Application of the Chebyshev pseudospectral method to van der Waals fluids

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A B S T R A C T

In this paper, we consider a class of van der Waals flows with non-convex flux functions. In these flows, nonclassical under-compressive shock waves can develop. Such waves, which are characterized by kinetic functions, violate classical entropy conditions. We propose to use a Chebyshev pseudospectral method for solving the governing equations. A comparison of the results of this method with very high-order (up to 10th-order accurate) finite difference schemes is presented, which shows that the proposed method leads to a lower level of numerical oscillations than other high-order finite difference schemes and also does not exhibit fast-traveling packages of short waves which are usually observed in high-order finite difference methods. The proposed method can thus successfully capture various complex regimes of waves and phase transitions in both elliptic and hyperbolic regimes.

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1. Introduction

Many problems in fluid mechanics and material sciences deal with liquid–vapor flows. In these flows, the ideal gas assumption is not accurate and the van der Waals equation of state is usually used. This equation of state is non-convex and causes the solution domain to have two hyperbolic regions separated by an elliptic region. Therefore, the governing equations of these flows have a mixed elliptic–hyperbolic nature.

Slemrod [8] investigated self-similar approximations to the Riemann problem. Considering a Riemann problem with left- and right-hand states in the hyperbolic regions of the solution, the standard entropy criterion for purely hyperbolic systems cannot be used to detect unphysical solutions for these flows. This is due to the possible presence of non-classical shock waves, namely phase boundaries, which violate the standard entropy criterion (see e.g., [4]). A special condition, the so-called kinetic relation, is needed to uniquely specify the solution.

Numerical modeling of these flows is a challenging problem. In particular, numerical methods may lead to inaccurate kinetic functions [5] for these flows, as is also shown in [4], using analysis of the modified equation. The present paper focuses on the quest for numerical methods able to deal with the mixed nature of the governing system of differential equations of these fluids. From the numerical point of view, the solution of this class of Riemann problem can be approached by augmenting the momentum equation with a viscous term as well as a dispersive term representing capillarity. However, the calculated kinetic function is sensitive to the ratio of numerical diffusion to numerical dispersion. Numerical oscillations usually appear with standard finite-difference space discretization schemes, and they persist when the order of accuracy of the semi-discrete scheme is increased. Such dispersive numerical oscillations can affect the accuracy of the numerical solution. Another problem arises from the elliptic part of the solution domain, which is very sensitive to small perturbations. From a physical point of view, it represents phase separation.

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In many problems in fluid mechanics only a low level of numerical diffusion is acceptable, such as in direct numerical simulations of turbulent flows. For such cases, spectral methods are usually preferred because of their high level of accuracy (see e.g., [6]). The two main groups of spectral methods which have been widely used in fluid mechanics are the Fourier and Chebyshev methods. In Fourier spectral methods, the basis functions are trigonometric functions, and therefore they are mainly used for periodic boundaries. On the other hand, in Chebyshev spectral methods, polynomials are used as basis functions, and are more popular for non-periodic boundaries. Generally in such methods, by adding a grid point the numerical error is reduced for two reasons, the reduction of grid size and the increase in the order of accuracy, because the degree of approximating polynomials increases. The numerical kinetic function associated with various high-order schemes for van der Waals fluids was calculated in [5], and they showed that the accuracy of the kinetic function increases by increasing the order of accuracy of spatial discretization schemes. Therefore, due to their high order of accuracy and in accordance with the conclusion of LeFloch and Mohammadian [5], the Chebyshev spectral method could be a good numerical method for modeling nonclassical shock waves and phase transition boundaries. In most nonlinear problems, direct application of spectral methods is not possible, and so pseudospectral methods are used instead. In such methods, the derivatives are calculated in the space of basis functions but the nonlinear terms are calculated in the physical space by transforming the calculated derivatives back from the space of basis functions to the physical space.

The objective of this paper is to evaluate the performance of the Chebyshev pseudospectral methods for van der Waals flows. This paper is structured as follows. The model equations are reviewed in Section 2, the Chebyshev pseudospectral method for numerical approximation of derivatives is presented in Section 3, and numerical experiments and comparisons with high-order finite difference methods are covered in Section 4. Some concluding remarks complete the study.

2. van der Waals fluids

With van der Waals fluids, the governing conservation laws may be written as:

\[ \begin{align*}
\partial_t \tau - \partial_t u &= 0, \\
\partial_t u + \partial_x p(\tau) &= \epsilon \partial_x u - \chi \epsilon^2 \partial_x \tau,
\end{align*} \]

(1)

where \( \tau \) is the specific volume of the fluid, \( u \) is the velocity of the fluid, \( \epsilon \) and \( \chi \) are respectively the viscosity and dispersion (capillarity) coefficients, and \( p \) is the pressure. The pressure can be expressed as a function of the specific volume of the fluid \( p = p(\tau) \) defined for \( \tau > 0 \). Note that the equations of motion have been linearized, since the system is assumed to be near critical. The pressure function in van der Waals fluids is characterized by two properties

\[ \lim_{\tau \to 0} p(\tau) = +\infty, \]

(2)

\[ \lim_{\tau \to +\infty} p(\tau) = 0, \]

(3)

and there exist two positive numbers, \( a \) and \( c \), such that \( 0 < a < c \) and,

\[ \begin{align*}
p''(\tau) &> 0, \quad \tau \in (0, a) \cup (c, +\infty), \\
p''(\tau) &< 0, \quad \tau \in (a, c), \\
p'(a) &> 0.
\end{align*} \]

(4)

As mentioned before, in the absence of diffusion and dispersion terms, the system (1) has a mixed elliptic-hyperbolic behavior. Assuming that there exist two positive numbers \( d \) and \( e \) such that

\[ p'(d) = p'(e) = 0 \]

and \( 0 < d < e < c \), then this system is elliptic for \( d < \tau < e \), where \( p'(\tau) \) is positive, and otherwise it is hyperbolic. Note that \( p'(\tau) \) is negative in the hyperbolic regime, and the system in that case has two left- and right-wave speeds, given by \( \sqrt{-p'(\tau)} \) and \( -\sqrt{-p'(\tau)} \).

As mentioned before, from a mathematical viewpoint the van der Waals system is a very special one because the pressure function has two inflection points. In a series of numerical experiments, LeFloch and Mohammadian [5] showed that the solutions of the van der Waals system are not unique, and the system may have several solutions. Indeed, the kinetic function for this system may be non-monotonic and non-single-valued [5]. That is, multiple intermediate states can exist for a given right-side state of the Riemann problem.

In this paper, as in [5], a pressure equation which has the same form as that of the van der Waals fluids is considered, which is written as

\[ p(\tau) := \frac{RT}{(\tau - \frac{1}{3})} - \frac{3}{\tau^2}, \]

(5)

with \( R = \frac{3}{2} \) and \( T = 1.005 \). As shown in Fig. 1, this flux function has two inflection points, at \( \tau = 1.00996 \) and \( 1.8515 \). Note that in the above equation, the variables (i.e., specific volume, temperature and pressure) denote their reduced value; i.e., their ratio with their critical value.
The solutions of the Riemann problem for the van der Waals system were numerically studied in [5] with the above pressure function. They identified three different regimes. In the first regime (regime A), a stationary shock wave is produced at the center, where the initial discontinuity is located. In the second regime (regime B), a nonclassical left-going non-stationary shock wave is generated. By increasing the velocity at the left-hand state of the Riemann problem, the shock wave speed decreases, and the kinetic function in this case is neither single-valued nor monotonic. In the third regime (regime C), a non-classical, non-stationary, left-going shock wave is generated. The left and right states of this shock wave are constant and are equal to the limiting values of regime B.

3. Numerical method

3.1. Space discretization scheme

In this paper we use the Gauss–Chebyshev–Lobatto (GCL) points for the positioning of unevenly spaced grid points for polynomial expansion

\[ x_j = \cos(j\pi/N), \quad j = 0, 1, \ldots, N. \] (6)

These points are the projections of equispaced points on the upper half of the unit circle onto \([-1, 1]\) over \(N + 1\) grid points. Note that in usual Fourier methods an even number of grid points are used. However, with Chebyshev polynomials, \(N\) could be odd or even. The numerical derivative of a grid function (here, the numerical flux) defined on the GCL points is calculated in two steps in the Chebyshev spectral method. In the first step, given the grid function on the Chebyshev points, the unique polynomial \(p\) of degree \(\leq N\) is constructed such that

\[ p(x_j) = w_j, \quad j = 0, \ldots, N, \] (7)

where

\[ w_j = \omega(x_j). \] (8)

The derivative of this polynomial \(p'(x)\) is calculated on grid points in the second step. As an essential feature of the Chebyshev polynomial method, the two steps can be efficiently combined in a single matrix form to calculate the derivative at grid points

\[ p'_N = D_N \omega, \] (9)

where

\[ p'_N = (p'(x_0), p'(x_0), \ldots, p'(x_N)), \] (10)

\[ \omega = (\omega(x_0), \omega(x_1), \ldots, \omega(x_N)), \] (11)

and \(D_N\) is the Chebyshev spectral differential matrix; an \((N + 1) \times (N + 1)\) matrix given by
where

\[
(D_N)_{00} = \frac{2N^2 + 1}{6},
\]

\[
(D_N)_{NN} = -\frac{2N^2 + 1}{6},
\]

\[
(D_N)_{ji} = \frac{-x_j}{2(1-x^2)}; \quad j = 1, \ldots, N - 1,
\]

\[
(D_N)_{ij} = \frac{C_j}{C_i} \left( \frac{-1}{x_i - x_j} \right)^i \quad i \neq j, \quad i, j = 0, \ldots, N,
\]

with

\[
C_i = \begin{cases} 
2, & i = 0 \text{ or } N, \\
1, & \text{otherwise}.
\end{cases}
\]

Note that the jth column of \( D_N \) corresponds to the derivative of polynomial interpolant \( p_j(x) \) of degree \( N \) to the delta function supported at \( x_j \), which is sampled at the GCL points \( x_j \) [9]. For \( N = 2 \), the differentiation matrix becomes

\[
D_2 = \begin{bmatrix}
\frac{3}{2} & -2 & \frac{1}{2} \\
\frac{1}{2} & 0 & -\frac{1}{2} \\
-\frac{1}{2} & 2 & -\frac{3}{2}
\end{bmatrix},
\]

where its first, second, and third rows, respectively, represent standard 2nd-order forward, centered, and backward finite difference schemes. The coefficients of higher-order Chebyshev spectral differentiation matrices also represent high-order finite difference methods on uneven grids. This is due to the fact that the Chebyshev method is a polynomial expansion over GCL points, and the polynomial expansions are unique.

The off-diagonal entries of \( D_N \) are calculated using (16). However, the diagonal components are usually calculated using an alternative formula

\[
(D_N)_{ii} = -\sum_{j=0}^{N} (D_N)_{ij}.
\]

This method reduces the instability of calculations due to rounding errors [1,2]. A derivation of (19) can be found in [9].

Note that the position of the GCL points and the corresponding matrix \( D_N \) do not change with time and therefore they need be calculated only once, at the beginning of calculations. Although the above formulas are given for the interval \([-1, 1]\), by a simple change of variables they could be also used for an interval \([0, L]\). In this paper, the above procedure is used for calculation of flux derivatives in the van der Waals system. However, the derivatives required to calculate the fluxes are obtained using the standard centered 4th-order finite difference scheme.

### 3.2. Time Marching Algorithm

In this paper, a Runge–Kutta scheme is employed for time integration of the semi-discretized system. For a vector \( U(t) \) defined by \( U(t) = (u_i(t))_{i=1}^{n} \), the semi-discretized scheme may be written as

\[
\frac{dU}{dt} = R[U(t)],
\]

where \( R[U(t)] \) is the right-hand side of the van der Waals system discretized using either a finite difference or a Chebyshev pseudospectral method. The resulting system of ordinary differential equations may be numerically solved by an s-stage Runge–Kutta scheme, given by

\[
g^k = R \left( U^n + \Delta t \sum_{j=1}^{k-1} a_{kj} g^j \right),
\]

\[
U^{n+1} := U^n + \Delta t \sum_{k=1}^{s} b_k g^k.
\]
In this study, a 4th-order Runge–Kutta scheme is used for temporal integration for which the non-zero coefficients are given by:

\[
a_{21} = 1/2, \quad a_{32} = 1/2, \quad a_{43} = 1, \quad b_1 = 1/6, \quad b_2 = 1/3, \quad b_3 = 1/3, \quad b_4 = 1/6.
\]  

(22)

Here, we also use the finite difference method used by LeFloch and Mohammadian [5] in order to evaluate the performance of the Chebyshev pseudospectral method. The corresponding discretized forms are briefly reviewed here. We represent the grid points by \( x_i \) and the approximated solution at those grid points by \( u_i \). Also, \( f_i \) corresponds to the value of the flux function at the grid points \( f(u_i) \). The semi-discrete schemes for the grid functions \( u_i = u_i(t) \) can be calculated with these notations by using standard finite difference methods or the pseudospectral scheme as given in the following. The 4th-order finite difference is written as

\[
\frac{du_i}{dt} = -\frac{1}{h} \left( \frac{1}{12} f_{i-2} - \frac{2}{3} f_{i-1} + \frac{2}{3} f_{i+1} - \frac{1}{12} f_{i+2} \right) + \frac{\epsilon}{h} \left( -\frac{1}{12} u_{i-2} + \frac{4}{3} u_{i-1} - \frac{5}{2} u_i + \frac{4}{3} u_{i+1} - \frac{1}{12} u_{i+2} \right) + \frac{2\epsilon^2}{h} \left( -\frac{1}{2} u_{i-2} + u_{i-1} - u_{i+1} + \frac{1}{2} u_{i+2} \right),
\]  

(23)

Fig. 2. Velocity and specific volume using the 2nd-order finite difference method.

Fig. 3. Velocity and specific volume using the 4th-order finite difference method.
where $h$ represents the grid size. It should be mentioned that the above system is fully conservative, e.g., with periodic boundary conditions. That is, $\sum \dot{u}_i(t)$ does not change in the absence of the boundary effects.

For completeness, the employed higher-order finite difference methods are also presented in the following.

The 4th-order discretization method is given by

$$hf_x = \frac{1}{12} f_{i-2} - \frac{2}{3} f_{i-1} + \frac{2}{3} f_{i+1} - \frac{1}{12} f_{i+2},$$

the 6th-order discretization scheme leads to

$$hf_x = -\frac{1}{60} f_{i-3} + \frac{3}{20} f_{i-2} - \frac{3}{4} f_{i-1} + \frac{3}{4} f_{i+1} - \frac{3}{20} f_{i+2} + \frac{1}{60} f_{i+3},$$

the 8th-order finite difference method has the following form

$$hf_x = \frac{1}{280} f_{i-4} - \frac{4}{105} f_{i-3} + \frac{1}{5} f_{i-2} - \frac{4}{5} f_{i-1} + \frac{4}{5} f_{i+1} - \frac{1}{5} f_{i+2} + \frac{4}{105} f_{i+3} - \frac{1}{280} f_{i+4}.$$

Fig. 4. Velocity and specific volume using the 6th-order finite difference method.

Fig. 5. Velocity and specific volume using the 8th-order finite difference method.
and the 10th-order finite difference method leads to

\[
h_{10} = -\frac{1}{1260} f_{-5} + \frac{5}{504} f_{-4} - \frac{5}{84} f_{-3} + \frac{5}{27} f_{-2} - \frac{5}{6} f_{-1} + \frac{5}{6} f_{0} + \frac{5}{84} f_{1} - \frac{5}{27} f_{2} + \frac{5}{6} f_{3} - \frac{5}{84} f_{4} + \frac{1}{1260} f_{5}.
\]

4. Numerical experiments

Here, two numerical experiments are performed to verify the performance of the pseudospectral method. In the first test case, the left and right states correspond to the hyperbolic regime, while the second test case deals with the performance of the scheme in the elliptic regime. In both test cases, boundaries are located far enough away that the waves do not reach the boundaries, and the influence of boundaries is thus avoided.

4.1. Test 1

In the first test case we consider a Riemann problem with the following left- and right-hand states:

\[
\begin{align*}
\tau_L &= 0.8, \\
\tau_R &= 2,
\end{align*}
\]

where subscripts \(R\) and \(L\) respectively represent right- and left-hand states. With the above values, the two inflection points of the pressure function are between the left- and right-hand states. The numerical modeling is conducted up to \(t = 0.065\) with a time-step of \(0.000042\) (non-dimensional units) and 700 grid points. The viscosity and dispersion coefficients were fixed to \(\epsilon = 5 \times 10^{-5}\) and \(\alpha = 10\) for all schemes. A sensitivity analysis regarding these parameters will be presented in the following. The above initial values lead to a right-going classical shock wave and a left-going rarefaction followed by a left-going non-classical shock wave, which makes this test case a challenging one for numerical methods. Figs. 2–6 show the velocity and specific volume profiles calculated by the 2nd-, 4th-, 6th-, 8th-, and 10th-order finite difference schemes respectively. The 2nd-order scheme, as observed in Fig. 2, leads to a high level of numerical oscillations. Moreover, the distinct intermediate region is not well represented in this scheme. The numerical oscillations are reduced and become more compact as the order of accuracy increases, as was also reported in [5]. All schemes lead to two fast noise structures going towards the left- and right-hand boundaries ahead of the rarefaction and shock waves. The results of the Chebyshev pseudospectral method are shown in Fig. 7. The pseudospectral method performs better than all other employed finite difference schemes and does not lead to fast short-wave noise packages which move to the right- and left-hand sides. Such an improvement in the results can be justified by the fact that the order of accuracy of the pseudospectral method is much higher than that of all other employed finite difference schemes. These results confirm the conjecture proposed in [5], which stated that the numerical solution converges with the analytical one by increasing the order of accuracy.

In order to observe the impact of the dispersion coefficient, a sensitivity analysis was performed. The value of the velocity at the middle state is shown in Fig. 8, where the dispersion coefficient is kept constant at \(\alpha = 10\) and the viscosity coefficient is variable. It is clear from this figure that the results of all schemes converge as the dispersion coefficient increases, and the value of \(\epsilon = 5 \times 10^{-5}\) may be considered as the typical value at which the results of higher-order schemes become very close. It is also observed that as the order of accuracy increases, the numerical methods converge, and the Chebyshev
pseudospectral scheme is the closest one to the limiting value. The fast noise structures are always present in the results of finite difference schemes (not shown), which is not the case for the Chebyshev pseudospectral method. Similar behavior is observed for $\alpha = 5$ and $\alpha = 1$, although the value of the intermediate state depends on $\alpha$. Therefore, it can be concluded that the Chebyshev pseudospectral method performs better than the other schemes over a large range of diffusion and dispersion coefficients.

Finally, it should be mentioned that in order to reduce dispersive oscillations within a finite-difference approach, a change of variables is proposed in [3], and more recently in [7]. This approach may be also possible with the Chebyshev pseudospectral method and is the subject of a future study.

4.2. Test 2

In the second case, we consider the following initial left and right states:

- $u_L = 0.1$, $\tau_L = 1.2$,
- $u_R = -0.1$, $\tau_R = 1.2$

![Fig. 7. Velocity and specific volume using the Chebyshev pseudospectral method.](image)

![Fig. 8. The value of the velocity at the middle state versus dispersion coefficient at $\alpha = 10$.](image)
Note that the initial specific volume is 1.2, which is in the elliptic region. Since $u_L > 0$ and $u_R < 0$, the above initial condition shows two streams that are colliding. Therefore, the specific volume after the collision should decrease in the intermediate region after the collision and a liquid phase may form. Therefore, the solution should consist of two shock waves followed by two phase transition boundaries moving outward. The numerical results using the Chebyshev pseudospectral method at time $t = 0.5$ using a time-step of 0.0001 with 700 grid points are shown in Fig. 9. Viscosity and dispersion coefficients were fixed to the same values of Test 1, $(\epsilon = 5 \times 10^{-5}$ and $\alpha = 10)$. As is observed, the Chebyshev pseudospectral method shows excellent performance and can efficiently capture both shock waves and phase transition boundaries with no significant numerical oscillations.

5. Conclusion

In this paper, the use of the Chebyshev pseudospectral method was proposed for a class of van der Waals flows with mixed hyperbolic–elliptic behavior. Such systems allow for undercompressive non-classical shock waves whose kinetic functions may be non-monotonic and non-single-valued. The numerical results of the Chebyshev pseudospectral method were compared with the high-order finite difference schemes (up to 10th-order) illustrated in [5], which showed that the proposed method leads to better results. The pseudospectral method performs better than all other employed finite difference schemes, with a lower level of numerical diffusion and oscillations. Moreover, it does not lead to fast short-wave noise packages which move to the right- and left-hand sides ahead of the rarefaction and shock waves, which is typically observed in finite difference schemes.

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References