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

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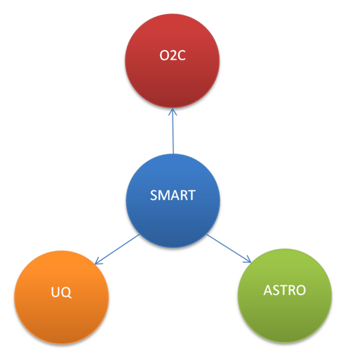
Outline

SMART PROJECT

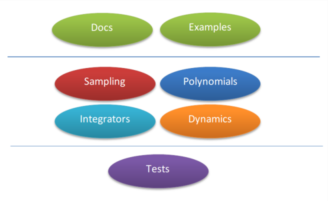
SMART

- **2015**: Strathclyde Mechanical and Aerospace Research Toolboxes
- **2016**: open source release of SMART-UQ under the MPL license
- GitHub `https://github.com/space-art`, C++, Doxygen



- **SMART-UQ** for Uncertainty quantification
- **SMART-O2C** for Optimisation and Optimal Control
- **SMART-ASTRO** for Astrodynamics

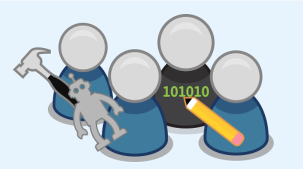
SMART-UQ



- **Sampling**: random sampling, Latin Hypercube sampling (LHS), low discrepancy sequence (Sobol).
- **Polynomial**: Tchebycheff and Taylor basis
- **Integrators**: fixed stepsize integrators (Euler, Runge-Kutta methods)
- **Dynamics**: Lotka-Volterra, Van der Pol, Two-body problem

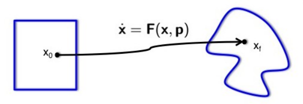
Interface

- **User**: can instantiate one of the available polynomial basis, sampling techniques, integration scheme, dynamical system
- **Developer**: can extend one of the abstract classes `base_dynamics`, `base_integrators`, `base_polynomial`, `base_sampling` to integrate new numerical strategies and problems

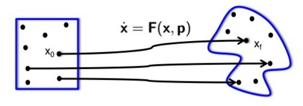


SMART-UQ: Background and Motivation

- **Intrusive methods**: they apply inside the model, modifying algebraic operators
  - *Advantages*: scalability
  - *Disadvantages*: requires more effort to implement



- **Non-intrusive methods**: evaluation of the model in sample points and construction of the response surface
  - *Advantages*: easy implementation
  - *Disadvantages*: curse of dimensionality



Generalised Intrusive Polynomial expansion (GIPE)

- **1982** (Epstein) Ultra Arithmetic
- **1986** (Berz) Taylor Differential Algebra
- **1997** (Berz) Taylor Models
- **2003** (Berz) Taylor Models and Other Validated Functional Inclusion Methods
- **2010** (Joldes) Formal comparison between Taylor, Tchebycheff, Newton Models (univariate)

IDEA

Develop a generic computer environment for multivariate polynomial algebra **Generalized Intrusive Polynomial Expansion (GIPE)**. Integrate the work already done in the team on non-intrusive techniques and apply them to problems in **astrodynamics**.

POLYNOMIAL APPROXIMATION

Multivariate Polynomials

Multivariate polynomial approximation

In d variables up to degree n

$$P(\mathbf{x}) = \sum_{\mathbf{i}, |\mathbf{i}| \leq n} p_{\mathbf{i}} \alpha_{\mathbf{i}}(\mathbf{x}) \in \mathcal{P}_{n,d}(\alpha_i)\,, \tag{1}$$

where $\mathbf{x} \in \Omega = [-1, 1]^d \subset \mathbb{R}^d\,,\ \mathbf{i} \in [0, n]^d \subset \mathbb{N}^d\,,\ |\mathbf{i}| = \sum_{r=1}^{d} i_r$ and $\alpha_{\mathbf{i}}(\mathbf{x})$ is the polynomial basis of choice.

- $\overline{\Omega} = [\mathbf{a}, \mathbf{b}] \subset \mathbb{R}^d$ and $\tau : \overline{\Omega} \to \Omega \to \alpha_{\mathbf{i}}(\mathbf{x}) = \alpha_{\mathbf{i}}(\tau(\mathbf{x}))$,
- **Taylor** $T_{\mathbf{i}}(\mathbf{x}) = \prod_{r=1}^{d} x_r^{i_r}$.
- **Tchebycheff** $C_{\mathbf{i}}(\mathbf{x}) = \prod_{r=1}^{d} C_{i_r}(x_r)$, where $C_0(x_r) := 1$, $C_{i_r}(x_r) := \cos(i_r \arccos(x_r))$. They form an **orthogonal basis** in $\mathcal{P}_{n,d}(\alpha_i)$

Polynomial Approximation

$f(\mathbf{x})$ multivariate function in d variables

$$f(\mathbf{x}) \sim \sum_{\mathbf{i}, |\mathbf{i}| \leq n} p_{\mathbf{i}} \alpha_{\mathbf{i}}(\mathbf{x}) \in \mathcal{P}_{n,d}(\alpha_i), \qquad |\mathbf{i}| = \sum_{r=1}^{d} i_r$$

$p_{\mathbf{i}}$ can be determined by means of **hyperinterpolation** techniques or **algebraic manipulations** of polynomials.

Approximation theory

- **Tchebycheff**: uniform convergence over the interval of definition (f is required to be more than continuous but less than differentiable)
- **Taylor**: convergence in a neighborhood of the expansion point (f is required to be n-th times differentiable)

Intrusive methods

Algebra Definition

$(\mathcal{P}_{n,d}, \otimes)$ is the Algebra on the space of polynomials such that being $P_{f(\mathbf{x})}$ and $P_{g(\mathbf{x})}$ the polynomial approximation of $f(\mathbf{x})$ and $g(\mathbf{x})$ respectively, in the chosen basis,

$$P_{f(\mathbf{x}) \oplus g(\mathbf{x})} = P_{f(\mathbf{x})} \otimes P_{g(\mathbf{x})},$$

where $\oplus \in \{+, -, *, /\}$ and $\otimes$ is the corresponding operation in the algebra.

- $\mathcal{N} = \dim(\mathcal{P}_{n,d}, \otimes) = \binom{n+d}{d} = \frac{(n+d)!}{n!d!}$
- Composition: $h(x) \in \{1/x, \sin(x), \cos(x), \exp(x), \log(x), ...\}$, $f(\mathbf{x})$ a multivariate function

$$h(f(\mathbf{x})) \sim H(x) \circ F(\mathbf{x}), \quad H(x) \in \mathcal{P}_{n,1}(\alpha_i), F(\mathbf{x}) \in \mathcal{P}_{n,d}(\alpha_i)$$

Manipulation in Monomial basis

- **Motivation**: computationally expensive multiplication in Tchebycheff basis
- **Solution**: transform the expansion of elementary functions into monomial base ϕ_i. Given $h(x) \in \{ 1/x, \sin(x), \cos(x), \exp(x), \log(x), \dots \}$ and $f(\mathbf{x})$ a multivariate function

$$h(f(\mathbf{x})) \sim \tau(H(x)) \circ F_\phi(\mathbf{x}) \,,$$

where $F_\phi(\mathbf{x})$ is the approximation in the monomial basis of f and τ is the transformation.
- New polynomial basis inherit a virtual method from the base class for **transformation to and from** monomial basis

Integration of Dynamical Systems

Expansion of the flow of an autonomous ODE

$$\begin{cases} \dot{\mathbf{x}} = f(\mathbf{x}) \\ \mathbf{x}(t_0) = \mathbf{x}_0 \end{cases}$$

Initialize $\mathbf{x}_0$ as an element of the algebra

$$\mathbf{X}_0(\mathbf{x}) = (\alpha_{\mathbf{1}_1}(\mathbf{x}), \ldots, \alpha_{\mathbf{1}_d}(\mathbf{x})) \in (\mathcal{P}_{n,d}(\alpha_i), \otimes)^d$$

Forward Euler scheme:

- Real Algebra: $\mathbf{x}_1 = \mathbf{x}_0 + dt\, f(\mathbf{x}_0)$
- Polynomial Algebra: $\mathbf{X}_1(\mathbf{x}) = \mathbf{X}_0(\mathbf{x}) + dt\, f(\mathbf{X}_0(\mathbf{x})) \in (\mathcal{P}_{n,d}, \otimes)^d$

Polynomial Expansion of the Flow

At the k-th iteration in the polynomial algebra environment

$$\mathbf{X}_k(\mathbf{x}) = \mathbf{X}_{k-1}(\mathbf{x}) + dt\, f(\mathbf{X}_{k-1}(\mathbf{x})) \in (\mathcal{P}_{n,d}, \otimes)^d$$

Implementation

- **Template library**: integration schemes and dynamical systems are implemented for real or polynomial evaluations
- **Operator overloading**: algebraic operators and elementary function have been overloaded
- **Abstract base classes**: if new polynomial basis, integrators, sampling techniques or dynamics are added to the toolbox a set of virtual functions need to be implemented (example `integrate(ti, tend, nsteps, x0, xfinal)` for integrators, `evaluate(t,state,dstate)` for dynamics, `evaluate(x)`) for polynomials and so on

Non-intrusive methods

Polynomial Interpolation

The **interpolation polynomial** on the grid nodes is computed as

$$F(\mathbf{x}) = \sum_{\mathbf{i} \in I(\Gamma_{n,d})} p_{\mathbf{i}}\, \alpha_{\mathbf{i}}(\mathbf{x})\,, \tag{2}$$

Where $\Gamma_{n,d}$ is the chosen sampling scheme. The unknown coefficients $p_{\mathbf{i}}$ are computed by **inverting the linear system** $HP = Y$

$$H = \begin{bmatrix} \alpha_0(x_1) & \dots & \alpha_{\mathcal{N}}(x_1) \\ \vdots & \ddots & \vdots \\ \alpha_0(x_s) & \dots & \alpha_{\mathcal{N}}(x_s) \end{bmatrix}, \qquad P = \begin{bmatrix} p_0 \\ \vdots \\ p_{\mathcal{N}} \end{bmatrix}, \qquad Y = \begin{bmatrix} Y_1 \\ \vdots \\ Y_s \end{bmatrix},$$

where $s = |\Gamma_{n,d}|$ is the number of nodes, $x_1, \dots, x_s$ are the nodes Y are the true values.

Implementation

- **Template library**: integration and polynomial evaluation are performed in the space of real numbers
- **Abstract class**: in the superclass the method for interpolating given a set of values (obtained through sampling and evaluation of the analysis or supplied as text file) is inherited by any polynomial

PROPAGATION OF UNCERTAINTY IN SPACE DYNAMICS

Two Body Problem

Problem Definition

In an inertial reference frame the dynamical equations are

$$\ddot{\mathbf{x}} = -\frac{\mu}{r^3}\mathbf{x} + \frac{\mathbf{T}}{m} + \frac{1}{2}\rho\frac{C_D A}{m}\|\mathbf{v}_{rel}\|\mathbf{v}_{rel} + \epsilon$$

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

$$\dot{m} = -\alpha\|\mathbf{T}\|$$

Problem parameters

- **Initial conditions** (circular LEO):

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

- **Atmosphere**: $\rho = \rho_0 \cdot exp\left(-\frac{r-r_0}{H}\right)[kg/m^3]$, $C_D A = 4.4[m^2]$
- **Thrust**: constant low thrust of 500 mN in the y direction with $\alpha = 3.33 \cdot 10^{-5}[s/m]$
- **Constant perturbation** ϵ is nominally zero

Uncertainity region

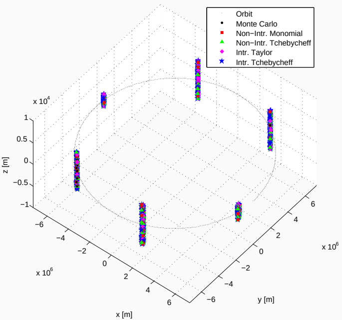
Table: Parameters and states uncertainties (% refers to the nominal value, d is the number of uncertain variables)

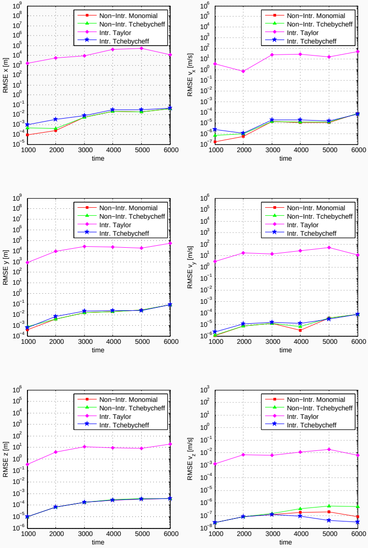
Test-case	1	2	3	4
$u_{\mathbf{x}(0)}$ [m]	10^3	10^3	10^3	10^3
$u_{\mathbf{v}(0)}$ [m/s]	5.00	5.00	5.00	5.00
$u_{m(0)}$ [Kg]	1.00	1.00	1.00	1.00
u_{T}, u_{α}	–	5%	5%	5%
u_{ρ_0}, u_H, u_{C_D}	–	–	1%	1%
u_{ϵ}	–	–	–	10^{-4}
d	7	11	14	17

Numerical set up

- **Integrator**: Runge-Kutta 4th order.
- **Polynomial approximation** of order 4
- **Validation**
  - *Monte Carlo:* sampling of $N = 10000$ points
  - *Error measure:* $RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\hat{x}_i - x_i)^2}$,
- **Comparison** of non-intrusive techniques (sampling on LHS and interpolation with Tchebycheff and monomial basis) and intrusive techniques (Taylor and Tchebycheff)

Results


Orbit
Monte Carlo
Non−Intr. Monomial
Non−Intr. Tchebycheff
Intr. Taylor
Intr. Tchebycheff
z [m]
x [m]
y [m]
x 10^4
x 10^6
x 10^6


Non−Intr. Monomial
Non−Intr. Tchebycheff
Intr. Taylor
Intr. Tchebycheff
RMSE x [m]
RMSE v_x [m/s]
RMSE y [m]
RMSE v_y [m/s]
RMSE z [m]
RMSE v_z [m/s]
time

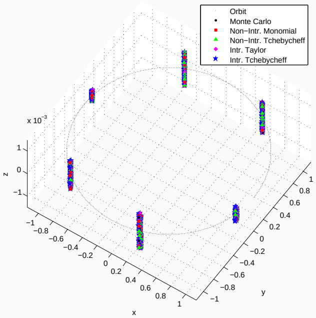
Scaled problem

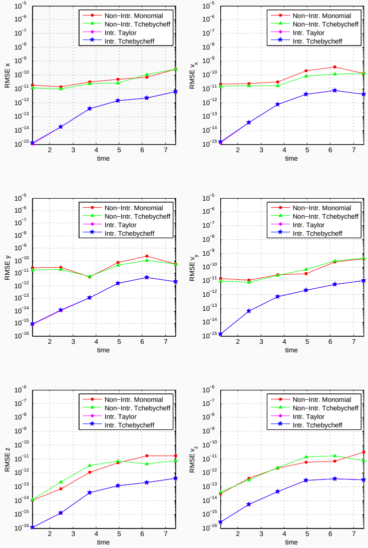
The fundamental scaling factors are the planetary canonical units of the Earth and the initial mass of the spacecraft, i.e.

$$DU = 6378136\,m\,, \quad TU = 806.78\,s\,, \quad m_0 = 2000\,kg\,.$$

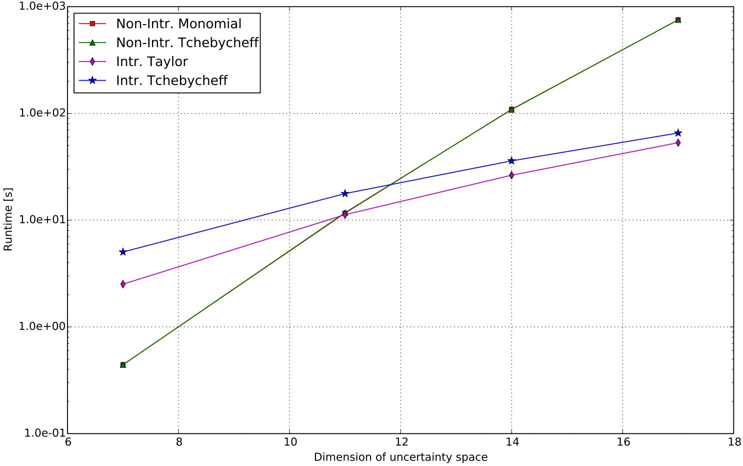
- position $x_{scaled} = x/DU$, $u_{x,scaled} = u_x/DU$
- velocity $v_{scaled} = v/(DU/DT)$, $u_{v,scaled} = u_v/(DU/DT)$
- mass $m_{scaled} = m/m_0$, $u_{m,scaled} = u_m/m_0$

Results (scaled problem)





Computational complexity



DISCUSSION & CONCLUSIONS

Discussion

- **SMART-UQ** is a **flexible** toolbox for uncertainity quantification and propagation by means of intrusive and non-intrusive polynomial approximation techniques
- The techniques currently available have been applied to a **space dynamic problem** and compared in terms of accuracy and computational costs
- **Intrusive** methods are **computationally more efficient** that non-intrusive one for large problems
- **Tchebycheff** intrusive method is **more robust** (unsensitive to scaling factors)

Future Work

- Treat of **singularity** in intrusive method by mean of domain splitting
- Extend the toolbox to include sparse grid sampling techniques and intrusive, non-intrusive techniques for **reduced polynomial basis**
- Populate the toolbox with **more test cases** for different applications
- **Increase the number of users** and finding more bugs ...

Questions?