eps_arr)                                      107
```

The ΔG value is again constant. The integration code is now instantiated with flat arrays of sampled values.

IV. *`LHS` sampling*. The Latin Hypercube Sampling is constructed using a perturbation of n_{sim} values of θ_i obtained using the percent point function.

```
# SAMPLING:                                                      108
# sampling probabilities (see Eq. 12), n_sim as above            109
j_arr = np.arange(1, n_sim + 1)                                  110
pi_arr = (j_arr - 0.5) / n_sim                                   111
# get the ppf values (percent point function)                    112
# using pdistrib objects defined at lines 7, 8                   113
theta_la_ppf = pdistrib_la.ppf(pi_arr)                           114
theta_xi_ppf = pdistrib_xi.ppf(pi_arr)                           115
# make random permutations of both arrays to diminish            116
# correlation (not necessary for one of the random variables)    117
theta_la = np.random.permutation(theta_la_ppf)                   118
theta_xi = theta_xi_ppf                                          119
                                                                 120
# INSTANTIATION:                                                 121
mu_q_fn = get_mu_q_fn(q_eq13, 1.0 / n_sim,                       122
                      theta_la, theta_xi)                        123
                                                                 124
# CALCULATION:                                                   125
mu_q_arr = mu_q_fn(eps_arr)                                      126
```

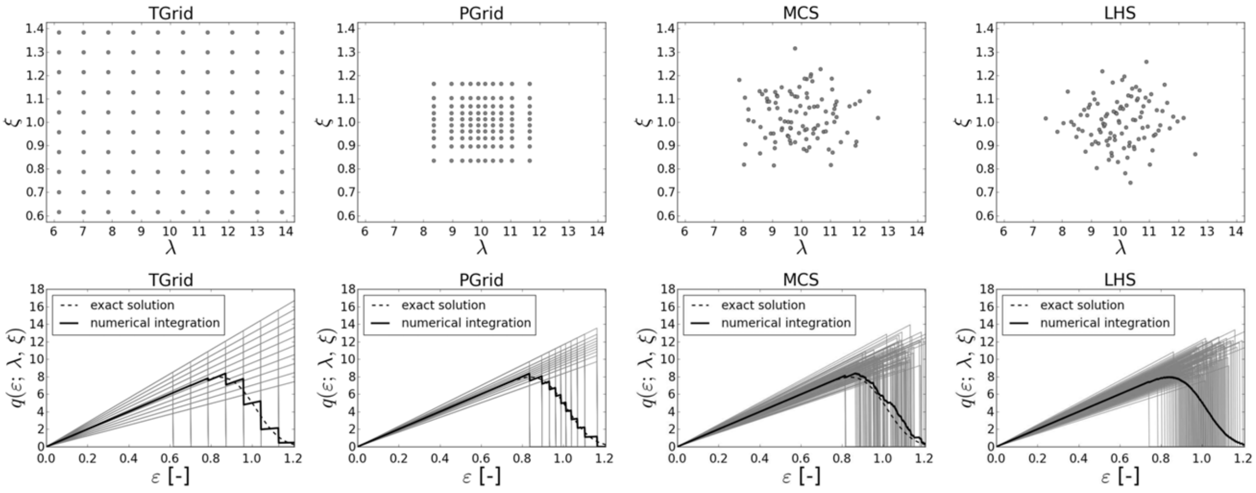


Fig. 3. Sampling structures within the random domain, and the calculated mean responses for the implemented integration schemes.

Fig. 3 shows the results for the four instantiated versions of the algorithm. For the sampling schemes using structured grid (`TGrid`, `PGrid`) $n_{\text{int}} = 10$ integration points are used in each direction. For the Monte Carlo types of sampling (`MCS`, `LHS`) the same number of sampling points, $n_{\text{sim}} = n^m = 10^2$, is used.

Let us summarize that all four examples could be realized using the generic template `get_mu_q` implemented at lines 61–66. Due to the use of implicit loops over `numpy` arrays the template code can handle both grid-based and Monte Carlo types of sampling. This documents the fact that using loopless code the algorithmic structure could be captured in an abstract way without strong assumptions about the particular representation of the sampling data.

5. Interactive algorithmic object

While the previous section was focused on capturing the structural commonalities of the algorithmic procedure in the generic code of the `get_mu_q_fn` template (lines 61–61), in this section we intend to generalize the code for the specification of the random problem, generation of sampling data and include also loop-based code as an alternative to the vectorized code described so far.

In the context of our running example, we want to avoid the part of code that is entitled as `SAMPLING` in the four implementations given in the previous section. At the same time, we want to represent the random problem, the sampling methods and the execution code in independent code entities so that they can be combined interactively.

The specified functionality has been provided in the form of an interactive algorithmic object. The random problem can be defined and interactively configured using the `SPIRRID` class by supplying an arbitrary response function and by specifying its control and random parameters. The complete list of attributes defining a general multi-variant random problem includes the following items:

`q` defines the response function. It is either a function or a "callable" object possessing the `()` call operator. An example is a standard Python function

```
def q(name1, name2, name3, name4, ...)
```

Parameter names are used for further specification of control and random variables included either in the `eps_vars` or `theta_vars` attributes.

`eps_vars` specifies the control variables as a dictionary of (name, value) pairs

```
eps_vars = {'name1' : value_arr1,
            'name2' : value_arr2}
```

where `value_arr` defines the evaluation range of the control variable.

`theta_vars` specifies random variables as a dictionary of (name, value) pairs

```
theta_vars = {'name3' : RV(distr3, loc3,
              scale3, n_i3),
              'name4' : RV(distr4, loc4,
              scale4, n_i4)}
```

where value objects constructed as `RV(distr_type, loc, scale, n_i)` define the random variables by specifying the type of probability distribution (`distr_type`) and its parameters `loc, scale` and the number of integration points `n_i` in the respective dimension of the random domain.

`sampling_type` within the random domain is specified using the option `sampling_type = ['TGrid', 'PGrid', 'MCS', 'LHS']`. By choosing the type of sampling, the corresponding arrays of Θ values and the associated statistical weights ΔG are generated for the integration algorithm.

`codegen_type` is selected using option `codegen_type = ['numpy', 'weave', 'cython']`. Based on this selection the integration code is generated on the fly for the currently configured random problem and sampling either using the vectorized `numpy` package or compiled looped-based C code produced using the `weave` or `cython` packages.

As an application example, let us reproduce the random problem defined previously at lines 108–123:

```
from stats.spirrid import SPIRRID, RV                        127
# DEFINITION: random problem, sampling type, code type       128
s = SPIRRID(q=q_eq13,                                         129
         eps_vars={'eps' : np.linspace(0, 1.2, 80)},          130
         theta_vars={'la' : RV(distr='norm', loc=10,          131
                        scale=1.0, n_i=10),                   132
                     'xi' : RV(distr='norm', loc=1,           133
                        scale=0.1, n_i=10)}                   134
```

```
          sampling_type='LHS',                                135
          codegen_type='numpy')                               136
# INSTANTIATION and CALCULATION                               137
print 'array of mean values', s.mu_q_arr                      138
```

Output values of the algorithmic object are obtained by accessing the `mu_q_arr` property attribute as indicated at line 138. This means that the actual calculation of the mean response using the `SPIRRID` object is not invoked explicitly but gets started on demand upon an access to the property attributes of the algorithmic object.

Except for the mean values, the `SPIRRID` class contains property attributes for accessing also other output data produced during the computation. In particular, variances and information about the last performed calculation (e.g. CPU times consumed for compilation, sampling and integration):

```
print 'array of variances', s.var_q_arr                       139
print 'execution time of the last calculation', s.exec_time   140
```

Using the listed input and output attributes of the `SPIRRID` class, the four sampling schemes introduced in Section 4 implemented at lines 67–126 can be reproduced using the algorithmic object defined at line 129 in a loop over the sampling schemes:

```
# plot results for all implemented sampling types             141
for sampling_type in ['TGrid', 'PGrid', 'MCS', 'LHS']:        142
    s.sampling_type = sampling_type                           143
    p.plot(s.eps_arr, s.mu_q_arr, label=sampling_type)        144
    print 'execution time for', sampling_type, s.exec_time    145
                                                              146
p.legend()                                                    147
p.show() # show all diagrams in a single figure               148
```

This loop produces a diagram showing the response obtained using the four sampling schemes and prints the execution times needed for the included types of sampling. In an indicated way, data on convergence and execution efficiency characterizing particular configurations of the algorithmic object can be gathered, processed and plotted. This is performed later in Sections 8 and 9 providing a systematic performance comparison of the discussed sampling methods on the one hand and of the implementation type, either vectorized, loopless or compiled, loop-based on the other hand.

6. Implementation of the `SPIRRID` class using traits

After a brief description of the user view of the `SPIRRID` class, let us shortly explain the approach to its implementation. The structure of the code is depicted in Fig. 4 in the form of a UML class diagram [20]. The diagram indicates the decomposition of the problem into three parts:

randomization: representing the specification of the random problem in terms of the response function and classification of its parameters into control and random.

sampling: delivering the sampling data `theta` and `dG` for the given randomization.

code generation: providing the instantiated execution method either as a vectorized `numpy` code or as a compiled `C` code generated with the help of `weave` or `cython` packages.

Our Python implementation of the class diagram uses the `traits` package provided within the *Enthought Tool Suite* (http://www.enthought.com). This package introduces an extended attribute definition into Python classes by including specification of the attribute's type and of its dynamic behavior. In our experience, traits can significantly contribute to a compact implementation of an object-oriented application since the implemented static class structure can be easily enhanced with the specification of state transitions involved in the life-cycle of an interactive object.

Let us demonstrate the implementation approach on a part of the code showing the definition of the classes `RV`, `Function Randomization` and `SPIRRID` depicted in Fig. 4:

```
from traits.api import Trait, Callable, Dict, \                149
    Str, Property, DelegatesTo, on_trait_change, \             150
    cached_property                                            151
from sampling import make_ogrid, \                             152
    TGrid, PGrid, MonteCarlo, LatinHypercube,                  153
from code_gen import \                                         154
    CodeGenNumpy, CodeGenWeave, CodeGenCython                  155
# import subsidiary class for probabilistic distributions      156
from stats.pdistrib import PDistrib                            157
                                                               158
class RV(HasTraits):                                           159
    """Class representing a random variable."""                160
    distr_type = Str('norm', desc='distribution type')         161
    loc = Float(0.0, desc='location parameter')                162
    scale = Float(0.0, desc='scale parameter')                 163
    shape = Float(1.0, desc='shape parameter')                 164
    n_i = Int(40, desc='number of integration points')         165
                                                               166
    # probability distribution                                 167
    distr = Property(depends_on='loc, scale, shape')           168
    @cached_property                                           169
    def _get_distr(self):                                      170
        # PDistrib class wraps the scipy.stats.distributions   171
        return PDistrib(type=self.distr_type, loc=self.loc,    172
                        scale=self.scale, shape=self.shape)    173
                                                               174
    # operators delegated to scipy.stats via PDistrib          175
    pdf = DelegatesTo('distr')                                 176
    cdf = DelegatesTo('distr')                                 177
    ppf = DelegatesTo('distr')                                 178
                                                               179
class FunctionRandomization(HasTraits):                        180
    """Specification of a multi-variate random problem."""     181
    q = Callable(rp_spec=True)                                 182
    eps_vars = Dict(Str, Array, rp_spec=True)                  183
    theta_vars = Dict(Str, RV, rp_spec=True)                   184
                                                               185
    @on_trait_change('+rp_spec')                               186
    def _validate_random_problem(self):                        187
        """Prepare the input data structure."""                188
        # ... skipped here ...                                 189
                                                               190
    # Mapping properties                                       191
    eps_lst = Property(depends_on='+rp_spec')                  192
    @cached_property                                           193
    def _get_eps_lst(self):                                    194
        """Order control variables according to q."""          195
        # ... skipped here ...                                 196
                                                               197
class SPIRRID(FunctionRandomization):                          198
    """Algorithmic class for multi-variate random problem.     199
    """                                                        200
    sampling_type = Trait('TGrid',                             201
                          {'TGrid' : TGrid,                    202
                           'PGrid' : PGrid,                    203
                           'MCS' : MonteCarlo,                 204
                           'LHS': LatinHypercube},             205
                          sp_spec = True)                      206
    sampling = Property(depends_on='sp_spec')                  207
    @cached_property                                           208
    def _get_sampling(self):                                   209
        """Getter method for the sampling generator."""        210
        return self.sampling_type_(randomization=self)         211
                                                               212
    codegen_type = Trait('numpy',                              213
```

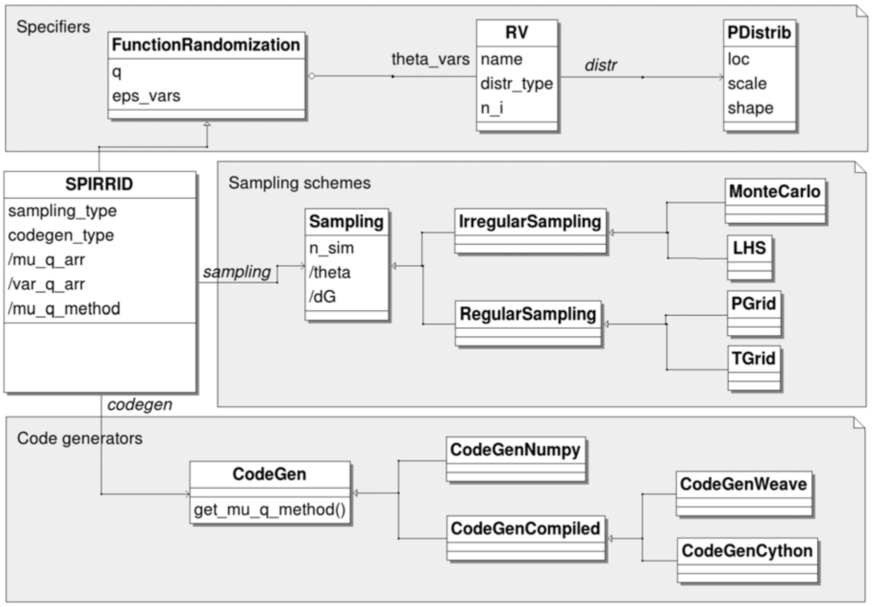


Fig. 4. UML class diagram with a general representation of the integration algorithm and extensible components for sampling schemes and implementations. Attribute names preceded by a slash indicate derived output values implemented as property traits.

```
                    {'numpy' : CodeGenNumpy(),              214
                     'weave' : CodeGenC(),                  215
                     'cython' : CodeGenCython()},           216
                    cg_spec = True)                         217
    codegen = Property(depends_on='+cg_spec')               218
    @cached_property                                        219
    def _get_codegen(self):                                 220
        """Getter method for the code generator."""         221
        return self.codegen_type_(spirrid=self)             222
                                                            223
    mu_q_arr = Property(depends_on=                         224
                   '+rp_spec,+sp_spec,+cg_spec')            225
    @cached_property                                        226
    def _get_mu_q_arr(self):                                227
        """Getter method for the mean value array."""       228
        eps_orth = make_ogrid(self.eps_lst)                 229
        mu_q_fn = self.codegen.mu_q_fn                      230
        mu_q_arr = mu_q_fn(*eps_orth)                       231
        return mu_q_arr                                     232
```

Let us summarize the aspects of the implementation in a list of remarks:

Remark 1 (*Imported Packages*)**.** In the import section, first the trait types included in the `traits.api` module of the Enthought package are imported at lines 149–151. After that (lines 152–155) specializations of the `Sampling` and `CodeGen` classes (compare class diagram in Fig. 4) are imported from the modules `sampling` and `code_gen` of the `spirrid` package, respectively. Finally, the class `PDistrib` utilizing the statistical distributions provided by the `scipy` package for an object-oriented application is imported from the `stats.pdistrib` module.

Remark 2 (*Representation of Random Variables*)**.** Random variables are introduced using the class `RV` shown at lines 159–178. The class consists of traits specifying the type of probability distribution `distr_type`, its parameters `loc`, `scale`, `shape` and the number of integration points `n_i`. Except for these input traits, `RV` class includes a property trait for the probability distribution `distr`. The `distr` property is defined as a `@cached_property` which means that there is a hidden attribute of a type `PDistrib` that gets automatically constructed upon first access to `distr`. If any of the traits listed in the `depends_on` specifier of the property has changed, the hidden `PDistrib` instance gets reconstructed upon the next access to the `distr` attribute by invoking the associated "getter" method `_get_distr()`. The last three traits (`pdf`, `cdf`, `ppf`) of the `RV` class defined as `DelegatesTo` traits are proxies accessing methods of the `distr` trait. These methods are used during the generation of the sampling data in the subclasses of `Sampling` class.

Remark 3 (*Specification of Multi-Variate Random Problem*)**.** Specification of the random problem including the response function, control variables and random variables is defined and managed by the `FunctionRandomization` class (lines 180–189). Based on the given control variables `eps_vars` and random variables `theta_vars` the response function `q` is inspected for the matching names of parameters. Note that these traits are grouped together by specifying the `rp_spec = True` metadata in the trait constructor. The `+rp_spec` specifier can then be used for compact specification of state dependencies. One way how to introduce a dynamic dependency is by using the decorator `on_trait_change('+rp_spec')`. This is exemplified at line 186 in order to trigger the validation method `_validate_random_problem()` whenever any of the `q`, `eps_vars` and `theta_vars` traits has been modified. Another example of dependency specification is provided for a lazy update of the list of control parameters in the cached property `eps_lst` (line 192) providing the input arrays in an order that corresponds with the specification given in the response function definition.

Remark 4 (*Integration of Algorithmic Features*)**.** The `SPIRRID` class defined at lines 198–232 inherits from the `FunctionRandomization` and integrates the algorithmic features for sampling types (`sampling_type`) and code types (`codegen_type`) as trait attributes containing the lists of available sampling methods and code generators, respectively. Depending on the current value of `sampling_type` and `codegen_type` the instances of the corresponding class given in Fig. 4 are provided through the `sampling` and `codegen` properties, respectively. In the associated "getter" methods, an instance of the sampling type (line 211) or code generator (line 222) is constructed and provided with a backward reference to the `SPIRRID` object (`self`). Using this reference, the algorithmic feature can extract information on the randomization or mapping of dimensions of the control/random domain and function parameters.

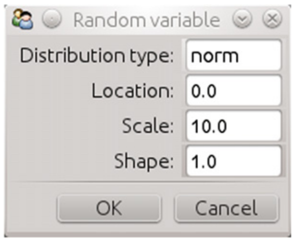
Remark 5 (*Instantiation of the Algorithm and of the Results*). The property trait `mu_q_arr` for the array of mean values (line 224) depends on attributes categorized as `+rp_spec`, `+sp_spec` and `+cg_spec`. In its getter method, the control variables for the parameters `eps_lst` are first arranged in an orthogonal array using the `make_ogrid` method at line 229. As a consequence, for more than one control variables, the broadcasting rules discussed previously in Section 4 in the context of the random domain apply. This means that for problems with more than one control variables (`eps_vars`) the mean values are automatically calculated for all combinations of their values. The particular calculation method `mu_q_fn` is instantiated for the current random problem and sampling method at line 230 upon the access to the equally named property of the current code generator `codegen`. The obtained vectorized function `mu_q_fn` accepts a list of control variables and runs the calculation.

In order to explain what is meant with the code generator let us briefly describe the definition of `CodeGenNumpy` class:

```
from code_gen import CodeGen                                   233
                                                               234
class CodeGenNumpy(CodeGen):                                   235
    """Code generator for vectorized numpy code."""            236
    mu_q_fn = Property(depends_on=                             237
                    '+spirrid.rp_spec,+spirrid.sp_spec')       238
    @cached_property                                           239
    def _get_mu_q_fn(self):                                    240
        """Return a method evaluating the mean of q()."""      241
        s = self.spirrid                                       242
        # construct dictionary of random variables             243
        theta_args = dict(zip(s.theta_var_names,               244
                              s.sampling.theta))               245
                                                               246
        def mu_q(*eps):                                        247
            # construct dictionary of control variables        248
            eps_args = dict(zip(s.eps_var_names, eps)          249
            # merge theta and eps dictionaries                 250
            args = dict(eps_args.items(), theta_args.items())  251
            # calculate the product                            252
            Q_dG = q(**args) * s.sampling.dG                   253
            return np.sum(Q_dG)                                254
                                                               255
        return np.vectorize(mu_q)                              256
```

The implementation of the getter method `_get_mu_q_fn` mimics the `get_mu_q_fn` template defined previously in Section 3 at lines 61–66. One significant difference, however, is that the getter method `_get_mu_q_fn` furnishes the generated `mu_q_fn` method with a sequence `*eps` of vectorized control parameters and, thus, supports broadcasting. Another difference is that the sampling data `theta` and `dG` are not passed as an argument of the instantiated `mu_q_fn` function but are accessed via the `sampling` attribute of the containing `SPIRRID` instance. As a consequence, a change of the sampling method is automatically reflected by the re-instantiation of the calculation method. Note that the generated method is stored as a cached hidden value and is reused if there was no change in its dependencies.

In our opinion the shown implementation of the `CodeGen Numpy` class provides a very compact and short code including a high flexibility with respect to the specification of the random problem and to the choice of the particular sampling method. The ingredients contributing to this kind of implementation are the dynamic typing of the Python language, notification mechanism introduced by the `traits` package and the broadcasting technique for vectorized implementation provided by the `numpy` package. Later in Section 9 we shall also comment on the implementation of the other generator classes (`CodeGenCython` and `CodeGenWeave`) producing compiled loop-based `C` code.


Random variable

Distribution type: norm
Location: 0.0
Scale: 10.0
Shape: 1.0

Fig. 5. View to an object defining a random variable.

7. User interface for an algorithmic object

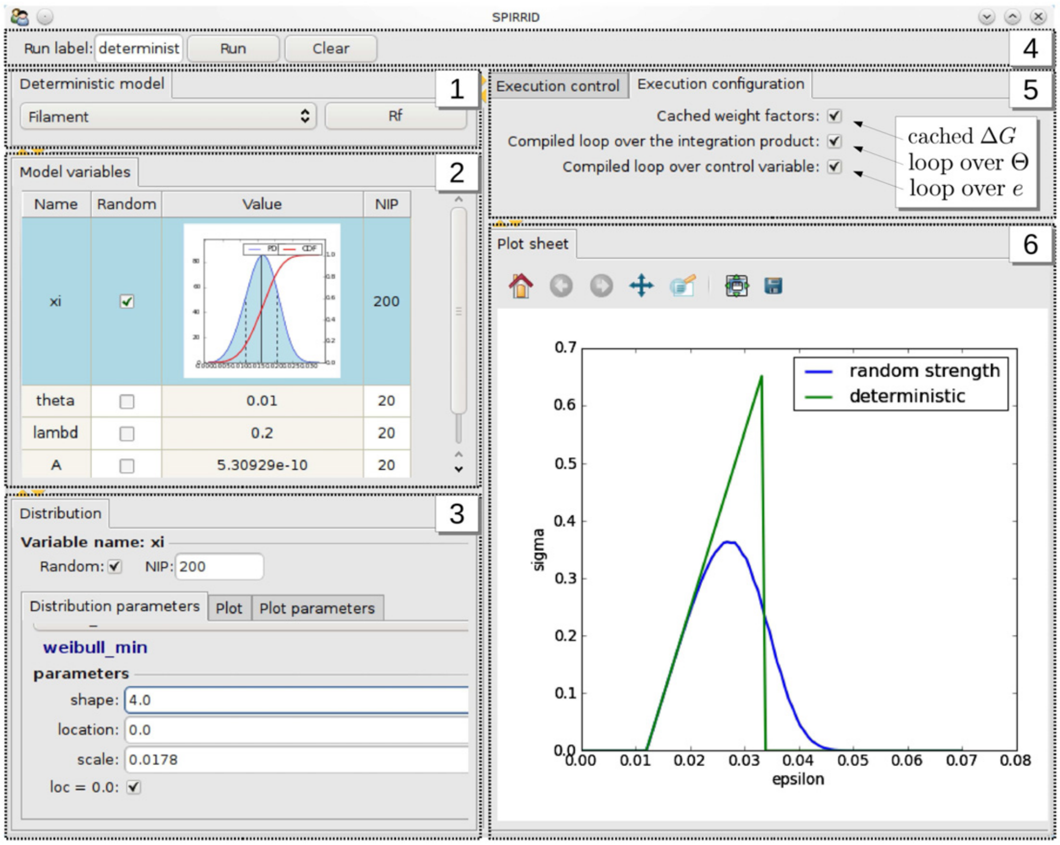
As already mentioned, the `SPIRRID` class is prepared for interactive use either through a command line or through a user interface. For a class defined using traits, the user interface can be constructed by specifying views to the object using the `traits.ui` package included in the Enthought suite. Views are defined declaratively by specifying lists of traits to be included in the user interface. For example, a view to the `RV` class (lines 159–178) can be defined and rendered into the UI window shown in Fig. 5 as follows:

```
from traits.ui import View, Item                               257
                                                               258
v = View(Item('distr_type', label='Distribution type'),        259
         Item('loc', label='Location'),                        260
         Item('scale', label='Scale'),                         261
         Item('shape', label='Shape'),                         262
         title='Random variable'                               263
         buttons=['OK', 'Cancel'])                             264
                                                               265
rv = RV(distr_type='norm', scale=10, shape=1)                  266
rv.configure_traits(view=v)                                    267
```

A more complex user interface is exemplified in Fig. 6 for an interactive `SPIRRID` instance. The example reflects the previously introduced computational components: (1) the response function, (2) specification of random parameters, (3) statistical distribution, (4) execution control, (5) configuration and (6) plotting of the calculated mean curves as movable tabs within the user interface window.

Besides views, traited classes also have an attached `Controller` class responsible for handling interaction events. By default, there is an automatically constructed view and controller object for each traited class instance. This means that even at the initial stages of development a simple user interface is automatically available. In the later stages, the views and controllers can be easily refined into a form suitable for a particular type of application.

The declarative mapping of class traits to a view makes it possible to define a user interface to an application without sticking to a particular UI library. Indeed, a switch between different types of user interface toolkits is done by switching between the UI backends. Currently, the back-ends for the `wx` and `Qt` libraries are available. Further details of the UI mapping machinery would go beyond the scope of the present paper and can be found in [21].



Run label: determinist

Filament

Name	Random	Value	NIP
xi	✓		200
theta	☐	0.01	20
lambd	☐	0.2	20
A	☐	5.30929e-10	20

Cached weight factors: ✓
Compiled loop over the integration product: ✓
Compiled loop over control variable: ✓

cached ΔG
loop over Θ
loop over e

Variable name: xi
Random: ✓ NIP: 200

weibull_min
parameters
shape: 4.0
location: 0.0
scale: 0.0178
loc = 0.0: ✓

Fig. 6. User interface view of an instance of the traited SPIRRID class.

8. Computational efficiency of the implemented sampling schemes

The implemented algorithmic object shall now be used for performance studies comparing the efficiency of the available algorithmic features. The studies have been implemented as scripts interacting with a single SPIRRID instance.

The convergence of the integration algorithm for the available sampling schemes shall be evaluated using an analytical solution available for our running example. The exact mean response of the two-parametric response function given in Eq. (13) with both parameters considered random and normally distributed can be obtained as:

$$\mu_q^{\text{exact}}(\varepsilon) = \frac{\mu_\lambda \varepsilon}{2}\left(1 - \operatorname{erf}\left(\frac{\varepsilon - \mu_\xi}{\sqrt{2}\sigma_\xi}\right)\right) \tag{15}$$

where $\operatorname{erf}(x)$ denotes the Gauss error function defined as $\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\,dt$. The convergence of the sampling schemes used for the numerical estimation of the mean has been studied depending on the number of sampling points and on executional time. The error has been defined both locally and globally. Since the estimate of the statistical characteristics of the peak value is of special significance, the local error measure has been defined as the relative maximum deviation along the control variable ε discretized using n_ε points:

$$e_{\max} = \frac{\max\limits_i \left|\mu_q(\varepsilon_i) - \mu_q^{\text{exact}}(\varepsilon_i)\right|}{\max\limits_i\left[\mu_q^{\text{exact}}(\varepsilon_i)\right] - \min\limits_i\left[\mu_q^{\text{exact}}(\varepsilon_i)\right]}, \quad i = 1 \cdots n_\varepsilon. \tag{16}$$

The global error measure has been introduced as the relative root mean square error within the range of the control variable ε:

$$e_{\text{rms}} = \frac{\sqrt{\frac{1}{n_\varepsilon}\sum\limits_i \left(\mu_q(\varepsilon_i) - \mu_q^{\text{exact}}(\varepsilon_i)\right)^2}}{\max\limits_i\left[\mu_q^{\text{exact}}(\varepsilon_i)\right] - \min\limits_i\left[\mu_q^{\text{exact}}(\varepsilon_i)\right]}, \quad i = 1 \cdots n_\varepsilon. \tag{17}$$

Fig. 7 shows the convergence behavior in double logarithmic scale for both types of errors for an increasing number of sampling points. Both diagrams document the fact that LHS covers the random domain in a significantly more efficient way than all the other implemented methods. The convergence behavior of the other three sampling methods is comparable.

A more relevant comparison of efficiency is given in Fig. 8 which shows the measured CPU time for the studied sampling methods instead of n_{sim}. Also in this view, the LHS method is superior to the other methods. PGrid sampling is revealed to be slightly more efficient than Monte Carlo and TGrid. The higher efficiency is due to the fact that during the response function evaluation, some interim results can be reused in the broadcasted dimension and, consequently, a significant number of operations can be saved. Such a caching of interim values within a random subspace is not possible in the Monte Carlo type of sampling due to the unstructured coverage of the m-dimensional space. The positive effect of vectorized evaluation increases as the number of random parameters grows. However, it also depends on the type of the response function and on the current choice of the random parameters. It must be also considered that the vectorized evaluation of the response function $q(\varepsilon)$ in the m-dimensional space is connected with the exponential growth of memory consumption. Further studies of convergence for varied sampling types and response functions, also including all permutations of

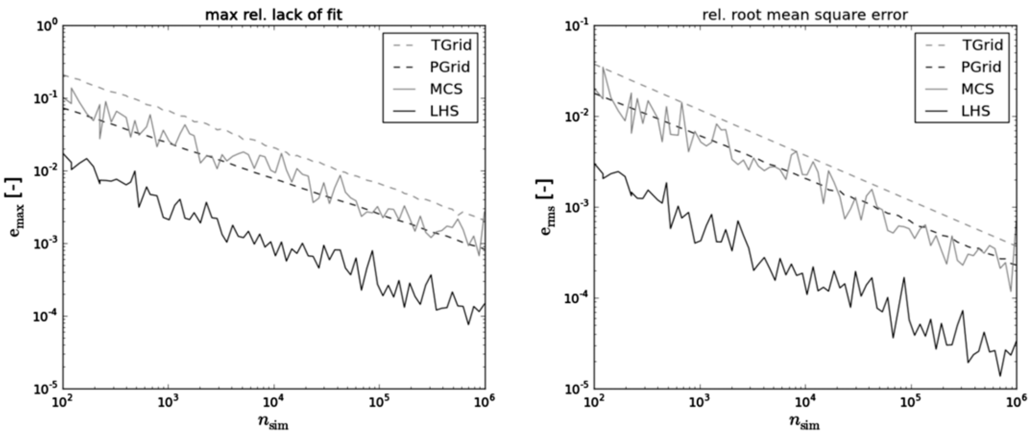


Fig. 7. Convergence to an exact solution with an increasing number of sampling points in terms of local and global error measures given in Eqs. (16) and (17), respectively.

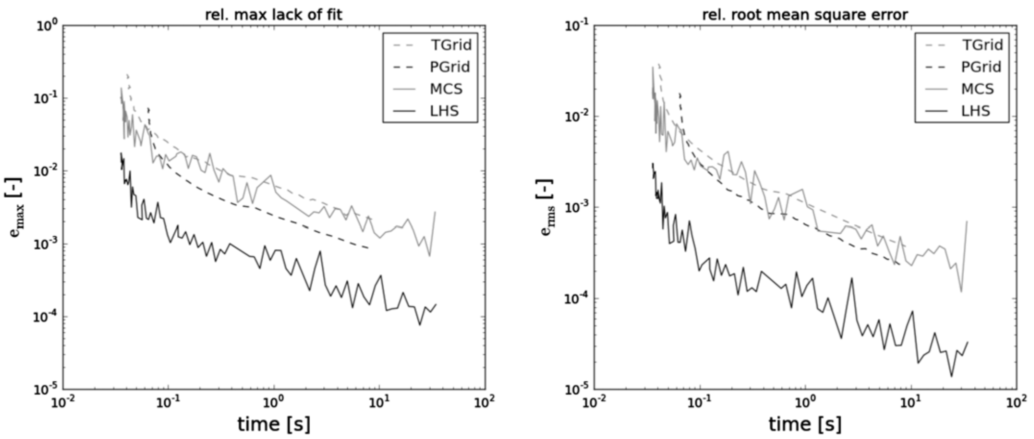


Fig. 8. Convergence to an exact solution with an increasing computational time in terms of local and global error measures given in Eqs. (16) and (17), respectively.

randomized parameters, have been provided in the documentation of the spirrid package [1].

9. Execution efficiency of vectorized and compiled code

Previous studies shown in Fig. 8 reveal that the CPU time required to achieve sufficiently accurate results ($e_{\mathrm{rms}} \leq 10^{-3}$) for a function with two random variables using the numpy code is less than 1 s. For more complex functions with more random variables further speedup might be desirable. There are several ways to improve the execution efficiency of Python code. An overview of speedup possibilities for numerical Python code has been provided in [22].

In order to accelerate the present application two options have been used: cython [23] and weave [24]. They have been incorporated into the spirrid package analogically to the numpy code generator as subclasses of the CodeGen class (see Fig. 4) providing the callable method mu_q_fn as a cached property. In comparison to the CodeGenNumpy described in Section 6 the generation of the code in CodeGenWeave and CodeGenCython is more complex and lengthy as it involves the string based assembly of the code, its subsequent compilation and integration into the running application.

The generation for loop-based cython code is sketched in Fig. 9. The codegen object in the middle box assembles the loops over the control and random domains, inserts the access operator to the particular values in the theta and dG arrays, inserts the call to the response function q for current theta value and, finally, inserts the expression for the weighted sum of the obtained response value. Let us remark that the code of the response function q must be provided in a form integrable into the code generator, i.e. both for cython in the form of Python code extended with type declarators and for weave code as a string in the C language.

Execution times have been measured for the two-parametric function in Eq. (13) of our running example with two types of sampling: LHS and PGrid. The size of the sample for both sampling schemes was chosen in order that a comparable level of accuracy was reached based on the studies of sampling efficiency shown earlier in Fig. 8. The accuracy required for the studies was $e_{\mathrm{rms}} \leq 5 \cdot 10^{-5}$, which corresponds to $n_{\mathrm{sim}} = 440^2$ for LHS and $n_{\mathrm{sim}} = 5000^2$ for PGrid. CPU time was measured for three phases of the computation:

- sampling time needed for preparing the arrays Θ_i (Eq. (5)) and ΔG_i within the sampling object,
- time needed to prepare and compile the method mu_q_method within the codegen object, and
- time needed to execute the integration procedure on the prepared data arrays.

Each version of the code was executed twice in order to show the difference between CPU time with and without the setup and compilation of the generated C code. CPU times obtained for LHS shown in Fig. 10 (left) reveal that a significant amount of time was spent on the permutation of $\boldsymbol{\theta}$ arrays. For all three types of code a standard permutation algorithm available in the numpy package was used so that the sampling time remained constant (≈0.19 s) in all runs.

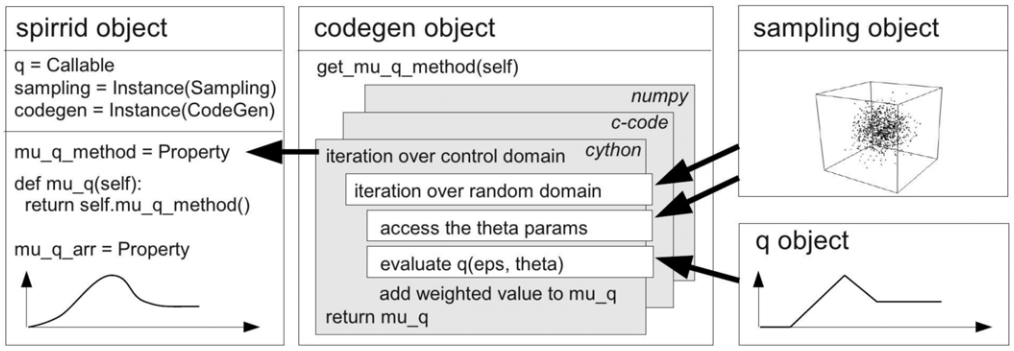


Fig. 9. Generation of the integration code for the current function, randomization, sampling and language.

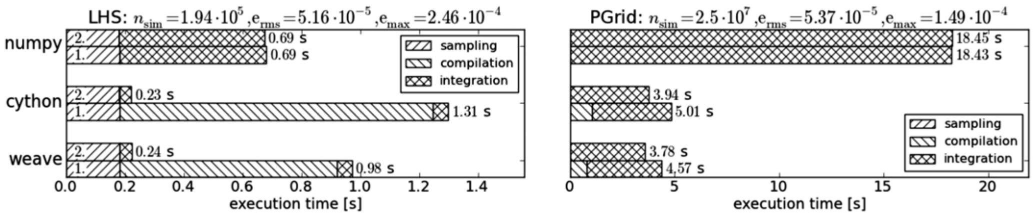


Fig. 10. Comparison of execution times for `LHS` and `PGrid` sampling needed in the first (1) and second (2) run of `numpy`, `cython` and `weave` code ($n_\varepsilon = 80$).

The shortest execution time was achieved in the second run of the compiled `weave` code.[4] The CPU time achieved by the `cython` version of the code was only insignificantly slower. This is not surprising since both compiled versions lead to an optimized C code with a similar structure. As already stated in [22] the efficiency of `weave` and `cython` can be regarded as equivalent. The overall CPU time of the scripting `numpy` version was about 2.5 times longer than for both compiled versions. Regarding the time required by the pure integration procedure, the compiled code is 12 times faster than the scripting code. This relation is in agreement with the studies published in [22].

Even though the grid-based sampling schemes are significantly slower than `LHS` it is interesting to examine the effect of compilation on the speedup for the `PGrid` sampling shown in the right diagram of Fig. 10. Regarding the CPU time required by the pure integration (`numpy`: 18.45 s, `weave`: 3.78 s) we can see that the speedup factor (≈5) is much smaller than in the case of `LHS` (≈12). As already discussed at the end of Section 8, the vectorized evaluation of the response function can increase the efficiency of `numpy` compared to the nested loop implementation in `weave` and `cython` due to the caching of interim results during broadcasting from a smaller subspace to the m-dimensional domain. Even though the increase in efficiency is not sufficient to compensate for the slower convergence of the sampling, it is helpful to keep this issue in mind when implementing scripts for the grid-based accumulation of values.

In the simple example used for this study, the setup and compilation time of the first run was longer than the time spent on computation. For larger problems with a more complex response function, more random variables and more sampling points, the proportion of time spent on setup and compilation would certainly diminish. A more detailed analysis of performance considering further factors affecting efficiency would go beyond the scope of this paper. Studies of more complex functions with different combinations of random variables have been included in the `spirrid` package. For the sake of completeness, let us remark that further speedup of the code would be possible using code parallelization and/or more advanced treatment of discontinuities in the response function. Regarding parallelization, an approach suggested in [25] exploiting the dynamic and generic nature of the Python language is a possible choice.

The effect of discontinuity representation deserves more detailed comment: The generic implementation of grid based sampling schemes (`PGrid` and `TGrid`) for compiled code uses nested loops. The code of the response function is simply inserted into the innermost loop over the random domain. This means that if the function body contains the control statements `if`, `else` introducing jumps in the response function, losses in performance occur since the argument of the `if`, `else` test does not necessarily occur directly at the intermediate level of iteration over its values. Performing the test in the innermost loop causes unnecessary passes through sampling points that would be skipped if the test occurred outside of the inner loop. For special cases it might be desirable to manually factor out the test to some higher level of iteration avoiding unnecessary passes through the inner loops. This case is not treated in the present implementation focused primarily on the flexibility of the algorithmic structure with interactively selectable integration variables. An expression analysis of the function would be necessary to provide an optimum placement of the control statements within the embedded iteration loops to achieve a general solution to this problem.

A similar problem occurs for the `numpy` code using the Heaviside function. Sampling points with zero Heaviside function values could be immediately skipped to avoid further calculation with zeros. A possible remedy might be the use of masked arrays provided by the `numpy` package. However, in our case the extra cost connected with access to values in a masked array turned out to be higher than the savings gained by skipping some operations in the masked sampling points.

10. Conclusions

In the present paper we have reported on the feasibility of the Python based environment for the development of scientific computing applications. We have gone through the whole development life-cycle including mathematical formulation, prototyping

[4] The compilation has been done using `gcc` compiler (version 4.5.2) with the following arguments: `-NDEBUG -fwrapv -O3 -march=native -ffast-math`.

using simple scripts, generalization of the algorithmic structure, designing an algorithmic object reflecting the state dependencies between the editable components and speeding up of the code to achieve the efficiency of low-level compiled code. The resulting algorithmic object for statistical integration can be interactively edited by modifying the response function, declaring its parameters as control or random variables, choosing and configuring probability distributions of the random variables, selecting from four types of sampling schemes and configuring the execution code for the integration.

During the implementation of the sampling schemes, an interesting possibility emerged covering the random domain using a regular grid with constant probabilities (`PGrid`). To the knowledge of the authors, this type of sampling has not yet been mentioned elsewhere. This type of sampling becomes interesting in connection with the vectorized evaluation as its efficiency grows with the increasing dimension m of the integration domain.

The vectorized evaluation of functions using implicit loops over m-dimensional arrays is sometimes referred to as loopless programming. It makes the scripting code in the early stages of prototyping very short and compact, which contributes to its scalability in the later stages of development. At the same time, the performance of the loopless code for calculations of moderately sized problems is within an acceptable range. For larger problems, including complex response functions with several random variables, it can even reach the level of optimized loop-based inlined C code. Further improvements of the loopless code are possible using techniques that accelerate algebraic operations with large vectors and arrays [26]. Further possibilities for speedup are provided by high-level libraries for vectorized programming using graphical processors [27] or library for optimization and evaluation of mathematical expressions involving multidimensional arrays [28].

The use of general numerical libraries in connection with the traited class provided by Enthought traits greatly simplifies the later stages of application development by alleviating the formulation of the interfaces both for the scripting interaction and for the construction of the user interface. The significant advantage of the Enthought environment is its multi-platform usage capability. It is very easy to extend the application with visualization features (`matplotlib`, `mayavi`), a graphics interface and persistence management of the data. It is a powerful environment for scientific computations based on the Python high-level programming language. The script constructed throughout the paper and the traited implementation of the `spirrid` package based on the Enthought traits library has been made available for downloading and testing through the Computer Physics Communications Program Library.

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References

[1] SPIRRID: tool for estimation of statistical characteristics of multi-variate random functions, http://github.com/simvisage/spirrid, 2011.
[2] P. Krysl, A. Trivedi, Instructional use of MATLAB software components for computational structural engineering applications, International Journal of Engineering Education 21 (2005) 778–783. WOS:000233032100004.
[3] H.P. Langtangen, A Primer on Scientific Programming with Python, first ed., Springer, 2009.
[4] H. Langtangen, A case study in high-performance mixed-language programming, in: B. Kågström, E. Elmroth, J. Dongarra, J. Wasniewski (Eds.), Applied Parallel Computing, State of the Art in Scientific Computing, in: Lecture Notes in Computer Science, vol. 4699, Springer, Berlin/Heidelberg, 2007, pp. 36–49.
[5] H.P. Langtangen, X. Cai, On the efficiency of Python for high-performance computing: a case study involving stencil updates for partial differential equations, in: H.G. Bock, E. Kostina, H.X. Phu, R. Rannacher (Eds.), Modeling, Simulation and Optimization of Complex Processes, Springer, Berlin Heidelberg, 2008, pp. 337–357.
[6] S.v.d. Walt, S.C. Colbert, G. Varoquaux, The NumPy array: a structure for efficient numerical computation, Computing in Science & Engineering 13 (2011) 22–30.
[7] J. Nilsen, MontePython: implementing quantum Monte Carlo using Python, Computer Physics Communications 177 (2007) 799–814.
[8] J. Unpingco, Some comparative benchmarks for linear algebra computations in matlab and scientific Python, in: DoD HPCMP Users Group Conference, 2008, DOD HPCMP UGC, pp. 503–505.
[9] J.C. Chaves, J. Nehrbass, B. Guilfoos, J. Gardiner, S. Ahalt, A. Krishnamurthy, J. Unpingco, A. Chalker, A. Warnock, S. Samsi, Octave and Python: high-level scripting languages productivity and performance evaluation, in: Proceedings of the HPCMP Users Group Conference, HPCMP-UGC '06, IEEE Computer Society, Washington, DC, USA, 2006, pp. 429–434.
[10] D.C. Morrill, J.M. Swisher, Traits 3 user manual, http://enthought.github.com/traits/traits_user_manual/front.html, 2011.
[11] R. Jarvis, D. Broadhurst, H. Johnson, N. O'Boyle, R. Goodacre, PYCHEM: a multivariate analysis package for Python, Bioinformatics 22 (2006) 2565–2566.
[12] W. Conover, On a better method for selecting input variables, 1975, Unpublished Los Alamos National Laboratories manuscript, reproduced as Appendix A of "Latin Hypercube Sampling and the Propagation of Uncertainty in Analyses of Complex Systems" by J.C. Helton and F.J. Davis, Sandia National Laboratories report SAND2001-0417, printed November 2002.
[13] J.C. Helton, F.J. Davis, Latin Hypercube Sampling and the Propagation of Uncertainty in Analyses of Complex Systems, Technical Report SAND2001-0417, Sandia National Laboratories Albuquerque, New Mexico and Livermore, California, 2002.
[14] M.D. McKay, W.J. Conover, R.J. Beckman, A comparison of three methods for selecting values of input variables in the analysis of output from a computer code, Technometrics 21 (1979) 239–245.
[15] M. Stein, Large sample properties of simulations using Latin Hypercube Sampling, Technometrics 29 (1987) 143–151.
[16] M. Vořechovský, D. Novák, Correlation control in small sample Monte Carlo type simulations I: a simulated annealing approach, Probabilistic Engineering Mechanics 24 (2009) 452–462.
[17] M. Vořechovský, Correlation control in small sample Monte Carlo type simulations II: analysis of estimation formulas, random correlation and perfect uncorrelatedness, Probabilistic Engineering Mechanics 29 (2012) 105–120.
[18] S.L. Phoenix, H.M. Taylor, The asymptotic strength distribution of a general fiber bundle, Advances in Applied Probability 5 (1973) 200–216.
[19] R. Chudoba, M. Vořechovský, M. Konrad, Stochastic modeling of multi-filament yarns I: random properties within the cross section and size effect, International Journal of Solids and Structures 43 (2006) 413–434.
[20] G. Booch, J. Rumbaugh, I. Jacobson, The Unified Modeling Language User Guide, first ed., Addison-Wesley Professional, 1998.
[21] L. Pierce, J. Swisher, Traits UI user guide, http://enthought.github.com/traits/TUIUG/front.html, 2011.
[22] I.M. Wilbers, H.P. Langtangen, A. Odegard, Using Cython to speed up numerical Python programs, Proceedings of MekIT 9 (2009) 495–512.
[23] S. Behnel, R. Bradshaw, C. Citro, L. Dalcin, D.S. Seljebotn, K. Smith, Cython: the best of both worlds, Computing in Science & Engineering 13 (2011) 31–39. WOS:000288053300004.
[24] Weave: tools for inlining C/C++ within Python code, http://www.scipy.org/Weave, 2011.
[25] J. Nilsen, X. Cai, B. Hoyland, H. Langtangen, Simplifying the parallelization of scientific codes by a function-centric approach in Python, Computational Science & Discovery 3 (2010) 1–24.
[26] F. Alted, I. Vilata, PyTables: hierarchical datasets in Python, http://www.pytables.org, 2002.
[27] A. Klöckner, N. Pinto, Y. Lee, B. Catanzaro, P. Ivanov, A. Fasih, PyCUDA and PyOpenCL: a scripting-based approach to GPU run-time code generation, Parallel Computing 38 (2012) 157–174.
[28] J. Bergstra, O. Breuleux, F. Bastien, P. Lamblin, R. Pascanu, G. Desjardins, J. Turian, D. Warde-Farley, Y. Bengio, Theano: a CPU and GPU math expression compiler, in: Proceedings of the Python for Scientific Computing Conference (SciPy).