SMART-UQ: UNCERTAINTY QUANTIFICATION TOOLBOX FOR GENERALISED INTRUSIVE AND NON INTRUSIVE POLYNOMIAL ALGEBRA

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ABSTRACT
The paper presents a newly developed opensource toolbox named Strathclyde Mechanical and Aerospace Research Toolbox for Uncertainty Quantification (SMART-UQ) that implements a collection of intrusive and non intrusive techniques for polynomial approximation and propagation of uncertainties. Non-intrusive approaches are mainly based on building polynomial expansions of the quantity of interest using sparse samples of the system response to the uncertain variables. Intrusive methods instead modify the analysis by redefining algebraic operators or by including polynomial expansions directly in the model. The paper will present the software architecture and development philosophy, its current capabilities and will provide an example where the available techniques are compared in terms of accuracy and computational cost on a test case of propagation of uncertainties in space dynamics.

Index Terms— uncertainty quantification, uncertainty propagation, polynomial algebra, polynomial interpolation, intrusive methods, non-intrusive methods

1. INTRODUCTION
The problem of quantify regions of uncertainties and their propagation through dynamics can be tackled numerically by intrusive and non-intrusive techniques. Non intrusive methods such as Polynomial Chaos Expansion and Stochastic collocation methods, do not require changes in the analysis code since it relies on multiple system responses and post processing of these information. Intrusive methods instead, such as Taylor Models, Galerkin projection modify the analysis code by redefinition of algebraic operators or embedding high order polynomial expansions of uncertain quantities.

For the time being only polynomial algebra intrusive methods and polynomial interpolation non-intrusive techniques are considered. The main advantage of sampling-based non intrusive methods is their range of applicability. The model is treated as a black box and no regularity is required. On the other hand, they suffer from the curse of dimensionality when the number of required sample points increases. Polynomial algebra intrusive techniques are able to overcome this limitation since their computational costs grow at a lower rate with respect to their corresponding polynomial interpolation non intrusive counterpart. Nevertheless, intrusive methods are harder to implement and cannot treat the model as a black box. Moreover intrusive methods are able to propagate nonlinear regions of uncertainties while non intrusive methods rely on hypercubes sampling.

The most widely known intrusive method for uncertainty propagation in orbital dynamics is Taylor Differential Algebra. The same idea has been generalised to Tchebycheff polynomial basis because of their fast uniform convergence with relaxed continuity and smoothness requirements. However the SMART-UQ toolbox has been designed in a flexible way to allow further extension of this class of intrusive and non-intrusive methods to other basis.

In the paper the different intrusive and non intrusive techniques integrated in SMART-UQ will be presented respectively in section 3 and 4 together with the architectural design of the toolbox in section 2. Test cases on propagation of uncertainties in space dynamics with the corresponding intrusive and non intrusive methods will be discussed in terms of computational cost and accuracy in section 5 and as final some conclusions and future development are presented.

2. SMART
The Strathclyde Mechanical and Aerospace Research Toolbox is an open source project initiated in 2015 by the Aerospace Center of Strathclyde University with the aim of releasing to the open source community the algorithm developed in the group, make research achievements freely accessible to the scientific community and push research one step further.

A modular approach has been preferred rather than developing one single comprehensive framework. Hence at the current state of development, one toolbox for optimisation and optimal control (SMART-O2C), one tool for astrodynamics (SMART-ASTRO) and one tool for uncertainty quantification and propagation (SMART-UQ) are being developed, see
SMART family

Figure 1. This approach allows experts from different fields to benefit from accessing optimisation and uncertainty quantification algorithms without the need of running the whole astrodynamical engine along with it. However, it will be given the possibility during compilation, to modify the configuration file to link the toolbox in use against one or more of the SMART tools to perform, for example, optimisation under uncertainties for space trajectory problems. All toolboxes are hosted on GitHub [https://github.com/space-art](https://github.com/space-art).

SMART-UQ is the first toolbox of the above-mentioned to be released open source under the MPL license in Spring 2016. SMART-UQ is a generic framework for uncertainty quantification and propagation. It has been developed in C++ with an heavy object oriented architecture. This allows the tool to be flexible enough for the integration of new techniques and test problems. The toolbox has been fully documented by the use of Doxygen [www.doxygen.org](http://www.doxygen.org) and few tutorials are available to get started. In Figure 2 the software layers are outlined.

On the top layer the information regarding documentation and tutorial are accessible for the user that is only interested in using the functionality of the tool for its own application. One level below are the modules of interest for the developers, people who wish to integrate their own techniques in the framework. One level more below is the unit test module, controlled by SMART maintainers that will ensure the consistency and quality of the code added by the developers.

At the current state of the art the core of the SMART-UQ toolbox includes the following techniques:

- **Sampling**: random sampling, Latin Hypercube sampling (LHS), low discrepancy sequence (Sobol).

- **Polynomial**: Tchebycheff and Taylor basis

- **Integrators**: fixed stepsize integrators (first and second order Euler, third, fourth and fifth order Runge-Kutta methods)

- **Dynamics**: Lotka-Volterra, Van der Pol, Two-body problem

The toolbox is at its first stage of development and it has been used as a benchmarking environment for the newly developed intrusive techniques. The inclusion of new components for each of the elements above is made easy by the object oriented structure of the toolbox. If for example a new dynamical system wants to be added it is enough to inherit from the base dynamics class and implement its virtual routines (evaluate dynamic in this case). The toolbox relies on one external dependency for fast multiplication in Tchebycheff basis FFTW3 [https://github.com/FFTW/fftw3](https://github.com/FFTW/fftw3) and the C++ template library for linear algebra Eigen [http://eigen.tuxfamily.org](http://eigen.tuxfamily.org) that is shipped with the toolbox. If FFTW3 is not found during the configuration process direct multiplication will be used instead.

For the time being only the C++ interface is available. The user has to provide in the main function the list of uncertain variables and their range of variability. At present only uniform distributions are handled. The toolbox will be expanded in the future to allow the definition of aleatory and epistemic uncertain variables and corresponding distribution(s). Depending on the type of analysis the user has to instantiate either a sampling technique and a polynomial class or only the latter one.

If non-intrusive techniques are used the interpolate method need to be called. Two options are available: provide a predefined set of points given as input and output matrices or provide the analysis code. In this case the model will be evaluated on specific sample points as specified by the sample technique instantiated. The method interpolate is then

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1. [www.doxygen.org](http://www.doxygen.org)
2. [https://github.com/FFTW/fftw3](https://github.com/FFTW/fftw3)
3. [http://eigen.tuxfamily.org](http://eigen.tuxfamily.org)
called on this set of new points and the polynomial coefficient of the interpolation, in the selected basis, are computed.

If intrusive methods are used the user has to initialise the uncertain variables as first degree polynomial in that variable in the selected basis. The analysis module need to be given as template function. Once the analysis module is evaluated in the algebra of polynomials therefore 

\[ T_1(x) = T_1(\tau_1(x)). \]

The generalised approach here proposed extends to any type of basis, hence the generic notation in equation 1 will be used.

3. INTRUSIVE TECHNIQUES

The Generalised Intrusive Polynomial Expansion (GIPE) approach, implemented in the toolbox and presented here in the paper, expands the uncertain quantities in a polynomial series in the chosen basis and propagates them through the dynamics using a multivariate polynomial algebra. Hence the operations that usually are performed in the space of real numbers now performed in the algebra of polynomials therefore a polynomial representation of system responses is available once the analysis code has been evaluated in the algebra.

To improve the computational complexity of the method, arithmetic operations are performed in the monomial basis. Therefore a transformation between the chosen basis and the monomial basis is performed after the expansion of the elementary functions.

Multivariate polynomial expansions of \( d \) variables up to degree \( n \), are defined as

\[
P(x) = \sum_{i | \|i\| \leq n} p_i \alpha_i(x),
\]

where \( x \in \Omega \), \( i \in [0,n]^d \subset \mathbb{N}^d \), \( |i| = \sum_{r=1}^{d} i_r \) and \( \alpha_i(x) \) is the polynomial basis of choice. The function space \( \mathcal{P}_{n,d}(\alpha_i) \) of all polynomials in the prescribed base, can be equipped with a set of operations, generating an algebra on the space of polynomial expansions. The multivariate basis here considered are

- Taylor
  \[
  T_1(x) = \prod_{r=1}^{d} s_{i_r}^r,
  \]
  where \( x \in \Omega = [-1,1]^d \)

- Tchebycheff
  \[
  C_1(x) = \prod_{r=1}^{d} C_i(x_r),
  \]
  where \( C_0(x_r) := 1 \), \( C_i(x_r) := \cos(i_r \arccos(x_r)) \) and \( x \in \Omega = [-1,1]^d \)

Being \( \tau_1 : \bar{\Omega} = [a,b] \subset \mathbb{R}^d \rightarrow \Omega \) the linear mapping between the two hyper-rectangular then the Tchebycheff polynomials are defined over \( \bar{\Omega} \) as

\[
C_1(x) = C_1(\tau_1(x)),
\]

where \( x \in \bar{\Omega} \). So without loss of generality the domain \( \Omega \) is considered for further considerations. Analogously Taylor approximations can be considered expanded around zero, as before the linear transformation \( \tau_1 \) can translate the initial interval into one centered in zero

\[
T_1(x) = T_1(\tau_1(x)).
\]

The elements of which belong to the polynomial ring in \( d \) indeterminates \( K[x] \) and have degree up to \( n \). Each element of the algebra \( P(x) \) is uniquely identified by the set of its coefficients \( p = \{ p_i : |i| \leq n \} \in \mathbb{R}^N \). The coefficients have been ordered using the scheme in Giorgilli and Sansottera\(^8\).

Being that the result of any algebraic operation or evaluation of elementary function still an element of the algebra, addition and multiplication are defined as on the ring \( K[x] \) while multiplication needs to be truncated. Division is treated as elementary function through the definition of a composition rule on the algebra such that

\[
g(y(x)) \sim G(x) \circ Y(x),
\]

where \( \circ \) is the composition function on \( (\mathcal{P}_{n,d}(\alpha_i), \otimes) \) and \( g(x) \) and \( y(x) \) are, respectively, a multivariate function and an array of \( d \) multivariate functions in the real space, with \( G(x) \) and \( Y(x) \) their polynomial expansions. Hence being \( h(x) \) any of the functions \{ 1/x, \sin(x), \cos(x), \exp(x), \log(x), \ldots \}, H(x) \) its univariate polynomial expansion and \( F(x) \) an element of the algebra that approximates the multivariate function \( f(x) \), their composition is approximated by

\[
h(f(x)) \sim H(x) \circ F(x),
\]

in which case \( \circ \) denotes the composition of an element of the algebra with an univariate polynomial.
Given that the computational cost of multiplying two polynomials not in the monomial basis is generally higher, the authors are proposing hereafter a methodology to overcome this issue. Being $H(x)$ the expansion of an elementary function in the current polynomial basis and being

$$
\tau_2 : P_{n,d}(\alpha_i) \rightarrow P_{n,d}(\phi_i)
$$

the transformation from the current basis into the monomial basis $\phi_i$, given $h(x)$ any of the functions \{1/x, sin(x), cos(x), exp(x), log(x), \ldots\} and $f(x)$ a multivariate function

$$
h(f(x)) \sim \tau_2(H(x)) \circ F_\phi(x),
$$

where $F_\phi(x)$ is the approximation in the monomial basis of $f(x)$. It needs to be noted that for the case of Tchebycheff expansions given that high order terms have contribution to low order terms in the monomial basis\(^1\), $H(x)$ is expanded up to 1.5 times the order of the algebra and $\tau_2(H(x))$ is truncated afterwards. This guarantees to not lose in accuracy when the changing of basis is performed. Hence just for the Tchebycheff case the transformation $\tau_2$ is between the functional spaces

$$
\tau_2 : C_{1.5n,d}(\alpha_i) \rightarrow P_{n,d}(\phi_i).
$$

All other algebraic operations are then performed in $P_{n,d}(\phi_i)$ and converted back to the current basis only at final. Note that since $H(x)$ is an univariate polynomial, the change-of-basis matrix is of order $n + 1$ ($1.5n + 1$ in case of Tchebycheff) instead of $\mathcal{N}$, rendering the conversion computationally cheaper than in the multivariate case.

From a software architecture point of view, if new polynomial basis are added to the toolbox they need to implement a method, virtually inherited from the base class, that performs the change from the current basis to the monomial one and viceversa.

### 3.2. Integration of dynamical systems

The aforementioned procedures allow one to create a new computational environment where each function, that can be defined by means of arithmetic operations and elementary functions, can be represented as an element of $(P_{n,d}(\alpha_i), \otimes)$. It follows that expanding the flow of the system of autonomous ordinary differential equations of the form

$$
\begin{align*}
\dot{\mathbf{x}} & = f(\mathbf{x}) \\
\mathbf{x}(t_0) & = \mathbf{x}_0
\end{align*}
$$

requires declaring the uncertain initial condition $\mathbf{X}_0(\mathbf{x}) = (X_1(\mathbf{x}), \ldots, X_d(\mathbf{x})) \in (P_{n,d}(\alpha_i), \otimes)^d$ as an element of the algebra:

$$
\begin{align*}
X_1(\mathbf{x}) & = \alpha_{1,1}(\mathbf{x}), \\
X_2(\mathbf{x}) & = \alpha_{1,2}(\mathbf{x}), \\
\vdots \\
X_d(\mathbf{x}) & = \alpha_{1,d}(\mathbf{x}),
\end{align*}
$$

where $\alpha_{1,j}(\mathbf{x})$ is the first order base in the $j$-th component, and applying any integration scheme with operations in the algebra to have at each integration step the full generalised polynomial expansion of the current state. For example, choosing forward Euler as integration scheme yields:

$$
\begin{align*}
\mathbf{X}_k(\mathbf{x}) & = \mathbf{X}_{k-1}(\mathbf{x}) + hf(\mathbf{X}_{k-1}(\mathbf{x})), \\
\mathbf{X}_k(\mathbf{x}) & = \mathbf{X}_{k-1}(\mathbf{x}) \in (P_{n,d}(\alpha_i), \otimes)^d,
\end{align*}
$$

where $\mathbf{X}_k(\mathbf{x})$ is the polynomial representation of the system flow at the $k^{th}$ time-step.

### 4. NON-INTRUSIVE TECHNIQUES

Non intrusive methods have been implemented for a set of sampling techniques for interpolation in the complete polynomial basis.

Given a set of $s$ sample point in the initial hyper-rectangular $\Omega$, $s$ numerical integration need to be performed to compute the polynomial expansion of the states at a given time. Hence given the dynamics

$$
\begin{align*}
\dot{\mathbf{x}} & = f(\mathbf{x}) \\
\mathbf{x}(t_0) & = \mathbf{x}_0
\end{align*}
$$

where $\mathbf{x}_0 \in \Omega$. Being $\mathcal{S}_0 = \{\mathbf{x}_{0,1}, \ldots, \mathbf{x}_{0,s}\}$ the point sampled with one of the techniques available in the toolbox or externally provided by the user, then applying a numerical integration scheme the set

$$
\mathcal{S} = \{\mathbf{x}_1, \ldots, \mathbf{x}_s\}
$$

where $\mathbf{x}_i = I(\mathbf{x}_{0,i})$ is the solution at time $t$ obtained with initial guess $\mathbf{x}_{0,i}$ and integration scheme $I(\cdot)$.

The generic polynomial interpolant on this set of nodes has the form

$$
F(\mathbf{x}) = \sum_{i, |i| \leq n} p_i \alpha_i(\mathbf{x}),
$$

where $p_i$ are the unknown coefficients computed by inverting the linear system

$$
HP = Y,
$$

with

$$
H = \begin{bmatrix}
\alpha_0(x_{0,1}) & \ldots & \alpha_N(x_{0,1}) \\
\vdots & \ddots & \vdots \\
\alpha_0(x_{0,s}) & \ldots & \alpha_N(x_{0,s})
\end{bmatrix},
\quad
P = \begin{bmatrix}
c_0 \\
\vdots \\
c_N
\end{bmatrix},
\quad
Y = \begin{bmatrix}
x_1 \\
\vdots \\
x_s
\end{bmatrix},
$$

\(^1\)If we consider for example the 4th order term of the univariate basis $C_4(x) = 8x^4 - 8x^2 + 1$, this has a contribution to the second order term of the monomial basis.
where \( s = |\mathcal{S}| \) is the cardinality of the set of grid points and the components of \( Y \) are the true values obtained integrating the dynamics in the initial sample points. The system cannot be inverted if the matrix \( H \) has not full rank. The minimum number of sample points is equal to the size of the space of the polynomial basis \( \mathcal{N} \). If more points are provided a Least Square approach is used to invert the system and find the unknown coefficients.

From a software architecture point of view if we are adding new polynomial basis to the toolbox a function that is able to evaluate the polynomial in a prescribed set of points is the only functionality need for using the non-intrusive technique.

5. CASE STUDY: PROPAGATION OF UNCERTAINTIES IN SPACE DYNAMICS

The toolbox capabilities are tested by applying the intrusive and non-intrusive techniques available on the propagation of uncertainties in a two-body dynamical problem where thrust, drag and an unknown force are modeled to increase the number of uncertainties and the complexity of the problem. Initially only uncertainties in the states are considered, then the uncertainties on the force parameters are added gradually to increase the dimensionality of the problem and to compare the available methods not only in terms of accuracy but also in term of computational complexity.

5.1. Problem

The two-body problem here considered is taking into account only three additional forces: a constant low thrust, atmospheric drag and an unknown constant perturbation. In an inertial reference frame the dynamical equations are

\[
\ddot{\mathbf{x}} = -\frac{\mu}{r^3} \mathbf{x} + \frac{\mathbf{T}}{m} + \frac{1}{2} \rho \frac{C_{DA}}{m} \| \mathbf{v}_{rel} \| \mathbf{v}_{rel} + \epsilon
\]

where \( r \) is the distance from the Earth, \( \mathbf{v}_{rel} \) is the Earth relative velocity and the mass of the spacecraft varies as

\[
\dot{m} = -\alpha \| \mathbf{T} \|
\]

5.2. Experimental set up

The dynamics is integrated with a fixed stepsize Runge-Kutta 4th order scheme, with nominal initial conditions

\[
\begin{align*}
x(0) &= 7338 \cdot 10^3, & v_x(0) &= 0, \\
y(0) &= 0, & v_y(0) &= 7350.21, \\
z(0) &= 0, & v_z(0) &= 0, \\
m(0) &= 2000.
\end{align*}
\]

Where all variables have I.S. units. This corresponds to a circular Low Earth Orbit. Constant low thrust of 500 mN in the \( y \) direction is considered with \( \alpha = 3.33 \cdot 10^{-5} \). Regarding drag, \( \rho \) is computed by means of the exponential atmospheric model

\[
\rho = \rho_0 \cdot \exp \left( -\frac{r - r_0}{H} \right),
\]

with \( \rho_0, r_0, H \) atmospheric parameters corresponding to the initial altitude, and \( C_{DA} = 4.4 \). Constant perturbation \( \epsilon \) is nominally zero.

Intrusive and non-intrusive methods are compared against a Monte Carlo sampling of \( 10^4 \) points. The Root Mean Square Error (RMSE) measure is used for the comparison defined as

\[
RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (\hat{x}_i - x_i)^2},
\]

where \( N \) is the number of samples, \( x_i \) is the true value of the state (obtained by forward integration in the sampling points) and \( \hat{x}_i \) is the approximated value computed evaluating the obtained polynomial approximation. Four techniques are compared:

- Non-intrusive with Tchebycheff basis and a LHS of \( N \) samples over the uncertain hypercube
- Non-intrusive with monomial basis and a LHS of \( N \) samples over the uncertain hypercube
- Intrusive with Tchebycheff basis over the uncertain hypercube
- Intrusive with Taylor basis centered in the mid point of the uncertain hypercube

The order of all polynomial expansions has been set to 4 after performing accuracy analysis on a simplified problem.

5.3. Uncertainty on initial states and model parameters

Four instances of the problem have been evaluated with identical nominal dynamics and progressively increasing dimension of the uncertain region. Case 1 only presents uncertainty on the initial states whereas cases 2 to 4 consider uncertainty in up to 10 model parameters. Finally a fifth case with full dimension but smaller uncertainty regions for the states has been run to assess the impact of the magnitude of the uncertainty on the accuracy of the methods. The definition of each test-case is detailed in Table 1.

5.4. Results

Cases 1 to 4 present similar accuracy results. This is due to the propagation being dominated by the uncertainties on the initial states, which are identical in all these cases.

For case 4, depiction of the uncertain regions and RMSE values in \( x \) and \( v \) are presented in Figures 3 to 5. The use of Taylor basis yields errors 4 to 5 orders of magnitude higher
than other methods, i.e. comparable to the size of the uncertain region. The uncertain space appears to be too large for this approach to capture its growth; Figure 4 illustrates this effect. The expansions obtained with the other three uncertainty propagation techniques attain mean final approximation errors of $10^{-1}$ m and $10^{-4}$ m/s in the plane of motion. [ht!]

Figures 6 to 8 show analogous results for case 5. The reduction in volume of the initial uncertain space has a positive impact on the absolute accuracy of the Taylor approach, but the same effect is encountered when comparing to the size of the propagated region. [ht!] [ht!]

These unexpectedly inaccurate results for the Taylor D.A. method called for further investigation. Hence yet another test-case is run, where the dynamics are identical to those of case 4 but have now been expressed with non-dimensional magnitudes. This aims at reducing the discordance in scale between different variables, which can have a negative effect in methods of local accuracy such as Taylor D.A.. The fundamental scaling factors are the planetary canonical units of the Earth and the initial mass of the spacecraft, i.e.

$$DU = 6378136 \, m, \quad TU = 806.78 \, s, \quad m_0 = 2000 \, kg.$$
The results are shown in Figures 9 to 11. As can be observed, all methods achieve accurate reproduction of the uncertain region by means of the proposed scaling. For both intrusive methods, final errors are in the order of $10^{-5}$ m, $10^{-7}$ m/s in the plane of motion, non-intrusive techniques yielding representations one to two orders of magnitude less accurate.

Figure 12 shows the simulation run-time necessary for cases 1 to 4. Intrusive methods require more operations for a single-step propagation than their non-intrusive counterparts, but have overall lower computational complexity. Hence they are advantageous for high-dimensional problems.

The two non-intrusive techniques present very similar times. The difference in run-time between Taylor and Tchebycheff intrusive methods is due to the transformation into monomial base of the latter for each of the elementary functions used, while the rest of operations have equivalent cost.
6. CONCLUSIONS

The paper presents a novel open source computational environment for uncertainties quantification and propagation. A set of intrusive and non-intrusive techniques have been integrated in a flexible architecture that allows further extension to different polynomial basis, sampling techniques, dynamical systems and integration schemes.

The available techniques have been compared in terms of accuracy and computational cost on a space-related problem with 17 uncertain variables. Non-intrusive and Tchebycheff-based intrusive techniques showed comparable results in terms of accuracy. Taylor-based intrusive method however is affected by a higher sensitivity to the scaling of the problem. Both intrusive methods have a lower computational cost for instances of the problem with more than 11 uncertain variables. Hence intrusive methods are recommended to be used for high-dimensional problems, wherever the model need not be treated as a blackbox but can be expressed in terms of algebraic operators and elementary functions.

Further work will be dedicated to the management of model discontinuities in intrusive techniques by means of
domain splittings and to the introduction of intrusive and non-intrusive methods on reduced set of polynomial basis.

7. REFERENCES


