CES Seminar WS 14 15

Uncertainty Quantification for Hyperbolic Equations

Jonas Kusch

RWTH Aachen University

Supervisor: Prof. Dr. Martin Frank,

Department of Mathematics and
Center for Computational Engineering Science,
RWTH Aachen University

1 Introduction

This paper has been developed for the CES seminar in the Master program of Computational Engineering Science at RWTH Aachen University. It aims at summarizing the derivation of the Intrusive Polynomial Moment Method presented in [4], focussing on its similarities to the minimal entropy closures used in Transport Theory and its advantages and disadvantages compared to commonly used methods in Uncertainty Quantification.
Today a lot of simulation applications make use of deterministic models in order to predict the behaviour of a physical system. However, the question arises whether these models allow a good investigation of the physical system in the case of non deterministic inputs. Deterministic inputs are often not available, as for example the choice of model parameters or measurements of boundary or initial conditions contain uncertainties. As a result, one might ask the question whether we can relie on the results of a solution computed without taking into account these known and present uncertainies.
Successful approaches have been proposed to treat these uncertainties in simple problems, such as the steady diffusion equation [5] or the advection equation [2] with Stochastic Galerkin Methods, which provide spectral convergence for smooth data. However, using discontinuous data can lead to oscillations in the solution. Furthermore, the problem can loose important characteristics, such as for the Euler equations hyperbolicity.
In [4] the Intrusive Polynomial Moment Method (IPMM) was introduced, which aims at preserving hyperbolicity of conservation equations and preventing oscillations in the space of uncertainties.
The paper is structured as follows: In Section 2, a model problem will be described and investigated by the use of standard methods of Uncertainty Quantification. Section 3 links the concepts of Transport Theory with Uncertainty Quantification and thereby presents the motivation and derivation of IPMM. In Section 4, results of the different methods of Uncertainty Quantification, including IPMM, are presented and compared. Section 5 summarizes the findings for the given model problem and points to some more interesting features of IPMM that have been investigated in [4].

2 Uncertainty Quantification

2.1 Model Problem

The following model problem is introduced in order to motivate the use of Uncertainty Quantification and to present its standard methods, focusing on their deficiencies.
The problem we look at is Burgers equation in the presence of uncertain initial conditions, namely

$$\partial_t u(t,x,\xi) + \frac{1}{2}\partial_x u^2(t,x,\xi) = 0 \tag{1a}$$

$$u_0(x,\xi) = \begin{cases} u_L & \text{if } x \leq x_0 + \sigma\xi \\ u_L + (u_R - u_L) \cdot \frac{x_0+\sigma\xi-x}{x_0-x_1} & \text{if } x_0 + \sigma\xi \leq x \leq x_1 + \sigma\xi \\ u_R & \text{if } x_1 + \sigma\xi \leq x \end{cases} \tag{1b}$$

where the uncertainty has been parametrized with the uniform random variable $\xi \sim U(-1,1)$. It is important to note that even though the uncertainty is only explicitly given for the initial

condition, it will influence the solution, meaning that the scalar solution $u(t, x, \xi)$ will depend on the random variable ξ for all times $t \in \mathbb{R}^+$ and the spatial coordinates $x \in \mathbb{R}$. The initial state can be thought of as two constant states u_L and u_R, which are linearly connected between x_0 and x_1. This function is then translated to the right by a factor of $\sigma\xi$.
Now, our goal is to compute moments of the underlying probability density of the solution at a fixed time t_{end}. An important moment is the expectation value which is a $0 - th$ order moment. It is given by

$$E[u(T, x, \xi)] = \int_{\mathbb{R}} u f_{U,T,x}(u) du = \int_{-1}^{1} u(T, x, \xi) f_{\Xi}(\xi) d\xi. \tag{2}$$

2.2 Monte Carlo Method

A straight forward approach to compute the expectation value is the Monte Carlo (MC) Method. The convergence of this method is guaranteed by the strong law of large numbers.

Theorem 2.1 *Let $U_1, U_2, ...$ be a sequence of independent and identically distributed random variables with expectation value μ. We have for every $\epsilon > 0$*

$$P\left(\lim_{M\to\infty} \left| \frac{1}{M} \sum_{i=0}^{M} U_i - \mu \right| < \epsilon \right) = 1.$$

Proof A proof can be found in [1]. □

This motivates the idea of repeating a random experiment M times, where M should be a large number. Averaging the results of all experiments will then give an approximation of the expectation value.
In order to apply this concept to the model problem (1), we assume that a routine, which computes the initial conditions for a given ξ, as well as a finite volume routine, which computes the solution of burgers equation at time t_{end} for a given initial condition u_0, are provided. Then a straight forward algorithm to compute the expectation value is

Algorithm 1 Monte Carlo Method

1: **for** $n = 1$ to M **do**
2: $\quad \xi = GenerateRandomVariable$
3: $\quad u_0 = InitialCondition(\xi)$
4: $\quad u_n = FVM(u_0)$
5: **end for**
6: $\mu = \frac{1}{M} \sum_{i=1}^{M} u_i$

A main advantage is the simplicity of this approach. One does not need great understanding of the method used to solve the Burgers equation as it can be treated as a black box. Furthermore, the Monte Carlo Method can easily be parallelized and is not affected by the curse of dimensionality, which often causes problems if several random parameters need to be used. The crucial disadvantage is, however, the relatively low convergence rate of $\frac{1}{\sqrt{M}}$, which can be derived with the central limit theorem. Therefore, one should look at other methods, that in the case of the Stochastic Galerkin Method potentially have spectral convergence rates.

2.3 Stochastic Galerkin Method

The idea of the Stochastic Galerkin (SG) Method is to propagate the random parametrization through the model. Note that in the case of the Monte Carlo Method, the random variable has been fixed before computation, allowing us to use standard finite volume methods. Clearly, we need to derive new numerical schemes as well as find some kind of discretization of the random parameter if we would like to propagate the randomness. This discretization is performed by assuming that the random space is spanned by finitely many basis function, meaning that

$$u(t,x,\xi) \approx u_N(t,x,\xi) = \sum_{i=0}^{N} u_i(t,x)\phi_i(\xi). \tag{3}$$

Plugging this ansatz into the Burgers equation will lead to one equation for $N+1$ unknown coefficients u_i. Additionally, this equation contains an unknown residual as we no longer solve for the exact solution. $N+1$ equations for the coefficients can be obtained by projecting the residual onto the space spanned by the basis functions. The coefficients should be chosen such that the residual is orthogonal to this ansatz space with respect to an inner product weighted by f_Ξ. This means one has to solve

$$\int_{-1}^{1} \left[\partial_t \left(\sum_{i=0}^{N} u_i\phi_i \right) + \frac{1}{2}\partial_x \left(\sum_{i,k=0}^{N} u_k\phi_k u_i\phi_i \right) \right] \phi_j f_\Xi d\xi = 0 \tag{4}$$

for $j = 0,\dots,N$. If we assume the basis functions to be orthonormal with respect to the weighted scalar product, simple transformations will lead to the system of equations

$$\partial_t \mathbf{u} + \partial_x \left(\frac{1}{2}\mathbf{u}^T \mathbf{C} \mathbf{u} \right) = 0 \tag{5a}$$

$$\text{with } \mathbf{C} = \left(\int_{-1}^{1} \phi_i\phi_j\phi_k f_\Xi d\xi \right)_{i,j,k=0,\dots,N} \tag{5b}$$

$$\mathbf{u} = (u_i)_{i=0,\dots,N} \tag{5c}$$

Note that for our uniform distribution of ξ, the corresponding basis functions are the Legendre polynomials, normalized for the interval $[-1,1]$ and the density $f_\Xi = \frac{1}{2}$. The resulting system no longer depends on the random parameter ξ. A discretization in time and space can be performed as in standard finite volume schemes. Let

$$\mathbf{u}_j^n := \mathbf{u}(t^n, x_j) \tag{6}$$

meaning the coefficient vector evaluated at time t^n in cell j. Let $G(\cdot,\cdot)$ be a numerical flux which is consistent with the physical flux

$$F(\mathbf{u}) = \frac{1}{2}\mathbf{u}^T \mathbf{C} \mathbf{u}. \tag{7}$$

We then have the following algorithm.

Algorithm 2 Stochastic Galerkin Method

1: compute $\mathbf{C}$ for the numerical flux
2: $\mathbf{u}_j^0 \leftarrow setupInitialConditions$ for all cells j
3: **for** $n = 1$ to $NTimeSteps$ **do**
4: **for** $j = 1$ to $NCells$ **do**
5: $\mathbf{u}_j^{n+1} = \mathbf{u}_j^n - \frac{\Delta t}{\Delta x}(G(\mathbf{u}_j^n, \mathbf{u}_{j+1}^n) - G(\mathbf{u}_{j-1}^n, \mathbf{u}_j^n))$
6: **end for**
7: **end for**

The moments of the underlying probability density function can now be easily computed with the definition of u_N. As an example, we compute the expectation value

$$\begin{aligned} E[u] \approx E[u_N] &= \int_{-1}^{1} \sum_{i=0}^{N} u_i(t,x)\phi_i(\xi) f_\Xi(\xi) d\xi \\ &= \sum_{i=0}^{N} u_i(t,x) \int_{-1}^{1} \phi_i(\xi) f_\Xi(\xi) d\xi \\ &= \sum_{i=0}^{N} u_i(t,x) \int_{-1}^{1} \underbrace{\phi_0(\xi)}_{=1} \phi_i(\xi) f_\Xi(\xi) d\xi \\ &= u_0(t,x) \end{aligned}$$

Obviously, the Stochastic Galerkin approach is more cumbersome than Monte Carlo, as one first needs to derive and analyze the system (5). Additionally, adding more random inputs will lead to huge systems. If, for example, we had P random parameters, the number of coefficients would grow in the order of N^p . This is called the curse of dimensionality.
The main advantage is that the potential rate of convergence is spectral for sufficiently smooth data. This is due to the fact that we use orthogonal polynomials to approximate the uncertainties in our solution. Our method actually returns approximations of the Fourier coefficients which are the optimal choice for approximation, as they minimize the approximation error with respect to the L^2 norm. However, in some cases the L^2 norm does not seem to be a good choice of measuring the approximation error. This can be seen when approximating discontinuities.

3 Intrusive Polynomial Moment Method

Two additional disadvantages of the Stochastic Galerkin Method are Gibbs phenomena as well as the possibility of loosing hyperbolicity in the case of conservation equations. Gibbs phenomena arise when trying to interpolate discontinuous data with the orthogonal basis functions of SG. They can lead to a poor approximation of the unknown solution as oscillations or overshoots are often non-physical and from a mathematical point of view no entropy solution. Furthermore, in the case of the Euler equations the oscillations can cause negative densities. As a result, the problem will loose hyperbolicity and standard numerical scheme will fail to compute the solution. The Intrusive Polynomial Moment Method (IPMM) aims at resolving these two problems. It is motivated by the minimal entropy closures, which are

used to ensure hyperbolicity in Transport Theory. In order to link IPMM to minimal entropy closures, a short description of Transport Theory and similarities to Uncertainty Quantification will be provided. The concepts of Transport Theory will be linked to Uncertainty Quantification, focusing on the similarities of PN-closures and the SG approach. The ideas to solve problems of the PN closure will then be used to derive IPMM.

3.1 Basic concepts of Transport Theory

Transport Theory describes the evolution of a probability density function $\tilde{f}(t, \mathbf{x}, \mathbf{c})$, which is the probability density of a particle having velocity $\mathbf{c}$ being at position $\mathbf{x}$ at time t. This probability density is then scaled with the number density n such that the scaled density f fulfills

$$n(t, \mathbf{x}) = \int_{\mathbb{R}^3} f(t, \mathbf{x}, \mathbf{c}) d\mathbf{c}. \tag{8}$$

Moreover, one has

$$n(t, \mathbf{x})\mathbf{u}(t, \mathbf{x}) = \int_{\mathbb{R}^3} \mathbf{c} f(t, \mathbf{x}, \mathbf{c}) d\mathbf{c} \tag{9}$$

and

$$\frac{3}{2} k_B n(t, \mathbf{x}) T(t, \mathbf{x}) = \int_{\mathbb{R}^3} \frac{m}{2} \|\mathbf{c} - \mathbf{u}\|^2 f(t, \mathbf{x}, \mathbf{c}) d\mathbf{c}. \tag{10}$$

$\mathbf{u}$ and T are the macroscopic velocities and temperature. k_B is the Boltzmann constant. The evolution of the scaled probability density function f is given by the Boltzmann equation

$$\partial_t f(t, \mathbf{x}, \mathbf{c}) + \mathbf{c} \cdot \nabla_{\mathbf{x}} f(t, \mathbf{x}, \mathbf{c}) = J(f, f), \tag{11}$$

where $J(f, f)$ is the collision operator which describes the rate of change due to collisions. It is difficult to solve this equation directly due to the complexity of the collision operator and most importantly due to the high dimensionality caused by the additional dependence on the three velocity components of $\mathbf{c}$. This is why one takes moments of this equation with respect to basis functions $\phi_i(\mathbf{c})$. Taking moments means that one multiplies the Boltzmann equation (11) with $\phi_i(\mathbf{c})$ and integrates over $\mathbf{c}$. First, we choose the basis functions to be the so called collision invariants

$$\phi_1(\mathbf{c}) = m \tag{12a}$$

$$\phi_{2,3,4}(\mathbf{c}) = m\mathbf{c} \tag{12b}$$

$$\phi_5(\mathbf{c}) = \frac{1}{2} m \|\mathbf{c}\|^2 \tag{12c}$$

with m being the molecular mass of each particle. This choice of basis functions is practical as the collision term will vanish and the resulting moments will become physically intuitive quantities. Therefore, we get

$$\partial_t \rho + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{u}) = 0, \tag{13a}$$

$$\partial_t (\rho \mathbf{u}) + \nabla_{\mathbf{x}} \cdot \int_{\mathbb{R}^3} \mathbf{c}\mathbf{c}^T f dc = 0, \tag{13b}$$

$$\partial_t \left(\frac{3}{2} n k_B T + \frac{1}{2} \rho \|\mathbf{u}\|^2 \right) + \nabla_{\mathbf{x}} \cdot \int_{\mathbb{R}^3} \frac{1}{2} m \|\mathbf{c}\|^2 \mathbf{c} f dc = 0. \tag{13c}$$

If one calculates the integral terms by expanding f around a local equilibrium for small Knudsen numbers, one obtains the Navier-Stokes equations.

3.2 The PN-closure and its relation to SG

Now we want to derive a system of equations which provides us with moments up to a desired order N. Therefore, we start with taking moments for arbitrary basis functions ϕ_i, where i indicates the polynomial order of the basis function. For every $i \in \mathbb{N}_0$, we obtain the equation

$$\partial_t \int_{\mathbb{R}^3} \phi_i(\mathbf{c}) f(t, \mathbf{x}, \mathbf{c}) d\mathbf{c} + \nabla_{\mathbf{x}} \cdot \int_{\mathbb{R}^3} \phi_i(\mathbf{c}) \mathbf{c} f(t, \mathbf{x}, \mathbf{c}) d\mathbf{c} = \int_{\mathbb{R}^3} \phi_i(\mathbf{c}) J(f, f) d\mathbf{c}. \tag{14}$$

Taking a closer look at the first term of this equation and remembering that f is a scaled probability density, we can interpret this term as the i^{th} moment of f, which we will call m_i. In order to solve these equations, we need to choose a finite number of moments, hence we only look at $i = 0, \dots, N$. The problem arising is the multiplication with $\mathbf{c}$ in the second term, which means that the equation of the N^{th} moment will contain some form of the $(N+1)^{st}$ moment for which we do not have an equation. Hence, we need to close this system by choosing

$$f(t, \mathbf{x}, \mathbf{c}) \approx f_N(t, \mathbf{x}, \mathbf{c}) = G(t, \mathbf{x}, m_0(\mathbf{c}), \dots, m_N(\mathbf{c})). \tag{15}$$

One possible ansatz is to choose orthonormal basis functions ϕ_i and to choose the closure to be

$$f_{PN}(t, \mathbf{x}, \mathbf{c}) = \sum_{i=0}^{N} m_i(t, \mathbf{x}) \phi_i(\mathbf{c}). \tag{16}$$

This seems plausible as the moments m_i are nothing more than the Fourier coefficients of the probability density f. The subscript PN is used because this closure is known as the PN-closure. It is clear that the $(N+1)^{st}$ moment in the equation for $i = N$ will drop out due to orthogonality and we are able to solve the system.
At this point, we would like to compare the concepts presented so far with those of Uncertainty Quantification. In both cases we are interested in obtaining moments of some probability function. In Uncertainty Quantification an equation is given for the solution $u(t, x, \xi)$ which has an underlying probability density function for every $\mathbf{x}$ and t. If we are not interested in the function u itself, but in for example expectation value and variance of u, we are actually computing moments of the underlying probability density function. In contrast to that, Transport Theory provides the Boltzmann equation which can be solved to directly obtain the probability density function f. However, due to high dimensionality, we are also

interested in the moments of f. Hence, in both cases we are looking for moments of a directly or indirectly given probability density.
When comparing the PN-closure with the SG Method, we directly see similarities. First of all, in both cases we choose orthonormal basis functions ϕ_i in order to approximate our unknown solution (compare equations (16) and (3)). If this (or any other) ansatz for f had been introduced before taking moments with respect to the basis functions ϕ_i, the step of taking moments could be seen as a Galerkin projection, meaning that we project the resulting residual onto the orthogonal space spanned by all ϕ_i with $i \in \{0, \cdots, N\}$. This is exactly what we did to derive the SG system.
Unfortunately, the PN-closure also suffers from deficiencies that we already pointed out for the SG Method. Most importantly, the PN-closure can lead to probability densities which are negative and therefore not admissible. However, this problem has been tackled for Transport Theory by the introduction of minimal entropy closures in [3]. This approach has been successfully applied to treat the problems of SG in [4], leading to the Intrusive Polynomial Moment Method. In the following, the concept of minimal entropy closures for Transport Theory and Uncertainty Quantification will be summarized.

3.3 The minimal entropy closure and its relation to IPMM

For the derivation of the minimal entropy closure, we recall the closure problem of equation (14) and the ansatz to solve this problem given by equation (15). The idea of the minimal entropy closures is to take the minimum of a mathematical entropy for the Boltzmann equation (11) to be the closure. However, we cannot choose any probability density function to be the closure as we need to make sure that the moments of our closure match the computed moments m_i for $i = 0, \ldots, N$. Note that we only need to match the moments up to order N as we only compute the moment equations up to this order. One can clearly see the necessity of this restriction when choosing the collision invariants (12) as basis functions, leading to system (13). If we did not restrict the closure to match the given moments, this would mean that the probability density function would not give us density ρ or momentum $\rho\mathbf{u}$ as moments, meaning that our choice of f is not admissible and the system for computing the moments, namely (13), no longer matches our problem.
Let us call the chosen mathematical entropy H and the closure which we would like to determine f_{ME}. We then need to determine f_{ME} by solving

$$\arg\min_f H(f) \tag{17a}$$

$$\text{s.t. } m_i = \int_{\mathbb{R}^3} \phi_i f d\mathbf{c} \;\; \forall i \in \{0, \cdots, N\}. \tag{17b}$$

This constraint optimization problem can be solved by minimizing the Lagrangian function

$$L(f, \vec{\lambda}) = H(f) + \sum_{i=0}^{N} \lambda_i \left(m_i - \int_{\mathbb{R}^3} \phi_i f d\mathbf{c} \right). \tag{18}$$

If we assume that the entropy H can be written as

$$H(f) = \int_{\mathbb{R}^3} h(f) d\mathbf{c}, \tag{19}$$

the Gateaux derivative for an arbitrary direction g is then given by

$$\delta L(f; g, \vec{\lambda}) = \int_{\mathbb{R}^3} \left(h'(f) - \sum_{i=0}^{N} \lambda_i \phi_i \right) g d\mathbf{c}. \tag{20}$$

In order for f_{ME} to be a minimizer of L, this derivative must be zero for all g, which means that we must have

$$h'(f_{ME}) = \sum_{i=0}^{N} \lambda_i \phi_i \tag{21}$$

or

$$f_{ME} = \left(h'\right)^{-1} \left(\sum_{i=0}^{N} \lambda_i \phi_i \right). \tag{22}$$

A moment system derived with the help of an entropy closure has several desirable features. For the choice $h(f) = fln(f) - f$ a proof for hyperbolicity of the moment system and the derivation of an entropy function can be found in [3]. This entropy for the moment system is given by H, which we defined in (19).
Now let us assume that a similar concept for Uncertainty Quantification, leading to a hyperbolic moment system with an entropy H, can be derived. Obviously, this would be desirable, as hyperbolicity will allow us to employ standard finite volume schemes to solve the system and the entropy could be used to limit oscillations. Before going into detail, we take a step back and write down our closure problem in the case of Uncertainty Quantification. By taking moments of the model problem (1), where we replaced the Burgers with a general physical flux $f(u)$ we arrive at

$$\partial_t \int_{-1}^{1} u(t, \mathbf{x}, \xi) \phi_i(\xi) f_\Xi(\xi) d\xi + \partial_x \int_{-1}^{1} f(u(t, \mathbf{x}, \xi)) \phi_i(\xi) f_\Xi(\xi) d\xi = 0 \tag{23}$$

We again identify the first term as the moment of the underlying probability density for u and call it u_i. In order to solve this equations we need to choose a finite number of moments, hence we only look at $i = 0, \dots, N$. The second term should now only depend on moments up to order N. The closure we choose is now motivated by the entropy closure, hence we look for a closure minimizing a convex mathematical entropy H under the condition that this closure returns our given moments. The entropy which we choose has the form

$$H(u(t, x, \xi)) = \int_{-1}^{1} h(u(t, x, \xi)) f_\Xi(\xi) d\xi. \tag{24}$$

We now proceed as in Transport Theory. In order to determine the minimizer of the constraint problem, we minimize the Lagrange function

$$L(u(t, x), \lambda) := H(u(t, x, \xi)) + \sum_{i=1}^{N} \lambda_i \left(u_i - \int_{-1}^{1} u(t, x, \xi) \phi_i(\xi) f_\Xi(\xi) d\xi \right). \tag{25}$$

The minimizer must fulfill

$$h'(u_{ME}) = \sum_{i=0}^{N} \lambda_i \phi_i, \tag{26}$$

meaning that

$$u_{ME} = (h')^{-1}\left(\sum_{i=0}^{N} \lambda_i \phi_i\right). \tag{27}$$

The choice of this closure is called the Intrusive Polynomial Moment Method. Now let us proof the desired properties of IPMM.

Theorem 3.1 *The moment system given by IPMM is hyperbolic.*

Proof Plugging the closure (27) into the moment system (23) leads to

$$\partial_t \int_{-1}^{1} u_{ME}(\Lambda)\phi_i(\xi) f_\Xi(\xi) d\xi + \partial_x \int_{-1}^{1} f(u_{ME}(\Lambda))\phi_i(\xi) f_\Xi d\xi = 0 \tag{28}$$

where we defined $\Lambda := \sum_{k=0}^{N} \lambda_k(t,x)\phi_k(\xi)$. We now derive a system for the unknowns λ_j and show that it is hyperbolic. By differentiation and applying the chain rule, we get

$$\sum_j \underbrace{\int_{-1}^{1} u'_{ME}(\Lambda)\phi_j\phi_i f_\Xi d\xi}_{=:M_{ij}} \partial_t \lambda_j + \sum_j \underbrace{\int_{-1}^{1} f'(u_{ME}) u'_{ME}(\Lambda)\phi_j\phi_i f_\Xi d\xi}_{=:A_{ij}} \partial_x \lambda_j = 0 \tag{29}$$

We have that

$$u'_{ME}(\Lambda) = \left((h')^{-1}\right)' = \frac{1}{h''(u_{ME})}, \tag{30}$$

which can be seen by differentiating $s'((s')^{-1}(\Lambda)) = \Lambda$ with respect to Λ. Let us now take a look at the matrix $\mathbf{M}$. Obviously, $\mathbf{M}$ is symmetric and due to strict positive definiteness of h, we can see from

$$\mathbf{d}^T \mathbf{M} \mathbf{d} = \int_{-1}^{1} \frac{1}{h''(u_{ME})} \left(\sum_i d_i \phi_i\right)^2 f_\Xi d\xi > 0 \tag{31}$$

that $\mathbf{M}$ is strictly positive definite. Clearly, $\mathbf{A}$ is symmetric. This is why we can write the system as

$$\partial_t \vec{\lambda} + \underbrace{\mathbf{M}^{-\frac{1}{2}}\mathbf{M}^{-\frac{1}{2}}\mathbf{A}\mathbf{M}^{-\frac{1}{2}}\mathbf{M}^{\frac{1}{2}}}_{=:\mathbf{C}} \partial_x \vec{\lambda} = 0, \tag{32}$$

where $\mathbf{M}^{-1} = \mathbf{M}^{-\frac{1}{2}}\mathbf{M}^{-\frac{1}{2}}$ with $\mathbf{M}^{-\frac{1}{2}}$ symmetric as $\mathbf{M}^{-1}$ is positive definite. Therefore, $\mathbf{C}$ is symmetric, meaning that $\mathbf{C}$ is diagonalizable with real eigenvalues, which means that the system is hyperbolic. □

Theorem 3.2 *The moment system given by IPMM fulfills the entropy inequality*

$$\partial_t H(u_{ME}) + \partial_x \Psi(u_{ME}) \leq 0, \tag{33}$$

where

$$H(u_{ME}) = \int_{-1}^{1} h(u_{ME}(\Lambda)) f_\Xi d\xi \tag{34}$$

and

$$\Psi(u_{ME}) = \int_{-1}^{1} \psi(u_{ME}(\Lambda)) f_\Xi d\xi. \tag{35}$$

The functions h and ψ are the entropy and the entropy flux of the model problem with general physical flux f.

Proof Let us first recall the derivation of h and ψ for a general scalar model problem. If u is not differentiable, we will not have a classical solution fulfilling

$$\partial_t u(t,x,\xi) + \partial_x f(u(t,x,\xi)) = 0. \tag{36}$$

Hence, we would like to look for the solution of the viscous problem

$$\partial_t u + \partial_x f(u) = \epsilon \partial_{xx} u. \tag{37}$$

An entropy can be derived by multiplication with $h'(u)$, which leads to

$$\partial_t h(u) + \underbrace{h'(u)f'(u)}_{=:\tilde{\psi}'(u)} \partial_x u = \epsilon h'(u) \partial_{xx} u. \tag{38}$$

Applying the reverse chain rule to the right hand side leads to

$$\partial_t h(u) + \partial_x (\underbrace{\tilde{\psi} - \epsilon h'(u)\partial_x u}_{=:\psi(u)}) = \underbrace{-\epsilon \partial_x u h''(u) \partial_x u}_{\leq 0}. \tag{39}$$

Therefore, the viscous limit, i.e. for $\epsilon \to 0$ fulfills

$$\partial_t h(u) + \partial_x \psi(u) \leq 0, \tag{40}$$

where equality holds for smooth data. Now let us derive the entropy counterpart of the moment system. We start by taking moments of the viscous problem (37). Applying the chain rule on f and u_{ME} yields

$$\int_{-1}^{1} u'_{ME}(\Lambda)\partial_t \Lambda \phi_i f_\Xi d\xi + \int_{-1}^{1} f'(u_{ME}) u'_{ME}(\Lambda) \partial_x \Lambda \phi_i f_\Xi d\xi = \epsilon \int_{-1}^{1} u_{xx} \phi_i f_\Xi d\xi. \tag{41}$$

We now multiply both sides with λ_i and sum over i. Let us start with the first term, where we get

$$\int_{-1}^{1} u'_{ME}(\Lambda)\partial_t \Lambda \underbrace{\sum_i \lambda_i \phi_i}_{=h'(u_{ME})} f_\Xi d\xi = \int_{-1}^{1} \partial_t h(u_{ME}(\Lambda(t,x,\xi))) f_\Xi d\xi. \tag{42}$$

The second term of (41) becomes

$$\begin{aligned}\int_{-1}^{1} f'(u_{ME}) u'_{ME}(\Lambda) \partial_x \Lambda \underbrace{\sum_i \lambda_i \phi_i}_{=h'(u_{ME})} f_\Xi d\xi &= \int_{-1}^{1} f'(u_{ME}) h'(u_{ME}) \partial_x u_{ME} f_\Xi d\xi \\ &= \int_{-1}^{1} \partial_x \tilde{\psi}(u_{ME}(\Lambda(t,x,\xi)))) f_\Xi d\xi. \end{aligned} \tag{43}$$

The third term of (41) becomes

$$\begin{aligned}\epsilon \int_{-1}^{1} \partial_{xx} u_{ME} \underbrace{\sum_i \lambda_i \phi_i}_{=h'(u_{ME})} f_\Xi d\xi &= \epsilon \int_{-1}^{1} \partial_x (\partial_x u_{ME} h'(u_{ME})) - \partial_x u_{ME} \partial_x h'(u_{ME}) f_\Xi d\xi \\ &= \epsilon \int_{-1}^{1} \partial_x (h'(u_{ME}) \partial_x u_{ME}) - \partial_x u_{ME} h''(u_{ME}) \partial_x u_{ME} f_\Xi d\xi \end{aligned} \tag{44}$$

Plugging (42), (43),(44) into (41) and remembering that h is strictly convex yields the entropy inequality (33). □

The hyperbolicity of the system now guarantees that one can use standard numerical schemes for solving the moment system. It is important to note that

$$h(u) = \frac{u^2}{2} \tag{45}$$

is a mathematical entropy of the scalar model problem. The same entropy function, where u is replaced by the scaled probability density f is also an entropy for the Boltzmann equation. Differentiating the entropy by u, or in the case of Transport Theory by f, shows that SG and the PN-Closure both lead to a hyperbolic moment system fulfilling an entropy inequality if a quadratic entropy is admissible. Note that a quadratic entropy is not always admissible if $u(t, x, \xi)$ is not scalar. Furthermore, the entropy inequality (33) can now be used to prevent oscillations in the solution. Integration over the entire spatial domain and the time domain $[0, T]$ leads to

$$\int_{-1}^{1}\int_{\mathbb{R}} h(u(\Lambda(T, x, \xi)))f_{\Xi}dxd\xi \leq \int_{-1}^{1}\int_{\mathbb{R}} h(u(\Lambda(0, x, \xi)))f_{\Xi}dxd\xi. \tag{46}$$

The fact that the entropy of the moment system is decreasing in time can now be used to prevent oscillations in the solution u. Let us choose the entropy h to be

$$h(u) = -ln(u - u_-) - ln(u_+ - u). \tag{47}$$

We now assume that the maximal value of the initial condition is smaller than u_+ and the minimal value is bigger than u_-. In this case the entropy is finite. As the entropy is decreasing in time, the solution can not obtain values that are bigger than u_+ or smaller than u_-, as in this case, the entropy would be bigger than the initial entropy. This means that oscillations are limited by the entropy decrease. It is important to point out that Theorem 3.2 can easily be extended to systems. In this case it is not straight forward to find an entropy, which satisfies the entropy inequality (40) and at the same time prevents oscillations.
We now look at an implementation of IPMM. Let $G(\cdot, \cdot)$ be a numerical flux which is consistent with the physical flux of our moment system, namely

$$F(\vec{\lambda}) = \partial_x \int_{-1}^{1} f\left(u_{ME}\left(\sum_k \lambda_k \phi_k\right)\right)\phi_i(\xi)f_{\Xi}d\xi \tag{48}$$

An algorithm for this method can now be written as

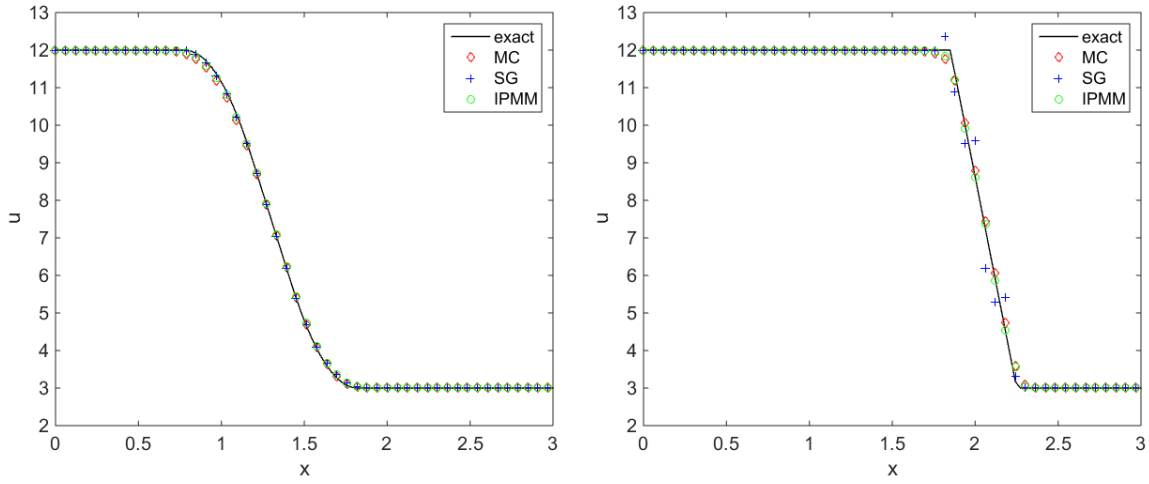
Algorithm 3 IPMM

1: $\vec{\lambda}_l^0 = \left(\int_{-1}^{1} s'\left(u_0(x_l, \xi)\right)\phi_j f_{\Xi}d\xi\right)_{j=0,\dots,N}$
2: **for** $n = 1$ to $NTimeSteps$ **do**
3: **for** $l = 1$ to $NCells$ **do**
4: $\mathbf{u}_l^n = \left(\int_{-1}^{1}(s')^{-1}\left(\sum_{k=0}^{N}\lambda_k(t^n, x_l)\phi_k\right)\phi_j f_{\Xi}d\xi\right)_{j=0,\dots,N}$
5: $\mathbf{u}_l^{n+1} = \mathbf{u}_l^n - \frac{\Delta t}{\Delta x}(G(\vec{\lambda}_l^n, \vec{\lambda}_{l+1}^n) - G(\vec{\lambda}_{l-1}^n, \vec{\lambda}_l^n))$
6: $\vec{\lambda}_l^{n+1} = \arg\min_{\lambda} L\left(u_N\left(\sum_{k=0}^{N}\lambda_k\phi_k\right), \vec{\lambda}\right)$
7: **end for**
8: **end for**

The last step inside the loop is necessary as the classical finite volume update only provides us with the updated moments $\mathbf{u}$. The corresponding Lagrange coefficients can be obtained by solving the dual problem.

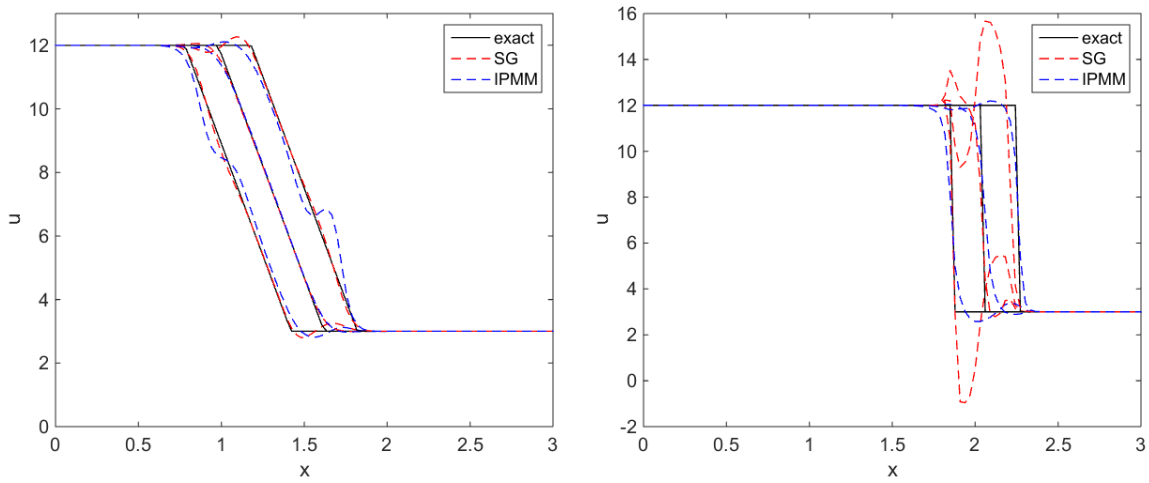
4 Results

In the last section, we will now look at and compare the solutions each method provides for the model problem (1). We choose the left state of our initial condition u_L to be 12.0 and the right state u_R to be 3.0. Furthermore, x_0 is chosen to be 0.5, x_1 has a value of 1.5 and σ is 0.2. The $x-$space, which ranges from 0.0 to 3.0 is discretized using 100 cells. Let us first take a look at the expectation value, which can also be computed by using the Monte Carlo Method. We can compare all computed expectation values with the exact solution, which can be calculated with the help of characteristics. It can be shown that at time $t^* = \frac{1}{9}$, a shock will form. For all times after t^* the exact entropy solution can be computed with the Rankine Hugoniot condition. In order to demonstrate the disadvantages of Stochastic Galerkin we will also look at the solution for $t_2 > t^*$. The IPMM method uses parameters $u_- = 2.0$ and $u_+ = 13.0$ to prevent significant oscillations. One can find the results in Figures 1. It can be seen that all methods return a good approximation of the exact expectation value for t_1. In this case, the SG method seems to be the best choice, as the error with respect to the L_2 norm and the runtime are the smallest: The runtime of SG is 0.6973, followed by the runtime of IPMM, which is 266.0448, and the runtime of MC, which is 535.3233 seconds. The errors are given by 0.17721 for SG, 0.20202 for IPMM and 0.24251 for MC. Even though the Monte Carlo Method does not seem to be a good choice to solve this problem, it must be stated that its implementation was by far the easiest, followed by the implementation of the Stochastic Galerkin Method. Another advantage of the Monte Carlo Method can be seen by looking at the results at time t_2. Here, the SG Method yields a quite bad approximation. The error for SG is given by 0.53336, the error of IPMM is 0.26259 and the error of MC is 0.33678. It is important to note that the SG result has values, which are bigger than those of the initial conditions. This behavior is due to oscillations, which arise when approximating discontinuities with the help of orthogonal polynomials. One can see the inadequate approximation behaviour by looking at Figures 2, in which the solution is plotted for $\xi \in \{-1, 0, 1\}$. While at t_1, both methods show small oscillations in their result, a clear difference between those two methods can be seen for t_2. Here, we can see strong oscillations for SG, whereas the oscillations of IPMM do not seem to be amplified over time. To actually see the approximation properties in the random space, we take a look at the solution plotted at two fixed critical values of x, which can be found in Figures 3. For time t_1, the fixed $x-$value is 1.6364, where the solution is not differentiable. Even though both methods cannot interpolate such an unsmooth function, the approximations of both methods seem to be reasonable. For time t_2, a critical region can be found at $x = 2.0606$. Here, we need to approximate a discontinuity, which for both methods leads to overshoots. Those overshoots are limited by u_- and u_+ for the IPMM Method. The approximation seems to be adequate for a shock, even though the shock appears to be smeared out. If we took more polynomials for approximation, we would see a sharper approximation of the shock. The solution of the SG Method shows clear overshoots, which are not limited.



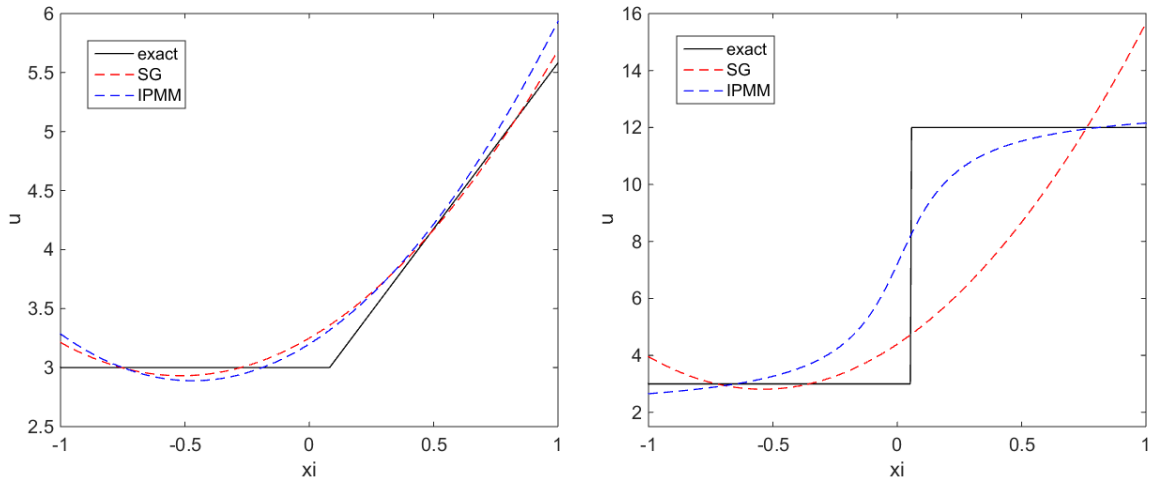
(a) Expecation values for $t_1 = 0.04$ (b) Expecation values for $t_2 = 0.14$

Figure 1: Exact expectation values compared with results from Monte Carlo, Stochatic Galerkin and IPMM at two different times. Both, SG and IPMM use polynomials up to order 2. The Monte Carlo Method uses 1000 samples.



(a) $t_1 = 0.04$ (b) $t_2 = 0.14$

Figure 2: Exact solution u for fixed values $\xi \in \{-1, 0, 1\}$, as well as the approximations provided by SG and IPMM. Both, SG and IPMM use polynomials up to order 2.



(a) $t_1 = 0.04$, $x = 1.6364$ (b) $t_2 = 0.14$, $x = 2.0606$

Figure 3: Plots of the random space for fixed t and x. Both, SG and IPMM use polynomials up to order 2.

5 Conclusion

In this paper, we have examined three different methods of Uncertainty Quantification and compared their behaviour when solving the Burgers equation with uncertain initial conditions. We have seen that while the Stochastic Galerkin Methods appears to be a good choice for sufficiently smooth data, it will yield large errors as soon as a shock appears in the solution. The Monte Carlo method has proven to be quite robust and easy to implement. However, it will take a long time to obtain a good approximation, which is caused by its small convergence rate. The findings of Transport Theory have been used to derive the Intrusive Polynomial Moment Method, which fulfills an entropy inequality. With this inequality we were able to limit oscillations and therefore obtained a good approximation of the unknown solution. It must be pointed out that the implementation of this method is not as straight forward as the implementation of Monte Carlo or SG. Furthermore, the runtimes of the Intrusive Polynomial Moment Method are by far larger than those of Stochastic Galerkin, which is caused by the optimization routine used to find the appropriate Lagrange multipliers. Especially if we had multiple random dimensions, it might be a better choice to use the Monte Carlo Method, which is actually a common problem in Uncertainty Quantification. However, IPMM appears to have some potential in the presence of a high dimensional random space, which can be seen in [4]. Here, convergence rates have been studied for smooth initial conditions, for which we can expect spectral convergence if we use SG or IPMM. For the smooth test case, IPMM showed better convergence than Stochastic Galerkin, which is why for smooth data less polynomial orders suffice to obtain good results. Hence, the number of unknown coefficients can be decreased if we use IPMM, which is especially useful in the case of multiple random variables. Furthermore, we have stated that Stochastic Galerkin is no longer an entropy closure if a quadratic function is not the entropy of the model problem. This is often the case for systems of equations. In [4], the Euler Equations have been investigated, where hyperbolicity is only preserved in the case of IPMM. There-

fore, one can conclude that the Intrusive Polynomial Moment Method should be used for systems of equations, in the presence of discontinuities in the random space as well as for multiple random dimensions, if we do not want to use the Monte Carlo Method.

References

[1] Nasrollah Etemadi. An elementary proof of the strong law of large numbers. *Zeitschrift für Wahrscheinlichkeitstheorie und verwandte Gebiete*, 55(1):119–122, 1981.

[2] David Gottlieb and Dongbin Xiu. Galerkin method for wave equations with uncertain coefficients. *Commun. Comput. Phys*, 3(2):505–518, 2008.

[3] C David Levermore. Moment closure hierarchies for kinetic theories. *Journal of Statistical Physics*, 83(5-6):1021–1065, 1996.

[4] Gaël Poëtte, Bruno Després, and Didier Lucor. Uncertainty quantification for systems of conservation laws. *Journal of Computational Physics*, 228(7):2443–2467, 2009.

[5] Dongbin Xiu and George Em Karniadakis. Modeling uncertainty in steady state diffusion problems via generalized polynomial chaos. *Computer Methods in Applied Mechanics and Engineering*, 191(43):4927–4948, 2002.