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Conservation/Balance Laws with Uncertainties

\[ U_t + F(U, x, z)x = R(U, x, z), \quad x \in \mathbb{R}, \ t > 0, \ z \in \Omega \subset \mathbb{R}^d \]

\( U = U(x, t, z) \) is the unknown vector function

\( x \): spatial variable

\( t \): time variable

\( z \): random variable

\( F \): flux vector function

\( R \): source term

Uncertainties can appear in the source terms, equations of state, initial or boundary data due to empirical approximations or measuring errors.
Quantifying Uncertainties – gPC Approach

Polynomial chaos or generalized polynomial chaos (gPC) approach:

- **Non-intrusive gPC method** – solves the original problem at selected sampling points, thus one can use the deterministic code, and then use interpolation and quadrature rules to numerically evaluate the statistical moments

[Xiu, Hesthaven; 2005]

[Mishra, Schwab, Sukys; 2012]

- **Intrusive gPC method** – uses the Galerkin approximation, which results in a system of deterministic equations, solving which will give the stochastic moments of the solution of the original uncertain problem
– **Pros**: lower computational cost; theoretical advantages;

[Elman, Miller, Phipps, Tuminaro; 2011]

– **Cons**: extra efforts are needed in order to obtain well-behaved discrete systems

[Xui; 2010]

[Tryoen, Le Maitre, Ndjinga, Ern; 2010]

[Després, Poëtte, Lucor; 2013]

[Pettersson, Iaccarino, Nordström; 2014, 2015]

[Hu, Jin, Xiu; 2015]
The solution is sought in terms of an orthogonal polynomial series in $z$:

$$U(x, t, z) \approx U_N(x, t, z) = \sum_{i=0}^{M-1} \hat{U}_i(x, t) \Phi_i(z), \quad M = \binom{d + N}{d}$$

- $\{\Phi_i(z)\}$ are multidimensional polynomials of degree up to $N$ of $z$:
  $$\int_{\Omega} \Phi_i(z) \Phi_\ell(z) \mu(z) \, dz = \delta_{i\ell}, \quad 0 \leq i, \ell \leq M - 1 \quad M = \dim\left(\mathbb{P}_d^N\right)$$
- $\mu(z)$: probability density function of $z$
- $\delta_{i\ell}$: Kronecker symbol
- The choice of the orthogonal polynomials depends on the distribution function of $z$. For example:
  - a Gaussian distribution defines the Hermite polynomials
  - a uniform distribution defines the Legendre polynomials
The gPC-SG method seeks to satisfy the system in a weak form by ensuring that the residual is orthogonal to the gPC polynomial space.

Substituting

\[ U_N(x, t, z) = \sum_{i=0}^{M-1} \hat{U}_i(x, t) \Phi_i(z) \]

into the governing system

\[ U_t + F(U, x, z)_x = R(U, x, z) \]

and using the Galerkin projection yield

\[ (\hat{U}_i)_t + (\hat{F}_i)_x = \hat{R}_i, \quad 0 \leq i \leq M - 1 \]

where

\[ \hat{F}_i = \int_{\Omega} F \left( \sum_{j=0}^{M-1} \hat{U}_j(x, t) \Phi_j(z), x, z \right) \Phi_i(z) \mu(z) \, dz \]

\[ \hat{R}_i = \int_{\Omega} R \left( \sum_{j=0}^{M-1} \hat{U}_j(x, t) \Phi_j(z), x, z \right) \Phi_i(z) \mu(z) \, dz \]
The gPC-SG Method – Challenges

\[ U_t + F(U, x, z)_x = R(U, x, z) \]

\[ (\hat{U}_i)_t + (\hat{F}_i)_x = \hat{R}_i \quad 0 \leq i \leq M - 1 \]

<table>
<thead>
<tr>
<th>Linear Hyperbolic</th>
<th>Hyperbolic</th>
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</thead>
<tbody>
<tr>
<td>Nonlinear Symmetric</td>
<td>Hyperbolic</td>
</tr>
<tr>
<td>Nonlinear Nonsymmetric</td>
<td>?</td>
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- **Our goal:** *Introduce an operator splitting for the original hyperbolic system, which will guarantee that the gPC-SG discretization of each of the split subsystems always results in a globally hyperbolic system*

- **Our strategy:** generic, but the splitting is problem specific

- **Our examples:** the compressible Euler equations and the shallow water equations
1-D Compressible Euler Equations

\[
\begin{align*}
\rho_t + m_x &= 0 \\
m_t + (\rho u^2 + p)_x &= 0 \\
E_t + (u(E + p))_x &= 0
\end{align*}
\]

- $\rho$: density
- $u$: velocity, $m = \rho u$: momentum
- $E$: total energy
- $p$: pressure with the equation of state $p = (\gamma - 1) \left( E - \frac{1}{2} \rho u^2 \right)$
- $\gamma$: specific heat ratio

We assume here that the data may depend on random variable $z$, i.e.,
\[
\rho(x, 0, z) = \rho_0(x, z), \quad u(x, 0, z) = u_0(x, z), \quad p(x, 0, z) = p_0(x, z), \quad \gamma = \gamma(z)
\]

Uncertainty may also arise from boundary data and other terms
1-D Euler Equations – Numerical Challenges

\[
\begin{align*}
\rho_t + m_x &= 0 \\
m_t + (\rho u^2 + p)_x &= 0 \\
E_t + (u(E + p))_x &= 0
\end{align*}
\]

\(\lambda = u, u \pm c, \quad c = \sqrt{\gamma p/\rho}\)

A direct application of the gPC-SG method to the system may fail due to the loss of hyperbolicity after the gPC-SG discretization.

**Operator Splitting:**

- Linear hyperbolic system

- Two degenerate nonlinear hyperbolic systems which are effectively scalar equations

The gPC-SG approximation is guaranteed to maintain the hyperbolicity for each of the subsystems.
1-D Euler Equations – Operator Splitting

\[ \begin{align*}
(I) \quad \begin{cases} 
\rho_t + m_x &= 0 \\
m_t + ((\gamma - 1)E + am)_x &= 0 \\
E_t - (aE)_x &= 0
\end{cases}
\end{align*} \]

\[ \begin{align*}
(II) \quad \begin{cases} 
\rho_t &= 0 \\
m_t + \left( \frac{3 - \gamma}{2} \cdot \frac{m^2}{\rho} - am \right)_x &= 0 \\
E_t &= 0
\end{cases}
\end{align*} \]

\[ \begin{align*}
(III) \quad \begin{cases} 
\rho_t &= 0 \\
m_t &= 0 \\
E_t + \left( \frac{m}{\rho} \left[ \gamma E - \frac{\gamma - 1}{2} \cdot \frac{m^2}{\rho} \right] + aE \right)_x &= 0
\end{cases}
\end{align*} \]

- We choose:
  \[-|a| \leq u - c < u + c \leq |a| : \text{subcharacteristic condition}\]
  \[a = \pm \sup(\max\{|u| + c, \gamma u, (3 - \gamma)u\}) : \text{convection coefficient should not change sign}\]
**Strang Splitting**

\[ U_t + F_I(U)x = 0 \quad \rightarrow \quad S_I \]
\[ U_t + F_{II}(U)x = 0 \quad \rightarrow \quad S_{II} \]
\[ U_t + F_{III}(U)x = 0 \quad \rightarrow \quad S_{III} \]

Here

\[ U = \begin{pmatrix} r \\ m \\ E \end{pmatrix}, \quad F_I = \begin{pmatrix} m \\ (\gamma - 1)E + am \\ -aE \end{pmatrix}, \quad F_{II} = \begin{pmatrix} 0 \\ \frac{3-\gamma}{2} \cdot \frac{m^2}{\rho} - am \\ 0 \end{pmatrix} \]
\[ F_{III} = \begin{pmatrix} 0 \\ 0 \\ \frac{m}{\rho} \left[ \gamma E - \frac{\gamma-1}{2} \cdot \frac{m^2}{\rho} \right] + aE \end{pmatrix} \]

- Assume that the solution of the original system is available at time \( t \)
- Introduce a (small) time step \( \Delta t \)
- One time step of the second-order Strang splitting method:

\[ U(x, t + \Delta t, z) = S_I(\Delta t/2)S_{II}(\Delta t/2)S_{III}(\Delta t)S_{II}(\Delta t/2)S_I(\Delta t/2)U(x, t, z) \]
Operator Splitting – Numerical Validation

- We consider the Sod shock tube problem – pure deterministic problem:

\[ \rho_0(x) = \begin{cases} 
1, & x < 0.5, \\
0.125, & x > 0.5, 
\end{cases} \quad u_0(x) \equiv 0, \quad p_0(x) = \begin{cases} 
1, & x < 0.5 \\
0.1, & x > 0.5 
\end{cases} \]

- We run numerical simulations for both the unsplit and split systems

- We compare the results computed by the central-upwind scheme
  
  - computational domain \([0,1]\)
  
  - non-reflecting boundary conditions
  
  - uniform grid with \(\Delta x = 1/400\)
  
  - final time \(t = 0.1644\)
$\rho$ (top left), $m$ (top right) and $E$ (bottom)
1-D Euler Equations – The gPC-SG Approximation

\[ \begin{align*}
\begin{cases}
\rho_t + m_x &= 0 \\
    m_t + ((\gamma - 1)E + am)_x &= 0 \\
    E_t - (aE)_x &= 0
\end{cases}
\quad \begin{cases}
\rho_t &= 0 \\
    m_t + \left(\frac{3-\gamma}{2} \cdot \frac{m^2}{\rho} - am\right)_x &= 0 \\
    E_t &= 0,
\end{cases}
\end{align*} \]

We define the gPC expansions of \( \rho, m, E \) and \( \gamma \) in the following form:

\[
\begin{align*}
\rho_N(x, t, z) &= \sum_{i=0}^{N} \hat{\rho}_i(x, t) \Phi_i(z), \\
m_N(x, t, z) &= \sum_{i=0}^{N} \hat{m}_i(x, t) \Phi_i(z), \\
E_N(x, t, z) &= \sum_{i=0}^{N} \hat{E}_i(x, t) \Phi_i(z), \\
\gamma_N(z) &= \sum_{i=0}^{N} \hat{\gamma}_i \Phi_i(z)
\end{align*}
\]

substitute them into the systems and derive the gPC-SG approximation ...

...
We define ...

\[
\gamma_N(z) - 1 = \sum_{i=0}^{N} \hat{\gamma}_i \Phi_i(z), \quad \frac{3 - \gamma_N(z)}{2} = \sum_{i=0}^{N} \hat{\gamma}_i \Phi_i(z),
\]

\[
\left( \frac{m^2}{\rho} \right)_N (x, t, z) = \sum_{i=1}^{N} \hat{\psi}_i(x, t) \Phi_i(z),
\]

\[
\left( \frac{\gamma m}{\rho} \right)_N (x, t, z) = \sum_{i=1}^{N} \hat{\psi}_i(x, t) \Phi_i(z),
\]

\[
\left( \frac{(\gamma - 1)m}{\rho} \right)_N (x, t, z) = \sum_{i=1}^{N} \hat{\psi}_i(x, t) \Phi_i(z).
\]

For example, \( \hat{\psi}_i \) can be computed by using \( \rho \psi = m^2 \), namely,

\[
\sum_{k, \ell=0}^{N} \hat{\psi}_k \hat{\rho}_\ell S_{ik\ell} = \sum_{k, \ell=0}^{N} \hat{m}_k \hat{m}_\ell S_{ik\ell}, \quad i = 0, \ldots, N
\]

\[
S_{ik\ell} = \int_{\Omega} \Phi_i(z) \Phi_k(z) \Phi_\ell(z) \mu(z) \, dz \quad \text{is computed once}
\]
... after implementing the Galerkin projection we obtain the corresponding three systems for the gPC coefficients $i = 0, \ldots, N$:

(I) \[
\begin{cases}
(\hat{\rho}_i)_t + (\hat{m}_i)_x = 0 \\
(\hat{m}_i)_t + \sum_{k,\ell=0}^{N} \hat{\gamma}_k (\hat{E}_\ell)_x S_{k\ell i} + (a\hat{m}_i)_x = 0 \\
(\hat{E}_i)_t - (a\hat{E}_i)_x = 0
\end{cases}
\]

(II) \[
\begin{cases}
(\hat{\rho}_i)_t = 0 \\
(\hat{m}_i)_t + \sum_{k,\ell=0}^{N} \hat{\gamma}_k (\hat{\psi}_\ell)_x S_{k\ell i} - (a\hat{m}_i)_x = 0 \\
(\hat{E}_i)_t = 0
\end{cases}
\]

(III) \[
\begin{cases}
(\hat{\rho}_i)_t = 0 \\
(\hat{m}_i)_t = 0 \\
(\hat{E}_i)_t + \sum_{k,\ell=0}^{N} (\hat{\psi}_k \hat{E}_\ell)_x S_{k\ell i} - \sum_{k,\ell=0}^{N} (\hat{\psi}_k \hat{\psi}_\ell)_x S_{k\ell i} + (a\hat{E}_i)_x = 0
\end{cases}
\]
For each $i = 0, \ldots, N$:

$$(\hat{U}_i)_t + (\hat{F}_I)(\hat{U}_i)_x = 0 \quad \rightarrow \quad S_I \quad \text{solution operator (CU scheme)}$$

$$(\hat{U}_i)_t + \hat{F}_{II}(\hat{U}_i)_x = 0 \quad \rightarrow \quad S_{II} \quad \text{solution operator (CU scheme)}$$

$$(\hat{U}_i)_t + \hat{F}_{III}(\hat{U}_i)_x = 0 \quad \rightarrow \quad S_{III} \quad \text{solution operator (CU scheme)}$$

- Assume that the solution of the original system is available at time $t$

- Introduce a (small) time step $\Delta t$

- One time step of the second-order Strang splitting method:

$$U_i(x, t + \Delta t, z) = S_I(\Delta t/2)S_{II}(\Delta t/2)S_{III}(\Delta t)S_{II}(\Delta t/2)S_I(\Delta t/2)U_i(x, t, z)$$
Central-Upwind Schemes

- Godunov-type finite-volume methods

- **Central**: Riemann-problem-solver-free methods designed without tracking complicated nonlinear waves

- **Upwind**: Use some information on wave propagation to reduce numerical dissipation and thus enhance the resolution of nonsmooth waves

- Can be applied as a “black-box” solver to (multidimensional) hyperbolic systems of PDEs

- Robust, efficient and highly accurate
[Kurganov, Tadmor; 2000]

[Kurganov, Petrova; 2001]

[Kurganov, Noelle, Petrova; 2001]

[Kurganov, Tadmor; 2002]

[Kurganov, Petrova; 2005]

[Kurganov, Lin; 2007]

[Kurganov, Prugger, Wu; preprint]
Numerical Examples

• Three examples for the Sod problem
  – Example 1 - Perturbed the initial conditions
  – Example 2 - Perturbed $\gamma$
  – Example 3 - Perturbed interface

• We always assume a 1-D random variable $z$ obeying the uniform distribution on $[-1, 1]$, thus the Legendre polynomials are used as the gPC basis

• The mean and standard deviation of the computed solution $U$, which are shown in the Figures below, are given by

$$E[U] = \bar{U}_0, \quad \sigma[U] = \sum_{i=1}^{N} (\bar{U}_i)^2,$$

where $\bar{U}_i, \ i = 0, \ldots, N$ are the computed gPC coefficients of $U$.

• In all the examples: Strang splitting + second-order semi-discrete central-upwind scheme was implemented for the spatial discretization
Example 1 – Perturbed Initial Data

We consider the Sod shock tube problem with $\gamma = 1.4$ and subject to the following initial condition:

$$\rho_0(x, z) = \begin{cases} 
1 + 0.1z, & x < 0.5, \\
0.125, & x > 0.5,
\end{cases} \quad u_0(x) \equiv 0, \quad p_0(x) = \begin{cases} 
1, & x < 0.5 \\
0.1, & x > 0.5
\end{cases}$$

- Computational domain $[0, 1]$
- Non-reflecting boundary conditions
- $N = 8$ – highest degree of the Legendre polynomials
- $\Delta x = 1/200$ and $\Delta x = 1/800$
- final time $t = 0.1644$
Mean (left) and standard deviation (right) of $\rho$
Mean (left) and standard deviation (right) of $m$
Mean (left) and standard deviation (right) of $E$
Example 2 – Perturbed $\gamma$

We consider the Sod shock tube problem with $\gamma(z) = 1.4 + 0.1z$ and subject to the following initial condition:

$$\rho_0(x, z) = \begin{cases} 
1, & x < 0.5, \\
0.125, & x > 0.5, 
\end{cases} \quad u_0(x) \equiv 0, \quad p_0(x) = \begin{cases} 
1, & x < 0.5 \\
0.1, & x > 0.5 
\end{cases}$$

- Computational domain $[0, 1]$
- Non-reflecting boundary conditions
- $N = 8$ – highest degree of the Legendre polynomials
- $\Delta x = 1/200$ and $\Delta x = 1/800$
- final time $t = 0.1644$
Mean (left) and standard deviation (right) of $\rho$
Mean (left) and standard deviation (right) of $m$
Mean (left) and standard deviation (right) of $E$
Example 3 – Perturbed Interface

We consider the Sod shock tube problem with $\gamma = 1.4$ and subject to the following initial condition:

$$\rho_0(x, z) = \begin{cases} 
1, & x < 0.5 + 0.05z \\
0.125, & x > 0.5 + 0.05z 
\end{cases}$$

$$u_0(x) \equiv 0$$

$$p_0(x) = \begin{cases} 
1, & x < 0.5 + 0.05z \\
0.1, & x > 0.5 + 0.05z 
\end{cases}$$

- Computational domain $[0, 1]$
- Non-reflecting boundary conditions
- $N = 8$ – highest degree of the Legendre polynomials
- $\Delta x = 1/200$ and $\Delta x = 1/800$
- final time $t = 0.1644$
Mean (left) and standard deviation (right) of $\rho$
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