Efficient Collocational Approach for Parametric Uncertainty Analysis[1]

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[1] Xiu, Dongbin. "Efficient collocational approach for parametric uncertainty analysis." Communications in computational physics 2.2 (2007): 293-309. [Xiu, 2007]

Why this paper?

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- I have not seen collocation applied this way before.
- This paper helps spark ideas to use this approach to set up optimization problems where a surrogate model is needed.

Outline

Primer on collocation methods for differential equations

Paper motivation and setup

Generalized polynomial chaos (gPC)

Stochastic collocation

Smolyak grids

Error Analysis

Numerical Results

Conclusion

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Collocation Methods

- Numerical methods that approximately solve ordinary differential equations.

- For ODE

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{f}(t, \mathbf{x}(t), \mathbf{p}), \quad t \in (t_0, t_f),$$
$$\mathbf{x}(t_0) = \mathbf{x}_0(\mathbf{p}),$$

  the goal is to approximate $\mathbf{x}(t)$ by a piecewise polynomial of degree s whose derivative coincides at given points with the vector field of the differential equation.

Collocation Discretization

- Partition $t_0 < t_1 < ... < t_{N+1} = t_f, \quad h_i = t_{i+1} - t_i.$
- Approximate ODE solution $\mathbf{x}$ by piecewise polynomial $\mathbf{x}^h$. On $[t_i, t_{i+1}]$, $\mathbf{x}_i^h$ is a polynomial of degree $\leq s$.
- Select s points

$$c_j \in [0, 1], \quad j = 1, ..., s$$

and set

$$t_{ij} = t_i + c_j h_i, \quad j = 1, ..., s, \quad i = 0, ..., N.$$

Collocation Discretization (cont.)

- To determine DoFs, require
  - collocation at s points $t_i + c_j h_i$,

$$\frac{d}{dt}\mathbf{x}_i^h(t_i + c_j h_i) = \mathbf{f}(t_i + c_j h_i, \mathbf{x}^h(t_i + c_j h_i), \mathbf{p}), \tag{1a}$$
$$j = 1, ..., s,\ i = 0, ..., N,$$

  - continuity at the subinterval boundaries,

$$\mathbf{x}_i^h(t_i) = \mathbf{x}_{i-1}^h(t_i), \quad i \in \{1, ..., N+1\}, \tag{1b}$$

  - initial condition is satisfied,

$$\mathbf{x}_0^h(t_0) = \mathbf{x}_0(\mathbf{p}). \tag{1c}$$

- (1) is a system of nonlinear eqns. in the DoFs
- Concrete form is determined by choice of polynomial basis.

Collocation Using Birkhoff Interpolation Basis

- For $c \in [0,1]$, $i = 0, ..., N$, we have

$$\mathbf{x}_i^h(t_i + ch_i) = \mathbf{x}_i^h(t_i) + h_i \int_0^c \frac{d}{dt}\mathbf{x}_i^h(t_i + \tau h_i)d\tau.$$

- $\mathbf{x}_i^h$ is poly. of deg. $\leq s$, so $\frac{d}{dt}\mathbf{x}_i^h$ is polynomial of deg. $\leq s - 1$.
- Represent $\frac{d}{dt}\mathbf{x}_i^h$ in Lagrange basis

$$\tilde{\ell}_j(\tau) = \prod_{\substack{k=1,\\ k\neq j}}^{s} \frac{\tau - c_k}{c_j - c_k}, \quad j = 1, ..., s$$

- Derivative can be written

$$\frac{d}{dt}\mathbf{x}_i^h(t_i + \tau h_i) = \sum_{j=1}^{s} \tilde{\ell}_j(\tau)\frac{d}{dt}\mathbf{x}_i^h(t_i + c_j h_i)$$

Collocation Using Birkhoff Basis (cont.)

- Substitute Lagrange representation in integral equation

$$\mathbf{x}_i^h(t+ch_i) = \mathbf{x}_i^h(t_i) + h_i \sum_{j=1}^{s} \Big(\int_0^c \tilde{\ell}_j(\tau) d\tau \Big) \frac{d}{dt} \mathbf{x}_i^h(t_i + c_j h_i).$$

- Define

$$a_{lj} = \int_0^{c_l} \tilde{\ell}_j(\tau) d\tau, \qquad b_j = \int_0^1 \tilde{\ell}_j(\tau) d\tau, \qquad 1 \le l, j \le s,$$

and

$$\mathbf{x}_i = \mathbf{x}_i^h(t_i), \qquad \mathbf{x}_{ik} = \mathbf{x}_i^h(t_i + c_k h_i), \qquad \dot{\mathbf{x}}_{il} = \frac{d}{dt} \mathbf{x}_i^h(t_i + c_l h_i).$$

- Gives Integral formulation

$$\begin{bmatrix} \dot{\mathbf{x}}_{i1} \\ \vdots \\ \dot{\mathbf{x}}_{is} \end{bmatrix} = \begin{bmatrix} \mathbf{f}(t_{i1}, \mathbf{x}_i + h_i \sum_{j=1}^s a_{1j} \dot{\mathbf{x}}_{ij}, \mathbf{p}) \\ \vdots \\ \mathbf{f}(t_{is}, \mathbf{x}_i + h_i \sum_{j=1}^s a_{sj} \dot{\mathbf{x}}_{ij}, \mathbf{p}) \end{bmatrix}, \qquad i = 0, ..., N$$

$$\mathbf{x}_i = \begin{cases} \mathbf{x}_0(\mathbf{p}), & i = 0, \\ \mathbf{x}_{i-1} + h_{i-1} \sum_{j=1}^s b_j \dot{\mathbf{x}}_{i-1,j}, & i \in \{1, ..., N+1\}. \end{cases}$$

Collocation Using Birkhoff Basis (cont.)

- Define

$$\dot{\mathbf{X}}_i = \begin{bmatrix} \dot{\mathbf{x}}_{i1} \\ \vdots \\ \dot{\mathbf{x}}_{is} \end{bmatrix} \in \mathbb{R}^{sn_x}, \quad \mathbf{t}_i = \begin{bmatrix} t_{i1} \\ \vdots \\ t_{is} \end{bmatrix}, \quad \mathbf{e} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \in \mathbb{R}^s,$$

$$\mathbf{A} = \begin{bmatrix} a_{11} & \cdots & a_{1s} \\ \vdots & & \vdots \\ a_{s1} & \cdots & a_{ss} \end{bmatrix} \in \mathbb{R}^{s\times s}, \quad \mathbf{b} = \begin{bmatrix} b_1 \\ \vdots \\ b_s \end{bmatrix} \in \mathbb{R}^s,$$

- Matrix-vector notation of collocation system is

$$\dot{\mathbf{X}}_i = \mathbf{F}\left(\mathbf{t}_i, \mathbf{e}\otimes\mathbf{x}_i + h_i(\mathbf{A}\otimes\mathbf{I})\dot{\mathbf{X}}_i, \mathbf{p}\right), \quad i = 0, ..., N \tag{2a}$$

$$\mathbf{x}_i = \begin{cases} \mathbf{x}_0(\mathbf{p}), & i = 0 \\ \mathbf{x}_{i-1} + h_{i-1}(\mathbf{b}\otimes\mathbf{I})^T\dot{\mathbf{X}}_{i-1}, & i \in \{1, ..., N+1\} \end{cases} \tag{2b}$$

Collocation Using Birkhoff Basis (cont.)

- Define

$$\dot{\mathbf{X}}_i = \begin{bmatrix} \dot{\mathbf{x}}_{i1} \\ \vdots \\ \dot{\mathbf{x}}_{is} \end{bmatrix} \in \mathbb{R}^{sn_x}, \quad \mathbf{t}_i = \begin{bmatrix} t_{i1} \\ \vdots \\ t_{is} \end{bmatrix}, \quad \mathbf{e} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \in \mathbb{R}^s,$$

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- Above system is an implicit Runge-Kutta method.

Collocation and IRK Methods

- Matrix-vector notation of collocation system is

$$\dot{\mathbf{X}}_i = \mathbf{F}\left(\mathbf{t}_i, \mathbf{e} \otimes \mathbf{x}_i + h_i(\mathbf{A} \otimes \mathbf{I})\dot{\mathbf{X}}_i, \mathbf{p}\right), \quad i = 0, ..., N \tag{3a}$$

$$\mathbf{x}_i = \begin{cases} \mathbf{x}_0(\mathbf{p}), & i = 0 \\ \mathbf{x}_{i-1} + h_{i-1}(\mathbf{b} \otimes \mathbf{I})^T \dot{\mathbf{X}}_{i-1}, & i \in \{1, ..., N+1\} \end{cases} \tag{3b}$$

Definition 7.1. Let b_i, a_{ij} $(i, j = 1, \ldots, s)$ be real numbers and let c_i be defined by (1.9). The method

$$k_i = f\Big(x_0 + c_i h, y_0 + h \sum_{j=1}^{s} a_{ij} k_j\Big) \qquad i = 1, \ldots, s$$
$$y_1 = y_0 + h \sum_{i=1}^{s} b_i k_i \tag{7.7}$$

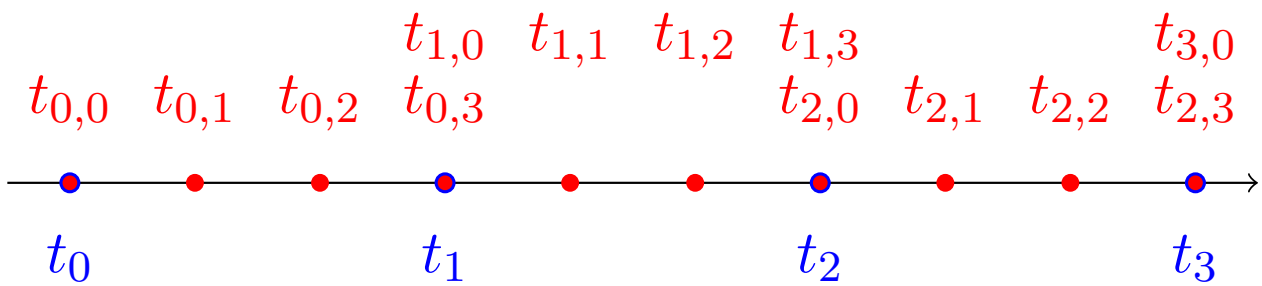
is called an *s-stage Runge-Kutta method.* When $a_{ij} = 0$ for $i \leq j$ we have an explicit (ERK) method. If $a_{ij} = 0$ for $i < j$ and at least one $a_{ii} \neq 0$, we have a

Figure: from [Hairer and Wanner, 1996]

- Collocation methods are IRK methods, but the opposite is not true.

Takeaway

- Collocation requires that:
  1. ODE is satisfied at $t_{ij} = t_i + c_j h_i$ where $i = 0, ..., N$, $j = 1, ..., s$.
  2. Piecewise polynomials are continuous at $t_i = t_{i,0} = t_i + c_0 h_i$ where $i = 0, ..., N$.



Simplified Illustration with N=3, K=3,
$0 = c_0 < c_1 = 1/3 < c_2 = 2/3 < c_3 = 1.$

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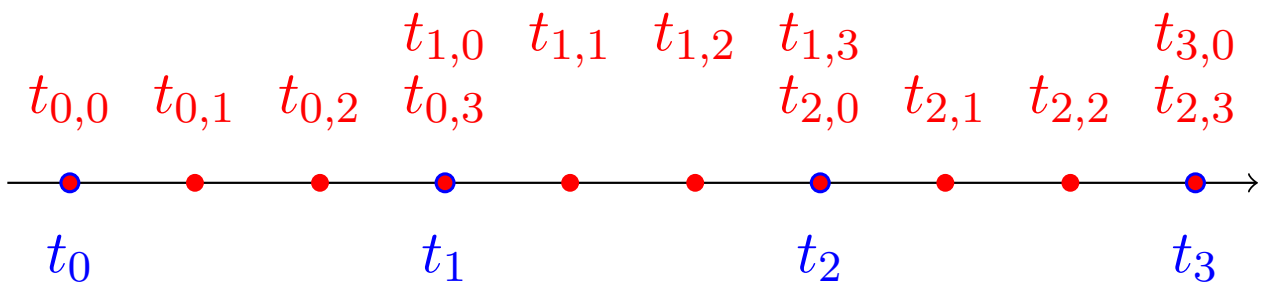

Simplified Illustration with N=3, K=3,
$0 = c_0 < c_1 = 1/3 < c_2 = 2/3 < c_3 = 1.$

- How do we choose the points $c_j, j = 1, ..., s$?

Collocation with Orthogonal Polynomials

- How should we choose collocation points c for best approximation?
- ODE can be written as implicit integral equation

$$\mathbf{x}(t_{i+1}) = \mathbf{x}(t_i) + \int_{t_i}^{t_{i+1}} \mathbf{f}(t, \mathbf{x}(t), \mathbf{p})\, dt,$$

and the numerical solution is given by the quadrature formula

$$\mathbf{x}(t_{i+1}) = \mathbf{x}(t_i) + \sum_{j=1}^{s} \omega_j \mathbf{f}(t_{ij}, \mathbf{x}(t_{ij}), \mathbf{p}), \quad \sum_{j=1}^{s} w_j = h_i.$$

- Choose c_j to maximize exactness of quadrature rule, i.e. roots of orthogonal polynomials.
- For example, in Gauss quadrature, if the nodes are roots of the sth degree Legendre orthogonal polynomial, the Gaussian quadrature formula will be exact for polynomials of degree $\leq 2s - 1$.

Do collocation points always include 0 and 1?

Theorem 344A *Let $c_1 < c_2 < \cdots < c_s$ be chosen as abscissae of the Radau I, the Radau II or the Lobatto quadrature formula respectively. Then*

I For the Radau I formula, $c_1 = 0$. This formula is exact for polynomials of degree up to $2s - 2$.

II For the Radau II formula, $c_s = 1$. This formula is exact for polynomials of degree up to $2s - 2$.

III For the Lobatto formula, $c_1 = 0, c_s = 1$. This formula is exact for polynomials of degree up to $2s - 3$.

Furthermore, for each of the three quadrature formulae, $c_i \in [0, 1]$, for $i = 1, 2, \ldots, s$ and $b_i > 0$, for $i = 1, 2, \ldots, s$.

Figure: Courtesy of [Butcher, 2008, Chapter 34, page 206]

Hermite-Simpson Collocation

An implicit Runge-Kutta method of stage 3 and order 4 with the following Butcher Table

0	0	0	0
1/2	5/24	1/3	-1/24
1	1/6	2/3	1/6
	1/6	2/3	1/6

Table: Butcher Table of LobattoIIA collocation

expressed explicitly as

$$\mathbf{x}_{i+1/2} = \mathbf{x}_i + h_i\left(\frac{5}{24}(t_i, \mathbf{x}_i, \mathbf{p}) + \frac{1}{3}(t_{i+1/2}, \mathbf{x}_{i+1/2}, \mathbf{p}) + \frac{-1}{24}(t_{i+1}, \mathbf{x}_{i+1}, \mathbf{p})\right),$$
$$\mathbf{x}_{i+1} = \mathbf{x}_i + h_i\left(\frac{1}{6}(t_i, \mathbf{x}_i, \mathbf{p}) + \frac{2}{3}(t_{i+1/2}, \mathbf{x}_{i+1/2}, \mathbf{p}) + \frac{1}{6}(t_{i+1}, \mathbf{x}_{i+1}, \mathbf{p})\right).$$

Radau IIA Collocation

An implicit Runge-Kutta method of stage 3 and order 5 with the following Butcher Table

$\frac{4-\sqrt{6}}{10}$	$\frac{88-7\sqrt{6}}{360}$	$\frac{296-169\sqrt{6}}{1800}$	$\frac{-2+3\sqrt{6}}{225}$
$\frac{4+\sqrt{6}}{10}$	$\frac{296+169\sqrt{6}}{1800}$	$\frac{88+7\sqrt{6}}{360}$	$\frac{-2-3\sqrt{6}}{225}$
1	$\frac{16-\sqrt{6}}{36}$	$\frac{16+\sqrt{6}}{36}$	$\frac{1}{9}$
	$\frac{16-\sqrt{6}}{36}$	$\frac{16+\sqrt{6}}{36}$	$\frac{1}{9}$

Table: Butcher table of the Radau IIA method, which is the (Flipped) Legendre-Gauss-Radau collocation.

Final Takeaway of Collocation

- Collocation methods approximate ODE solution by piecewise polynomial of certain degree.
- They require roots of orthogonal polynomials.
- They are pseudo-spectral methods, enjoying spectral convergence.

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Paper motivation and setup

Generalized polynomial chaos (gPC)

Stochastic collocation

Smolyak grids

Error Analysis

Numerical Results

Conclusion

Focus of paper

- Paper focuses on efficient numerical methods for DAE equations with random/uncertain parameters.
- These parameters are modeled as random variables.
- The resulting DAEs become stochastic equations.

Problem Setup

- Consider system of DAEs

$$\begin{cases} F(t, y, y', .., y^{(l)}, p) & = 0, \quad t \in (t_0, T], \\ g(t_0, y(t_0), ..., y^{(l)}(t_0), p) & = 0, \end{cases} \tag{4}$$

where $y = (y_1, ..., y_J) \in \mathbb{R}^J$ are state variables and $p = (p_1, ..., p_N) \in \mathbb{R}^N$ are parameters of interest.

- Assume parameters $p_1, ..., p_N$ are mutually independent.
- Define $z = (z_1, ..., z_K) \in \mathbb{R}^K$ as observables.
- Interested in numerically determining the function $z(p)$.

Probabilistic Framework

- Let $p = (p_1, ..., p_N)$ be an N-variate random vector in probability space $(\Omega, \mathcal{A}, \mathcal{P})$
- Let $\rho_i : \Gamma_i \to \mathbb{R}^+$ be the PDF of random variable p_i and its image $\Gamma_i = p_i(\Omega) \in \mathbb{R}$ for $i = 1, .., N$.
- The joint probability density of $p = (p_1, ..., p_N)$ is

$$\rho(p) = \prod_{i=1}^{N} \rho_i(p_i)$$

with hypercube

$$\Gamma = \prod_{i=1}^{N} \Gamma_i \in \mathbb{R}^N.$$

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gPC expansion setup

- Goal is to approximate random function via orthogonal polynomials of random variables in finite dimensional random space Γ.
- Define one-dimensional orthogonal polynomial space wrt measure $\rho_i(p_i)dp_i$ in Γ_i

$$W^{i,d_i} = \left\{ v : \Gamma_i \to \mathbb{R} : v \in \text{span}\{\phi_m(p_i)\}_{m=0}^{d_i} \right\}, \quad i = 1, .., N,$$

where $\{\phi_m(p_i)\}$ are a set of orthogonal polynomials satisfying

$$\int_{\Gamma_i} \phi_m(p_i)\phi_n(p_i)\rho_i(p_i)dp_i = \delta_{mn}$$

- The choice of pdfs dictate the type of orthogonal polynomials used.
- Uniform dist. is associated with Legendre poly., and Gaussian dist. is associated with Hermite poly.

gPC expansion setup (continued)

- Corresponding N-variate orthogonal polynomial space in Γ is

$$W_N^P = \bigotimes_{|\mathbf{d}| \leq P} W^{i,d_i}.$$

- This tensor product is over all possible combinations of multi-index $\mathbf{d} = (d_1, ..., d_N) \in \mathbb{N}_0^N$ satisfying

$$\sum_{i=1}^{N} d_i \leq P$$

where P is total degree of orthogonal polynomial.

- Basis functions satisfy

$$\int_\Gamma \phi_m(p)\phi_n(p)\rho(p)dp = \mathbb{E}[\phi_m(p)\phi_n(p)] = \delta_{mn}$$

for all $1 \leq m, n \leq \dim(W_N^P) = \binom{N+P}{N}$.

gPC approximation

- P-th order gPC approximation of the observable z is

$$z(p) \approx \mathbb{P}_N^P z = z_N^P(p) = \sum_{m=1}^{M} \hat{z}_m \phi_m(p), \quad M = \binom{N+P}{N}$$

where $\mathbb{P}_N^P$ is projection operator of Γ onto W_N^P and

$$\hat{z}_m = \mathbb{E}[z(p)\phi_m(p)] = \int_\Gamma z(p)\phi_m(p)\rho(p)dp, \quad m = 1, ..., M.$$

- Define

$$\epsilon_G = ||z - \mathbb{P}_N^P z||_{L^2_\rho(\Gamma)} = (\mathbb{E}[(z(p) - z_N^P(p))^2])^{1/2}$$

as mean square error of finite-term gPC approximation.

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Stochastic collocation approach

- Goal is to find an approximate solution to observable z in form of gPC expansion as

$$z(p) \approx \mathbb{I}_N^P z = v_N^P(p) = \sum_{m=1}^{M} \hat{v}_m(t)\phi_m(p), \quad M = \binom{N+P}{N}$$

where $\mathbb{I}_N^P$ is another operator of Γ onto W_N^P and

$$\hat{v}_m(t) = \sum_{j=1}^{Q} z(t, p^j)\phi_m(p^j)\alpha_j, \quad m = 1, ..., M.$$

- Recall the gPC expansion coefficients

$$\hat{z}_m = \mathbb{E}[z(p)\phi_m(p)] = \int_\Gamma z(p)\phi_m(p)\rho(p)dp, \quad m = 1, ..., M.$$

- Notice $\hat{v}_m$ approximates $\hat{z}_m$ via quadrature with $\{p^j, \alpha^j\}_{j=1}^Q$ as set of nodes and weights.
- Define mean square error $\epsilon_Q = ||\mathbb{I}_N^P z - \mathbb{P}_N^P z||_{L^2_\rho(\Gamma)}$.

Quadrature Nodes

- For each direction $i = 1, .., N$, construct a 1D quadrature rule

$$\mathcal{U}_i^{q_i}[f] = \sum_{i=1}^{q_i} f(p_i^j)\alpha_i^j$$

based on nodal set

$$\Theta_i^1 = (p_i^1, ..., p_i^{q_i}) \in \Gamma_i.$$

- Optimal choice is quadrature rule based on orthogonal polynomials.
- For $N > 1$, we get a tensor product formula

$$\mathcal{U}^Q[f] = (\mathcal{U}_i^{q_i} \otimes ... \otimes \mathcal{U}_N^{q_N})[f] = \sum_{j_1=1}^{q_1} ... \sum_{j_N=1}^{q_N} f(p_1^{j_1}, ..., p_N^{j_N})(\alpha_1^{j_1} ... \alpha_N^{j_N})$$

- We need $Q = \prod_{i=1}^N q_i = q^N$ points if we choose the same number of points q in each direction.
- Need sparsity!

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Smolyak sparse grids

- First proposed in 1963 [Smolyak, 1963]
- The Smolyak algorithm is a linear combination of product formulas, and linear combination is chosen in a way than an integration property for $N = 1$ is preserved for $N > 1$.
- The Smolyak algorithm is given by

$$\mathcal{U}^Q[f] \equiv A(J,N) = \sum_{J-N+1 \leq |\mathbf{i}| \leq J} (-1)^{J-|\mathbf{i}|} \binom{N-1}{J-|\mathbf{i}|} (\mathcal{U}_{i_1} \otimes ... \otimes \mathcal{U}_{i_N})$$

  where $\mathbf{i} = (i_1, i_2, ..., i_N) \in \mathbb{N}^N$.

- Only need function evaluations on the sparse grid

$$\Theta_N \equiv H(J,N) = \bigcup_{J-N+1 \leq |\mathbf{i}| \leq J} (\Theta^1_{i_1} \times ... \times \Theta^1_{i_N})$$

Updated nodal set

- The paper uses extrema of Chebyshev polynomials (Clenshaw-Curtis nodes) as quadrature nodes.
- For any $q_i > 1$, the nodes are

$$p_i^j = -\cos\frac{\pi(j-1)}{q_i - 1}, \quad j = 1, ..., q_i.$$

- Define $p_i^1 = 0$ if $q_i = 1$ and choose $q_1 = 1,\ \ q_i = 2^{i-1} + 1$ for $i > 1$.
- Nodal sets Θ_i^1 are nested and thus $H(J, N) \subset H(J + 1, N)$.
- If $J = N + P$ then $A(N + P, N)$ exact for polynomials in W_N^P and number of nodes is

$$Q \equiv \dim(A(N + P, N)) \approx \frac{2^P}{P!} N^P.$$

Example

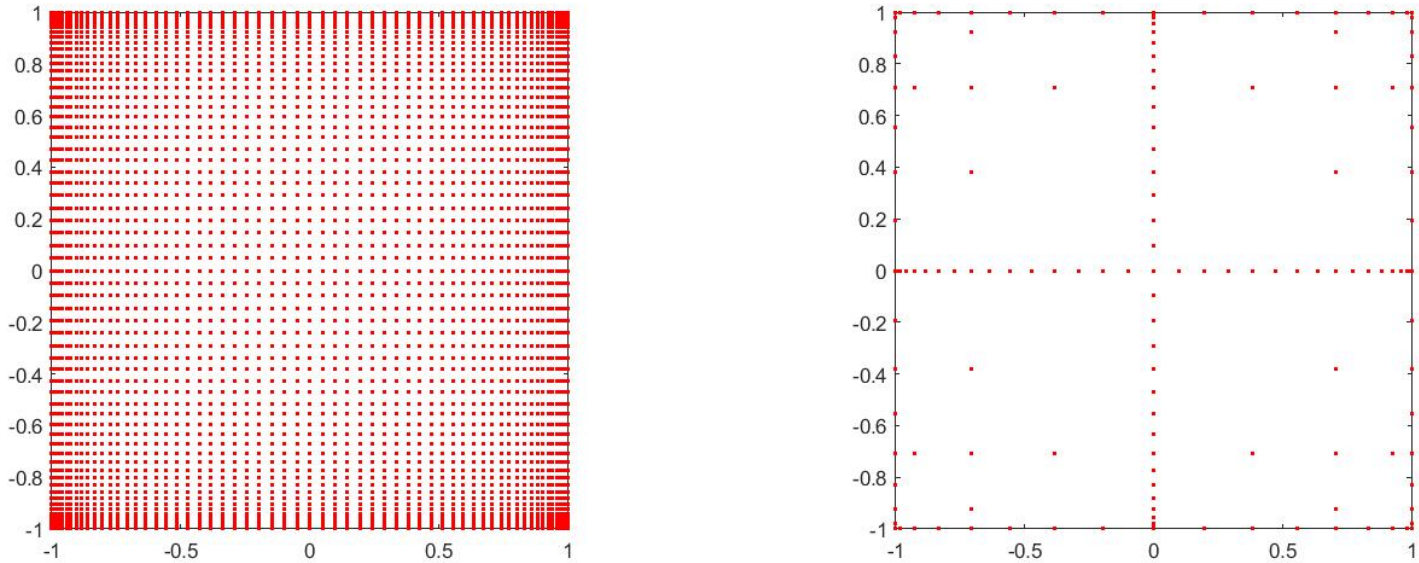

Figure: $N = 2$ dimensional nodes based on extrema of Chebyshev polynomials. Left: 145 points from Level 5 Smolyak grid $H(N + 5, N)$. Right: 1089 points from tensor product formula. Generated using codes from [Nobile et al., 2008, Driscoll et al., 2014]

Collocational Algorithmic Summary

1. Choose collocation nodal set $\{p^j, \alpha^j\}_{j=1}^{Q}$.

2. For each $j = 1, ..., Q$, numerically solve DAE system with fixed parameter set $p^j = (p_1^j, ..., p_N^j)$ and evaluate observables $\tilde{z}(p^j)$. (only expensive offline step)

3. Evalute approximate gPC expansion coefficients

$$\hat{w}_m = \mathcal{U}^Q[\tilde{z}(p)\phi_m(p)] = \sum_{j=1}^{Q} \hat{z}(p^j)\phi_m(p^j)\alpha^j, \quad m = 1, ..., M$$

4. Construct N-variate, P-th order gPC approximation

$$w_N^P = \sum_{m=1}^{M} \hat{w}_m \phi_m(p), \quad M = \binom{N+P}{N}$$

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What are the errors?

- Recall mean square error of gPC approximation

$$\epsilon_G = ||z - \mathbb{P}_N^P z||_{L^2_\rho(\Gamma)} = (\mathbb{E}[(z(p) - z_N^P(p))^2])^{1/2}$$

- Recall aliasing error of approximating gPC expansions

$$\epsilon_Q = ||\mathbb{I}_N^P z - \mathbb{P}_N^P z||_{L^2_\rho(\Gamma)}.$$

- Define error for numerical scheme employed for computing numerical solution $\tilde{z}(p^j)$

$$\epsilon_\Delta = \max_j |z(p^j) - \hat{z}(p^j)|, \quad j = 1, .., Q.$$

Error superposition

- Proposition 4.1 states that the mean-square error of N-variate, P-th order gPC stochastic collocation w_N^P satisfies

$$\epsilon = \left(\int_\Gamma [z(p) - w_N^P(p)]^2 \rho(p) dp \right)^{1/2} \leq [\epsilon_G^2 + \epsilon_Q^2 + M \epsilon_\Delta^2 C_Q^2]^{1/2},$$

  where $C_Q = \max_m \left| \mathcal{U}^Q[\phi_m(p)] \right|$,

- All of these errors can be controlled/refined in practice.

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Numerical Example 1

Here we set the observables with the following explicit definition

$$\begin{aligned} z_1 &= p_1 \cdot e^{p_2}/(1+p_3^2), \\ z_2 &= \cos(p_1)\ln\left(\frac{1}{2}+p_2^2+p_3^2\right), \end{aligned} \tag{5.1}$$

where $p = (p_1, p_2, p_3)$ are three independent Gaussian random variables with zero mean and standard deviation $\sigma = 0.1$. This can be considered as an exact solution to certain differential equations whose dependence in physical space/time has been suppressed. Therefore, the deterministic numerical error ϵ_Δ (4.16) is eliminated. Corresponding the Gaussian distribution, the gPC basis functions are Hermite polynomials. The random space is three-dimensional ($N = 3$), and we adopt tensor product of one-dimensional Hermite quadrature as integration rule. Each dimension has the same number of node, $q = q_1 = q_2 = q_3$, and the total number of nodes is $Q = q^3$.

Numerical Example 1 Continued

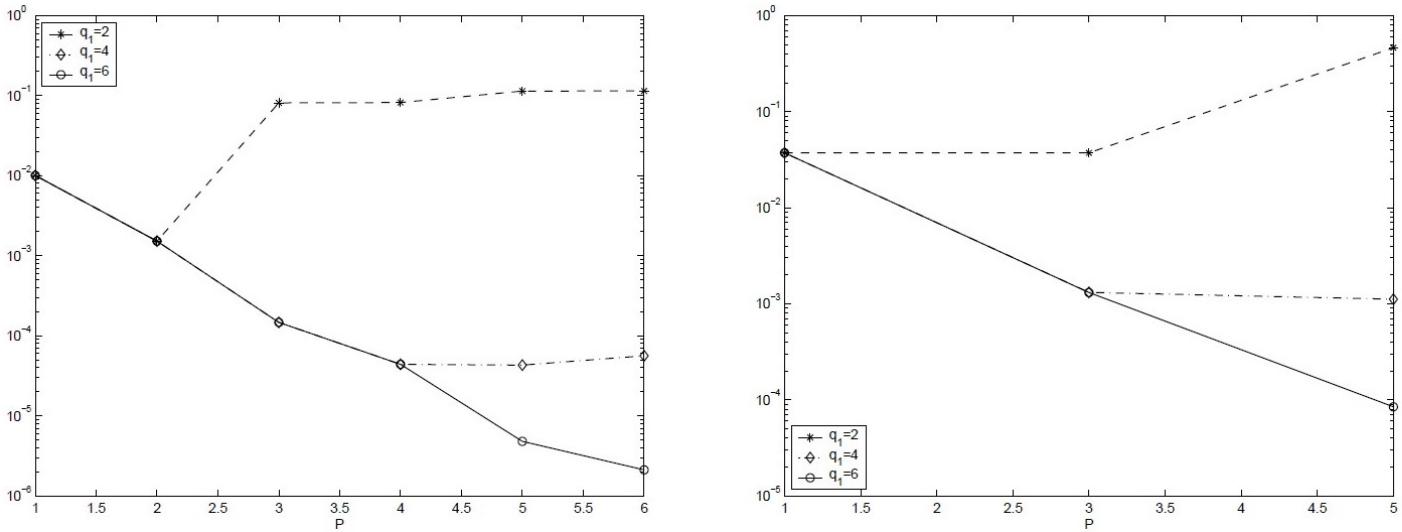


Figure 2: Mean-square error of model problem (5.1), with increasing order of gPC expansion and different number of integration nodes in each dimension. Left: errors in z_1; Right: errors in z_2.

Numerical Example 2: Cell Signaling Cascade

Here we consider a mathematical model for autocrine cell-signaling loop developed in [22]. Let e_{1p}, e_{2p}, and e_{3p} denote the dimensionless concentrations of the active form of the enzymes. The model for dynamics of e_{1p}, e_{2p}, and e_{3p} has the following form

$$\frac{de_{1p}}{dt} = \frac{I(t)}{1+G_4 e_{3p}} \frac{V_{\max,1}(1-e_{1p})}{K_{m,1}+(1-e_{1p})} - \frac{V_{\max,2}e_{1p}}{K_{m,2}+e_{1p}}, \tag{5.5}$$

$$\frac{de_{2p}}{dt} = \frac{V_{\max,3}e_{1p}(1-e_{2p})}{K_{m,3}+(1-e_{2p})} - \frac{V_{\max,4}e_{2p}}{K_{m,4}+e_{2p}}, \tag{5.6}$$

$$\frac{de_{3p}}{dt} = \frac{V_{\max,5}e_{2p}(1-e_{3p})}{K_{m,5}+(1-e_{3p})} - \frac{V_{\max,6}e_{3p}}{K_{m,6}+e_{3p}}. \tag{5.7}$$

For detailed biological background of the model, see [22]. In [22], the parameters are chosen as $K_{m,1-6} = 0.2, V_{\max,1} = 0.5, V_{\max,2} = 0.15, V_{\max,3} = 0.15, V_{\max,4} = 0.15, V_{\max,5} = 0.25,$

Numerical Example 2 Continued

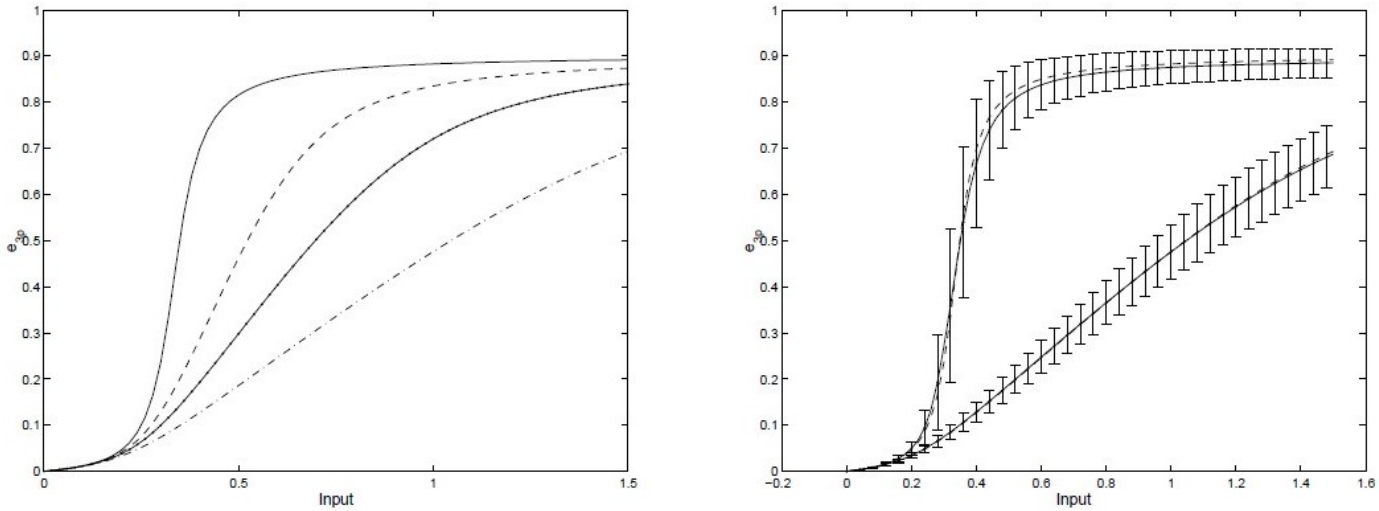


Figure 4: Steady input-out behavior computed for several values for gain of the negative feedback Left: deterministic simulation. The four curves from top to bottom correspond to $G_4 = 0, 1, 2$, and 4, respectively. Right: stochastic computation with 10% uncertainty in parameters $V_{\max,1-6}$ Results of $G_4 = 0$ and $G_4 = 4$ are shown in error bars, with the corresponding deterministic results in dotted lines.

4

Outline

Primer on collocation methods for differential equations

Paper motivation and setup

Generalized polynomial chaos (gPC)

Stochastic collocation

Smolyak grids

Error Analysis

Numerical Results

Conclusion

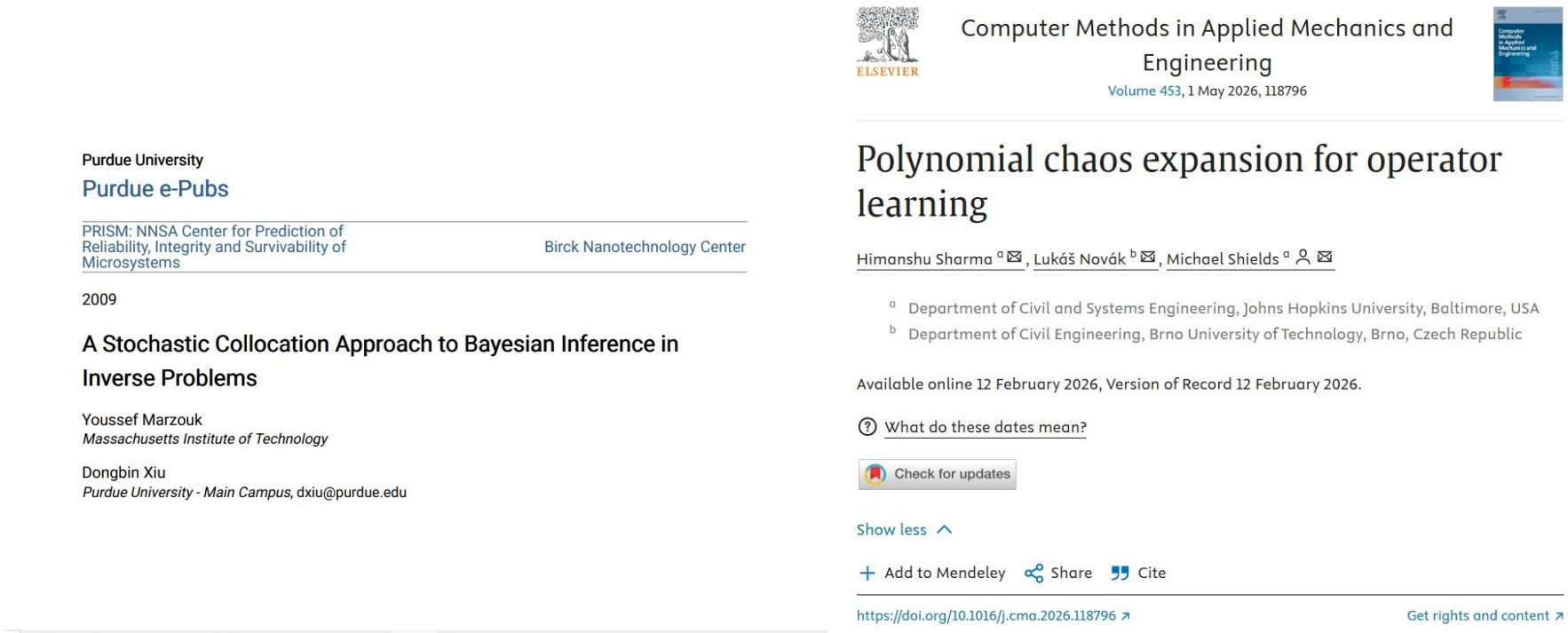
Stochastic Collocation combines advantages of other methods

- Monte Carlo sampling requires repetitive deterministic simulations but solution statistics converge relatively slowly.
- Galerkin projection methods and gPC-Galerkin methods enjoy high accuracy and fast convergence but are intrusive methods (require modifying eqns) and can be difficult to implement.
- Stochastic collocation algorithm combines advantages of Monte-Carlo sampling and Galerkin projections.

Classical Collocation vs Stochastic Collocation

Classical Collocation	Stochastic Collocation
points in time/space	points in parameter space
solves ODE/PDE at nodes	solves model at parameter samples
interpolates solution	builds surrogate

This research is still relevant today



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Polynomial chaos expansion for operator learning

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Figure: Left: [Marzouk and Xiu, 2009], Right:[Sharma et al., 2026]

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