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Automatic computation of Chebyshev polynomials for the study of parameter dependence for hyperbolic systems

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Abstract

We introduce a new intrusive method for studying the parameter dependence of solutions of hyperbolic systems having sharp discontinuities. Two applications to the study of solutions of Euler's system are presented.

1 Introduction

In the paper [AG] the authors have introduced a method for the computation of the dependence of a hyperbolic partial differential equation based on the automatic computation of Taylor expansions. We refer to [AG] and references therein for an extensive introduction to the topic. It was observed that a Taylor expansion fails close to the smoothed representation of a sharp discontinuity, because the functions that are expanded appear to have singularities close to the real axis; since a Taylor series necessarily converges in a disk, the presence of singularities binds the radius of convergence. A technique to modify the region of convergence was introduced, based on the use of a conformal map to transform a disk in a region thinner in the direction of the imaginary axis. Here, we want to push further that approach and find a series expansion that better adapts to the study of sharp discontinuities.

In Section 2 we describe and motivate the choice of the Chebyshev polynomials. In Section 3 we describe the system used as an example. In Section 4 we present the results of the shock tube experiment obtained with the Chebyshev expansion and we compare them with the results obtained in [AG] with the Taylor expansion. In Section 5 we describe a new experiment where the effectiveness of the Chebyshev expansion is particularly manifest.

2 The Chebyshev expansion

Consider an hyperbolic system depending on a parameter x. With no restriction, we assume $x \in [-1,1]$. We approximate a function f depending on x by means of a truncated series

$$(Cf)(x) = \sum_{k=0}^{K} \hat{f}_k T_k(x)\,, \tag{1}$$

where $T_k(x)$ is the Chebyshev polynomial of order k. Here, in the case when we are solving a hyperbolic partial differential equation with some numerical discretization, the function f can be the value of the solution at one point of the grid, or the coefficient of some expansion, if we are using spectral methods. We recall that the Chebyshev polynomials satisfy

$$T_k(x) = \cos(k \arccos x) \quad k = 0,1,2,... \tag{2}$$

and they are a complete orthogonal set for the weighted Hilbert space $L^2_w := L^2_w([-1,1])$ defined by

$$L^2_w := \left\{ f : [-1,1] \to \mathbb{C},\ \int_{-1}^{1} f^2(x) w(x) dx < \infty \right\}, \tag{3}$$

with $w(x) = (1-x^2)^{-1/2}$ and

$$(f,g) = \int_{-1}^{1} f(x)\overline{g(x)} w(x) dx\,.$$

The reason because Chebyshev polynomials should be more effective in the study of a shock with a fine grid lies in the way they transform regions of the complex plane. In order to study the effect of a Chebyshev polynomial on the region around the segment $I = \{z \in \mathbb{C} \,:\, Re(z) \in [-1,1],\, Im(z) = 0\}$, let $w = e^{iz}$, so that $\cos z = g(w) = \frac{1}{2}(w + w^{-1})$, $\cos nz = g(w^n)$ and $T_n(z) = g([g^{-1}(e^{iz})]^n)$. Note that, for all $\alpha \in \mathbb{R}$, the image of the circle $|w| = e^{\alpha}$ through the map g is an ellipse centered at 0 and with semiaxes $(\cosh\alpha, \sinh|\alpha|)$. We call such ellipse E_α and we call $\mathcal{E}_\alpha$ the open set bounded by E_α (note that $E_0 = I$). More precisely, if we call A_α the annulus of radii $(e^{-\alpha}, e^{\alpha})$ punctured at $z = \pm 1$, that is $A_\alpha = \{z \in \mathbb{C} \,:\, e^{-\alpha}, < |z| < e^{\alpha}\,,\, z \neq \pm 1\}$, then g is a conformal map from A_α onto $\mathcal{E}_\alpha \setminus \{1,-1\}$ with the property that $g(z) = g(z^{-1})$. It follows that, if $z = \cosh\rho\cos\vartheta + i\sinh\rho\sin\vartheta$, then $T_k(z) = \cosh k\rho\cos k\vartheta + i\sinh k\rho\sin k\vartheta$. Consider now the expansion with respect to the orthogonal system $\{T_k\}$:

$$f(x) = \sum_{k=0}^{+\infty} \hat{f}_k T_k(x)\,, \tag{4}$$

choose $\rho > 0$ and consider the Banach space $B_\rho \subset L^2_w$ of the functions f such that the expansion (4) satisfies

$$\|f\| := \sum_{k=0}^{+\infty} \left|\hat{f}_k\right| e^{\rho k} < +\infty\,.$$

Theorem 2.1 *Let $\rho' > \rho > 0$. If $f \in B_\rho$, then f is analytic in $\mathcal{E}_\rho$. If f is analytic in $\mathcal{E}_{\rho'}$, then $f \in B_\rho$.*

Proof. Assume that $f \in B_\rho$ and let $\{\hat{f}_k\}$ be its Fourier coefficients as in (4). Choose α, $0 < \alpha < \rho$. If $z \in E_\alpha$, then $T_k(z) \in E_{k\alpha}$, so that $|T_k(z)| \le Ce^{k\alpha}$ and

$$\sup_{z\in\mathcal{E}_\alpha} \left| \sum_{k=K}^{+\infty} \hat{f}_k T_k(z) \right| \le C \sum_{k=K}^{+\infty} e^{-\rho k} \sup_{z\in\mathcal{E}_\alpha} |T_k(z)| \le C \sum_{k=K}^{+\infty} e^{-(\rho-|\alpha|)k} \to 0 \text{ as } K \to +\infty\,; \tag{5}$$

therefore (4) converges uniformly in $\mathcal{E}_\alpha$ and the sum is analytic.

Conversely, assume that f is analytic in $\mathcal{E}_{\rho'}$. Then, $f \in L^2_w$, so the coefficients $\{\hat{f}_k\}$ are well defined. Consider the map

$$F(z) = \sum_{k=0}^{+\infty} \hat{f}_k g(z^n) = \frac{1}{2} \sum_{k=0}^{+\infty} \hat{f}_k (z^k + z^{-k})\,; \tag{6}$$

if $g(z) = x$, then $F(z) = f(x)$, and since f is analytic in $\mathcal{E}_{\rho'}$, then F is analytic in $A_{\rho'}$. This implies that (6) converges absolutely for all z such that $e^{-\rho} \le |z| \le e^{\rho}$, hence $f \in B_\rho$. □

2.1 Implementation of the Chebyshev polynomials

As with the Taylor polynomials (see [AG]), it is easy to implement on a computer an arithmetic of Chebyshev polynomials. More precisely, one represents a truncated Chebyshev expansion as the list of the coefficients and then implements a procedure that, given a scalar α and two Chebyshev expansions T_1, T_2 and an arithmetic operation $*$ (either addition or multiplication), computes the Chebyshev expansion corresponding to $\alpha(T_1 * T_2)$. This implies that, given a polynomial $p(x)$, it is possible to compute the Chebyshev expansion of $p(T_1)$, and since all analytic functions $f(x)$ can be approximated with polynomials, it is also possible to compute the Chebyshev expansion of $f(T_1)$. Furthermore, since $T_0(x) = 1$ and $T_1(x) = x$, then an interval $[a, b]$ can be represented by the Chebyshev expansion

$$\frac{a+b}{2}T_0(x) + \frac{a-b}{2}T_1(x) \text{ with } x \in [-1, 1]\,. \tag{7}$$

Since the addition of two Chebyshev expansions is straightforward, we describe here the algorithm used for the multiplication. Given two Chebyshev expansions of order n, say $P_1(x) = \sum_{k=0}^{n} c_k^1 T_k(x)$ and $P_2(x) = \sum_{l=0}^{n} c_l^2 T_l(x)$, let

$$P(x) = P_1(x) * P_2(x) = \sum_{j=0}^{2n} c_j T_j(x)\,.$$

In order to compute the coefficients c_j of $P(x)$ we observe that

$$T_k(x)T_l(x) = \frac{1}{2}T_{k+l}(x) + \frac{1}{2}T_{k-l}(x).$$

Then, we have

$$\begin{aligned} P(x) &= \left(\sum_{k=0}^{n} c_k^1 T_k(x)\right)\left(\sum_{l=0}^{n} c_l^2 T_l(x)\right) = \sum_{k=0}^{n}\sum_{l=0}^{n} c_k^1 c_l^2 T_k(x) T_l(x) \\ &= \sum_{k=0}^{n}\sum_{l=0}^{n} c_k^1 c_l^2 \left(\frac{1}{2}T_{k+l}(x) + \frac{1}{2}T_{k-l}(x)\right)\,, \end{aligned}$$

so that

$$c_j = \frac{1}{2}\sum_{k+l=j} c_k^1 c_l^2 + \frac{1}{2}\sum_{k-l=j} c_k^1 c_l^2\,.$$

As it was pointed out in [AG], once the addition and the multiplication have been implemented, it is straightforward to implement the computation of polynomials and analytical functions.

3 The Euler system of equations

As in [AG], we test the method on the *shock tube problem* introduced in [S] for the one dimensional Euler system of equations. We refer to [AG] for all details concerning the experiment. Here, we recall that the equation is

$$U_t + F(U)_x = 0$$

in $(t, x) \in [0, T] \times [0, 1]$, where

$$U = \begin{pmatrix} \rho \\ \rho v \\ \rho e \end{pmatrix} \quad \text{and} \quad F(U) = \begin{pmatrix} U_2 \\ \frac{U_2^2}{U_1} + p \\ (U_3 + p)\frac{U_2}{U_1} \end{pmatrix}\,.$$

We choose $T = 0.15$, since the waves which characterize the solution have time to fully develop, without reaching the boundaries of the tube. $\rho(t, x)$ is the density of the gas, $v(t, x)$ is the velocity, $e(t, x)$ is the energy density and $p(t, x)$ is the pressure. In order to have a closed set of equation, we need a relation between p, e, ρ, v, that is the equation of state of the gas. We choose the equation of state for a polytropic ideal gas, that is

$$e_i = \frac{p}{\rho(\gamma - 1)}$$

where $\gamma = c_p/c_v$ is the ratio of specific heats at constant pressure and at constant volume and e_i is the internal energy density, defined by

$$e = e_i + \frac{1}{2}v^2 \, .$$

The initial conditions of the experiment are:

$$(\rho(0, x), v(0, x), p(0, x)) = \begin{cases} (1, 0, 1) & \text{if} \quad x \in [0, 1/2] \\ (1/8, 0, 1/10) & \text{if} \quad x \in (1/2, 1] \, . \end{cases}$$

Since the nodes close to the boundary are uneffected by the experiment, the boundary conditions are irrelevant, as long as they do not introduce any kind of new dynamics. We use absorbing boundary conditions, implemented by adding one ghost cell at each end of the tube, and using a zeroth order extrapolation to assign values to them. The variable parameter is γ; since monoatomic gases have $\gamma = 5/3$ and biatomic gases have $\gamma = 7/5$, we consider γ varying in the interval $[7/5, 5/3]$. The shock wave travels to the right at speed $v + c(\gamma)$, where the speed of sound $c(\gamma)$ is given by $c(\gamma) = \sqrt{\gamma p/\rho}$, the rarefaction wave travels to the left at speed $v - c(\gamma)$ and the contact discontinuity travels at speed v (to the right if $v > 0$ or to the left if $v < 0$). So, when γ takes values in an interval, the velocities of the shock and rarefaction waves also take values in an interval.

We compute a solution of the system with Roe's approximate Riemann solver. We point out that we implemented it "as is", except for the fact that we used "objects Chebyshev" instead of floating point numbers (but see Section 5 on a detail concerning the spectral projection of the linearized matrix).

4 Comparison between Taylor and Chebyshev expansions

First, we wish to compare the accuracy of the Taylor expansion and the Chebyshev expansion. In Figure 1 on the left, we compare the error $\epsilon(x, t)$ on the density obtained with the expansion of order $k = 5$ and with a grid of $N = 100$. Note that the Chebyshev expansion has an error higher than the Taylor expansions of equal order. The maximum error is once again close to the shock wave and its magnitude is quite similar to that obtained with the Taylor expansion with holomorphic correction. It is clear that, at low order, neither the Chebyshev expansion nor the Taylor expansion with holomorphic correction are as efficient as the plain Taylor expansion. On the other hand, at higher order the Chebyshev expansion becomes more efficient as we can see in Figure 1 on the right, where we compare the errors of the expansions at order $k = 10$. At this order, the Chebyshev expansion outperforms the Taylor expansion with the holomorphic map correction: more precisely, the error with the Taylor expansion with holomorphic correction is almost one order of magnitute larger at every point of the domain. As we have seen for the Taylor expansions with or without the holomorphic correction, an increase of the order implies a decrease of the error, until we reach an order when a larger order does not help anymore. Note that an increase of the order cuts down the errors close to the rarefaction and contact waves, while the error close to the shock wave remains the highest.

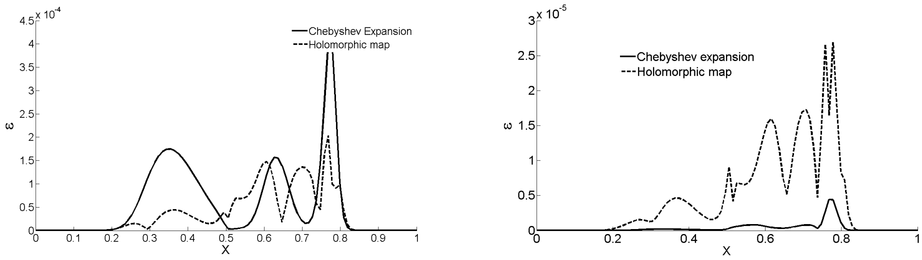

Figure 1: Error on the density at $t = T$ with $k = 5, 10$

An important advantage of the Chebyshev expansion consists in the fact that it is possible to achieve a description of the discontinuities as accurate as desired with the parameter taking values in the whole interval, by choosing a sufficiently fine grid and high order. More precisely, it is not necessary to choose a priori the region of convergence of the expansion, as in the Taylor case, but, as long as there are no singularities on the real axis, it is possible to perform the computation for an arbitrary interval of variability, and the coefficient of the Chebyshev expansion will adapt to the region analiticity, according to the statement of Theorem 2.1. As we have seen in the experiments performed in [AG], we expect that the region of analyticity shrinks to a narrow strip around the interval $[-1, 1]$ in the rescaled parameter, when the grid is refined. The table below shows the estimated values of ρ (see the definition of B_ρ in Section 2) for the function representing the density computed in the middle of the shock wave, for different grids.

N	ρ
400	1.0095
600	0.7714
800	0.6180
1000	0.5177

Since $\sinh \rho$ is the length of the semiaxis of the ellipse of convergence, it is quite evident that such region shrinks when a finer grid is used. Furthermore, since the coefficients of the expansion are roughly bounded by $Ce^{-\rho k}$, it is also clear that a finer grid will require a higher order, to mantain a desired maximal error.

Figure (2) shows the reconstruction of density at $\xi = -1$ and $t = T$ for $N = 200, 400, 600, 800, 1000$ with an expansion of order 10.

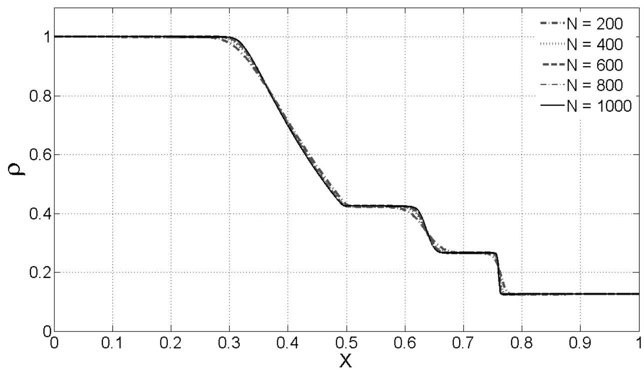

Figure 2: Density reconstruction at $\gamma = 7/5$ and $t = T$ with different grids

It turns out that the Chebyshev expansion can provide an accurate description of the discontinuity when γ ranges in the whole interval, with a maximum error $\epsilon(t, x) \leq 10^{-3}$ and a spatial discretization $N = 1000$.

We can also enlarge the interval of variability of the parameter γ to take in account poliatomic gas characterized by $\gamma = 9/7$. Figure 3 shows the physical variables reconstruction for monoatomic ($\gamma = 5/3$), biatomic ($\gamma = 7/5$) and poliatomic ($\gamma = 9/7$) gases at time $t = T$ with $N = 1000$. Note that, while the speed of the waves is not dramatically different for different values of γ, it is nonetheless evident that there are points where each of the waves has already passed, or has not arrived yet, depending on the value of the parameter.

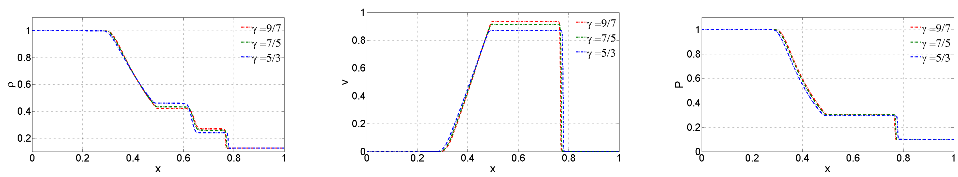

Figure 3: The physical variables for $\gamma = 5/3$, $\gamma = 7/5$ and $\gamma = 9/7$, at $t = T$

5 A more challenging test

In order to better show the performance of the Chebyshev expansion, we change example test. We still consider the shock tube as before. Again we test a pipe of length 1 that we discretize in 500 cells and we choose a time step corresponding to Courant number equal to 0.9. But now the parameter is the initial pressure: more precisely we set

$$p^0(x,\xi) = \begin{cases} 0.75 + 0.25\xi & \text{if } x \leq 1/2 \\ 0.75 - 0.25\xi & \text{if } x > 1/2 \end{cases}$$

with $\xi \in [-1,1]$. We also set $v^0(x) = 0$ for $x \in [0,1]$ and we choose $\rho^0(x)$ satisfying isothermal conditions.

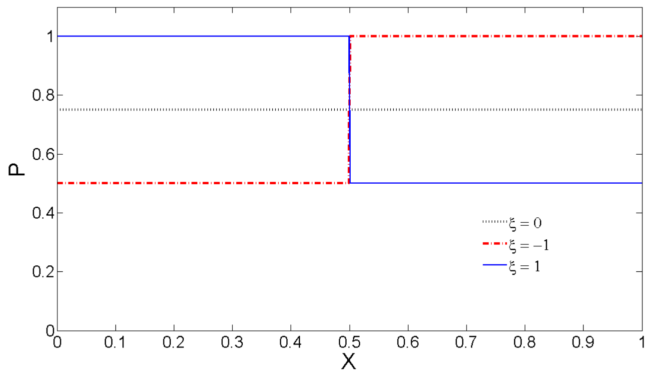

Figure 4: Initial condition on the pressure, with $\xi = -1, 0, 1$.

Figure 4 shows the initial condition on the pressure for $\xi = 0$ (green line), $\xi = -1$ (red line) and $\xi = 1$ (blue line). These initial conditions imply that the rarefaction, contact and shock waves propagate in both directions, to the left and to the right, depending on the value of ξ. Note that for $\xi = 0$ we have the steady state solution with no waves at all.

We recall that the eigenvalues of the Jacobian matrix $f'(u)$ of the system of the Euler equations are

$$\lambda_1 = v - c, \quad \lambda_2 = v, \quad \lambda_3 = v + c.$$

Then, with the initial conditions defined above, the eigenvalue λ_2 assumes both positive and negative values for different values of ξ. This is a potential problem with Roe's algorithm, since it determines the numeric flux at the cell interfaces by treating the positive and the negative eigenvalues (and corresponding eigenspaces) separately. More precisely, the algorithm requires the implementation of the function "positive part", defined by $x^+ = \frac{|x|+x}{2}$, and since we are using

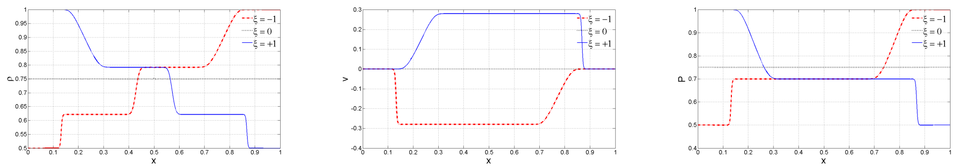

Figure 5: Physical variables reconstruction through evaluation of Chebyshev expansion for $\xi = -1$, $\xi = 0$ and $\xi = 1$ at time $t = T$.

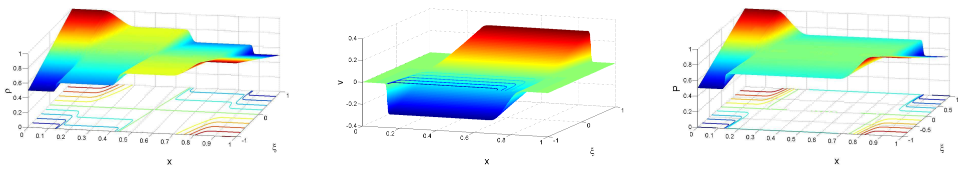

Figure 6: Physical variables evaluated by a Chebyshev expansion of order $k = 20$, for all values of ξ at time $t = T$.

Chebyshev expansions instead of numbers, we need to be able to compute the expansion of $f^+(x)$, given the expansion of $f(x)$. This can be easily achieved by taking into account that the coefficients of a Chebyshev expansion of a function $f : [-1, 1] \to \mathbb{R}$ can be computed by

$$\tilde{f}_k = \frac{2}{n d_k} \sum_{j=0}^{n} \frac{1}{d_j} \cos\left(\frac{kj\pi}{n}\right) f\left(-\cos\left(\frac{\pi j}{n}\right)\right),$$

with $d_0 = d_n = 2$ and $d_j = 1$ otherwise.

Figures 5 and 6 show the physical variables value at time $t = T$ obtained through evaluation of order $k = 20$ of the Chebyshev expansion at $\xi = -1, 0, 1$ and for all ξ respectively. Note that, with the same numerical integration, we can describe with a good accuracy three completely different configurations at each point x along the tube: the rarefaction wave, the shock wave and the steady state condition. Moreover we can describe in the same simulation discontinuities that travel in opposite directions depending on the value of the parameter.

6 Conclusion

In this paper we extended the results obtained in [AG] by considering truncated Chebyshev series instead of truncated Taylor series. The numerical complexity of these approaches is very similar, with a slight advantage for the Taylor expansion, due to a simpler formula for the multiplication of a Taylor series. Also, the Taylor series has the advantage of providing directly the values of the derivatives of the functions under consideration, and for this reason it looks more useful e.g. for sensitivity analyses. On the other hand, the Chebyshev expansion is much more powerful when one wishes to be able to represent sharp discontinuities (which will nonetheless appear smoothed by the numerical discretization), or when one need to compose the expansion with a less than smooth function (such as the positive part used in Roe's algorithm). In these cases, by choosing a sufficiently high order, it is possible to obtain an approximation as good as required.

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