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IRREVERSIBILITY IN REVERSIBLE SYSTEMS I: THE COMPRESSIBLE EULER EQUATIONS IN 1D

JOHAN HOFFMAN AND CLAES JOHNSON

Abstract. This is the first part of a series, where we present a new approach to resolving the classical paradox of irreversibility in reversible Hamiltonian systems. We base our solution on finite precision computation in the form of General Galerkin G2, instead of statistical mechanics. In the present Part I we consider as Hamiltonian model the Euler equations for an inviscid compressible perfect gas with focus on model problems in one space dimension. We show that the irreversibility arsises because G2 reacts by introducing a dissipative weighted least squares control of the residual if the Euler equations lack solutions with pointwise vanishing residual, which is the general case because of the appearance of shocks and/or turbulence. In particular, we prove that the Second Law of Thermodynamics is a consequence of the First Law of Thermodynamics combined with G2 finite precision computation.

1. Introduction

There are great physicists who have not understood it.
(Einstein about Boltzmann's statistical mechanics)

This is the first part of a series, where we present a new approach to resolving the classical paradox of irreversibility in reversible Hamiltonian systems. We base our solution on finite precision computation instead of statistical mechanics, which is the standard approach. We thus stay within a deterministic Hamiltonian framework and only add a restriction of finite precision computation, and we do not use any form of statistics. A World governed by Hamiltonian mechanics combined with finite precision computation, follows the laws of mechanics as far as possible taking the finite precision into account, but is not a game of roulette as in statistical mechanics. The difference of scientific paradigm is fundamental. Einstein expresses his reservation to statistical mechanics in: *God does not play dice.* We seek to follow this device ourselves.

In the present Part I we choose as Hamiltonian model the Euler equations for an inviscid compressible perfect gas with focus on model problems in one space dimension. In Part II we consider the Euler equations for incompressible inviscid flow in three dimensions,

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and expand to compressible flow in Part III. We continue in Part IV with a study of the kinetic theory of gases. We hope to ultimately approach also quantuum mechanics using the same computational deterministic point of view, again avoiding the conventional statistical interpretation. In the present introductory Part I, we expose the basic ideas, with a certain amount of repetion, from different perspectives with the hope of this way reaching a broader audience also outside computational mathematics.

The origins of irreversibility in reversible systems is a main unsolved mystery of mechanics and physics. A Hamiltonian system is reversible in time and does not have a preferred (forward) direction of time: From a given configuration both the future and past are equally well determined. The reversibility follows from the invariance of a Hamiltonian system under a change of sign of time and velocity. It follows in particular that letting a Hamiltonian system evolve in time from an initial configuration to a final configuration and there reversing the velocity and changing the direction of time, will bring the system back to the initial configuration. As a result, one may in Hamiltonian mechanics construct a perpetuum mobile of the first kind, which is a machine that will run forever without consuming any energy. Both celestial mechanics and quantum mechanics are Hamiltonian and the motion of the planets in our Solar system as well as the electrons in an atom represent reversible perpetuum mobile of the first kind.

On the other hand, in the real World there is a preferred direction of time and we are all familiar with irreversible processess in which initial configurations cannot be recovered, and the impossibility of constructing a perpetuum mobile of the first kind, as well as of the second kind supposed to reversibly convert energy back and forth from heat to mechanical work without consuming any net energy. The irreversibility is expressed in the Second Law of Thermodynamics, which states that in an isolated system a certain scalar quantity, named *entropy*, cannot decrease with time. As a consequence, an isolated system becomes irreversible if its entropy increases, since time reversal would correspond to decreasing entropy, which is impossible. In a Hamiltonian system the entropy is equal to minus the total energy being the sum of kinetic and potential energy, and energy conservation reflects reversibilty and entropy constancy. The observation that a perpetuum mobile of the second kind seems impossible, because converting mechanical energy into heat does not seem to be fully reversible, indicates the existence of real processes which are irreversible and thus not Hamiltonian. Dropping a stone to the ground will convert its potential energy into heat making the stone warmer, but the reverse process of the stone lifting itself by getting colder, is impossible. The question is why?

So if now the World ultimately is governed by reversible Hamiltonian (quantuum) mechanics, the scientific challenge thus becomes to explain how irreversibility may arise in systems based on reversible Hamiltonian mechanics. In the late 19th century when the existence of an Aether filling empty space was still contemplated, the irreversibilty was suggested to possibly result from some small viscosity of the Aether, but since no one could ever detect any Aether, this belief faded. Similarly, the idea of putting in just a tiny bit of friction (coming from somewhere) to explain irreversibility, is not convincing, since then the planets and electrons would be constantly retarding a little bit, but they don't seem to do that. And if there would be some friction in some system, the challenge would be to explain how friction can arise in a system governed by Hamiltonian reversible mechanics without friction. Thus the irreversibility paradox can be phrazed: How can there be friction in a system without friction?

Another attempt to explain irreversibility in a macroscopic system based on reversible microscopic mechanics, claims that irreversibility is simply a result of perspective, where the macroscopic irreversibility would be a consequence of a (possibly subjective) macroscopic view. The basic principle is then stated as an irreversible tendency of a macroscopic system to proceed from ordered to less ordered states, for some reason yet to explain, while microscopically the same system would be reversible. Moreover, the subjectivity in this approach does not harmonize well with a desired scientific objectivity. Although this type of reasoning has become quite popular, it does have several weak points, as indicated. In particular, no answer is offered to the question how initial ordered states can occur, if progress always is towards less order.

In Boltzmann's kinetic theory of gases the mystery shows up in the form of Loschmidts paradox: Kinetic theory is based on a model of a gas as a reversible Hamiltonian system of very many molecules in the form of very small rigid spheres interacting by elastic collisions, yet Boltzmann's equation is irreversible. ¿From Translators Foreword to Lectures on Gas Theory by Boltzmann [2], we cite: *There is apparently a contradiction between the law of increasing entropy and the principles of Newtonian mechanics, since the latter do not recognize any difference between past and future times. This is the so-called reversibility paradox which was advanced as an objection to Boltzmann's theory by Loschmidt 1876-77.*

Loschmidts paradox forced Boltzmann to invent statistical mechanics, which is an expansion of deterministic Hamiltonian mechanics using concepts from statistics and probability. In expanding Hamiltonian deterministic mechanics by statistics, Boltzmann assumed that a gas as a system of elastically colliding rigid spheres, would tend to evolve from less probable towards more probable states, which would define a preferred direction of time and result in irreversibility. The assumption of Boltzmann can alternatively be expressed as statistical independence of molecules before collisions, but not after, which again defines a preferred direction of time and results in irreversibility. In Boltzmann's words from [2] the assumption is formulated: *Each molecule flies from one collision to another one so far away that one can consider the occurence of another molecule, at the place where it collides the second time, with a definite state of motion, as being an event completely independent (for statistical calculations) of the place from which the first molecule came (and similarly for the state of motion of the first molecule).*

Cercigniani writes in his Boltzmann biography [1]: *The answer to Loschmidt's paradox is roughly as follows: If one obeys the laws of mechanics, one can use the equation to "predict" either the future or the past. When deriving the Boltzmann equation we expressed the distribution functions corresponding to an aftercollision state in terms of the distribution function corresponding to the state before the collision, rather than the latter in terms of the former. It is clear, however, that that this choice introduced a connection with the everyday concepts of past an future which are extraneous to molecular dynamics. In other words, we prepared the way to a definition of these concepts on the basis of the statistical behaviour of many-particle systems.*

The irreversibility is expressed in Boltzmann's famous H-Theorem stating that a certain scalar quantity denoted by H (which with a change of sign is an entropy) defined for a solution to Boltzmann's equation, cannot increase. Boltzmann claims in response to Loschmidts paradox: *If at an intermediate stage we reverse all velocities, we get an exceptional state where H increases for a certain time and decreases again. But the existence of such cases does not disprove our theorem. On the contrary the theory of probablity iteself shows that the probability of such cases is not mathematically zero, only extremely small.*

In the Stanford Encyclopedia of Philosophy we read: *Boltzmann's responses to the reversibility objections are not easy to make sense of, and varied in the course of time. In his immediate response to Loschmidt he acknowledges that certain initial states of the gas would lead to an incraese of the H-function, and hence a violation of the H-Theorem. The crux of this rebuttal was that such initial states were extremely improbable, and could safely be ignored.... This rebuttal is far from satisfactory.*

Boltzmann's statistical mechanics was met with much scepticism by e.g. Maxwell and Einstein. Maxwell states: *By the study of Boltzmann I have been unable to understand him. He could not understand me on account of my shortness, and his length was and is an equal stumbling-block to me. Hence I am very much obliged to join the glorious company of supplanters and to put the whole business in about six lines.* Einstein expresses his reservations in the quote in the Introduction. Neither could Karl Popper accept the idea of explaining irreversibility by statistical mechanics and suggested instead a connection to radiation, but did not develop convincing details.

Boltzmann's idea about natures preference to move from less towards more probable states seems to be seriously circular (a motion from a probable to a less probable state would not seem very probable, would it?), and Boltzmann's assumption of statistical independence before collision (also referred to as "molecular chaos"), has been difficult to either verify or disprove. However, today it should be possible to check if Boltzmann's assumption is valid or not by very careful computation in Hamiltonian particle systems, and we will present the results of such a study in [9]. Moreover, the fact that even Boltzmann himself acknowledges that his H-theorem sometimes is violated, although he claims this only can occur for very special (rare) inititial conditions, of course is potentially catastrophical from a scientific point of view. If Newton's apple occasionally would not fall down, there would seem to be some serious flaw in his universal theory of gravitation. Neverheless, lacking any other convincing explanation of the appearance of irreversibility in reversible systems, statistical mechanics has not only survived into our time, but also opened the way to the statististical interpretation of quantuum mechanics with the modulus of the wave function squared supposedly expressing the probability of finding electrons at specific locations in space/time.

In 1993 Evans, Cohen and Morriss tackled the paradox in their Fluctuation Theorem again using statistical methods. Evans et al suggest that the Second Law may be violated for small microscopic systems, while it would still hold macroscopically for large systems with a very high probability.

Altogether, as far as we can understand, the true origins of irreversibility in reversible systems has not been given a scientifically convincing explanation. The literature is vast with contributions from mathematicians, physicists, chemists, engineers, philosophers, linguists, authors of science fiction and the general public.

2. Finite Precision Computation

We now focus on the new mode of explanation based on finite precision computation, which we advocate. The finite precision computation appears in two forms: First, it necessarily appears in digital solution of Hamiltonian equations using computers. Secondly, it probably appears also in Natures evolution in time from one state to the next in some form of analog computation. In this note we focus on finite precision computation from digital solution of the Hamiltonian equations using computers, but we also speculate about possible forms of finite precision analog computation in Nature.

The solution of the paradox of irreversibility in reversible system based on finite precision computation, is not trivial in the sense that it may be blamed simply on something like round-off errors in digital computing or the inevitable approximations in solving differential equations numerically. This would be similar to explaining irreversibility as an effect of a slightly viscous Aether, a mode of explanation we have already rejected.

The solution of the paradox is much deeper and more fundamental and directly couples to our recent work on computational turbulence exposed in [6]. In short, the secret we uncover is the following: We consider a set of Hamiltonian equations describing the evolution in space/time of a certain system in Nature. We seek to solve the equations computationally using a numerical method implemented on a computer. Doing so we meet two different situations: In the first case, which is the simple standard case without surprise, the Hamiltonian equations have pointwise solutions which are computable, and if so we simply compute these solutions and find them to be reversible. A pointwise solution has a residual which is pointwise zero, obtained by inserting the solution in the equation, and we can compute approximate solutions with residuals being small pointwise. Accordingly, computed solutions are approximately reversible by the reversible nature of the equations they are approximately solving pointwise.

In the second case, which contains the secret, the Hamiltonian equations do not admit pointwise solutions, which means that there simply are no (stable) solutions with residual being zero pointwise. This reflects the appearance of small scale phenomena such as turbulence and/or shocks in the case of inviscid fluid mechanics, which represents a basic example of Hamiltonian mechanics. In this second case the computational method cannot produce an approximate solution with small pointwise residual, and the computational method we are using reacts by producing an approximate solution for which the residual is small in a weak average sense combined with a certain weighted least squares control of the residual, which turns out to be possible to achieve. We refer to the numerical method with this property as General Galerkin or G2. In the case the Hamiltonian equations do not admit pointwise solutions, which may correspond to the appearence of turbulence and/or shocks, G2 thus produces an approximate solution with the residual being small in a weak sense and with a certain weighted least squares control of the size of the pointwise residual, while the pointwise residual itself is not small.

We shall see that this is about the best that can be done in the situtation when the Hamiltonian equations do not admit pointwise solutions, but it turns out to be good enough if we as quantities of interest or output quantities choose certain mean values of the solution, rather than point values. In the case the Hamiltonian equations do not admit pointwise solutions, corresponding to turbulence/shocks, we can thus nevertheless by G2 compute certain mean value outputs accurately. From a physically point of view, we may say that even though the Hamiltonian equations cannot be satisfied pointwise, they can be satisfied in an average sense with the pointwise residual not being too large, and that is enough for the system to evolve. The pointwise violation but average satisfaction of the Hamiltonian laws in this sense, corresponds to a physical system in pointwise non-equilibrium, but in average local equilibrium with some control of the pointwise non-equilibrium. In such a physical system the laws of physics serve as goals, which cannot be satisfied pointwise, and the search of satisfaction in a suitably approximate sense is what drives the evolution of the system. It is like the Law in our society, which is never followed pointwise by all citizens, only in some average sense, but yet has the important role to secure that society does not fall apart.

Now, the catch is that the weighted least squares control of the residual in G2 adds a dissipative term in an energy balance, which effectively makes the system irreversible. It is thus the appearance of turbulent/shock small scales and the resulting impossibility of computing solutions with pointwise small residuals, which necessarily introduces the irreversibility. Facing the impossibility of pointwise solution, the system reacts by producing an approximate solution in which some of the energy is lost in a dissipative least squares term implying irreversibility. Moreover, the size of the dissipation and the energy loss does not decrease with increasing precision: In turbulence the dissipation always occurs on the finest scales available, but the total amount of the turbulent dissipation (turning into heat), stays (approximately) constant under scale refinement. A shock in compressible flow has a similar nature. Mean value outputs thus show an independence of the scale of resolution in the computation, while pointwise solution is impossible even if the computational scale is refined indefinitely.

Our proposal for solution connects to the following scenario presented by the always visionary Leibniz: *I had maintained that the vis viva (live force or momentum) are conserved in the world. It has been objected that in a collision two soft or inelastic bodies would loose their live force. I answer that things are not so. It is true that the bodies as a whole loose it as far as their total motion is concerned, but their parts acquire it, because the collision strength creates an inner agitation. Thus this loss is only apparent. The forces are not destroyed, but everything goes as if somebody wanted to change a coin into smaller pieces.*

The basic idea is thus that in certain Hamiltonian processes necessarily small scale features in the form of turbulence/shocks appear, and when faced with these small unresolvable scales, which physically correspond to heat, the system reacts by introducing a dissipative least squares control of the residual, which implies irreversibility in which the small scales cannot be recovered. Thus, in turbulence/shocks, large scale mechanical energy may be turned into small scale motion, corresponding to generation of heat, and this process is irreversible since the details of the small scales cannot be kept and thus cannot be recovered.

The key here is to realize that the dissipative damping (i) is necessary, (ii) is substantial, (iii) is not a numerical artifact which can be diminished by increasing the precision. The key new fact behind (i)-(iii) is the non-existence of solutions to the Hamiltonian equations!

The appearance of turbulence/shocks in inviscid compressible flow is an example of an irreversible process satisfying (i)-(iii), where inevitably and irreversibly energy is turned into heat. As is well known, a shock solution is not a pointwise solution to the Euler equations. As we will show, neither turbulence corresponds to a pointwise solution.

One may ask why the non-existence of pointwise solutions, has to result in dissipation in approximate solutions? An answer is that anyway this is the way G2 works, and G2 corresponds to a best approximate solution in cases when exact solution is impossible. G2 is designed so as to satisfy the mathematical equations expressing the physical laws in a weak average sense, which is necessary, combined with a weighted least squares control of the pointwise residual, where the weight is chosen so that mean value outputs are maximally correct. Thus, one may say that G2 handles the non-existence of an exact solution as well as possible, and that includes a dissipative least squares control of the pointwise residual. One could of course hope that Nature handles the situation equally well, but further studies to settle this issue are clearly required. At least there is G2 model to look for.

One may view the least squares dissipation as a fine paid because the laws of the system are violated. Necessarily a fine has to represent a postive cost. If we would get paid by breaking the Law, society would quickly collaps.

3. The Second Law of Thermodynamics

We may summarize our results as proving that the Second Law of Thermodynamics is a consequence of the First Law of Thermodynamics (which expresses conservation of energy) combined with finite precision computation. We may thus propose a new foundation of gas dynamics based on deterministic mechanics expressed by the First Law combined with finite precision computation, as opposed to a usual foundation with the Second Law as an additional postulate.

Finite precision computation of course appears in digital solution of the differential equations of deterministic mechanics, but it necessarily also has to appear in some form in the analog computation performed in the physics of the real World. We may analyze the consequences of finite precision computation of digital solution, and then seek to find analogs in physics.

This brings us back to a deterministic World as a giant Clock in the spirit of Laplace, but our Clock has finite precision and that changes the game. In particular, it takes us out of the classical paradox of the existence of free will in a deterministic World. With finite precision computation, the future is no longer fully determined by the present, and there is room for something like a free will. And there are necessarily irreversible processess.

Google gives 160.000 hits searching on "Second Law of Thermodynamics", while "First Law of Thermodynamics" gives 70.000, which gives an indication of the mystery surrounding the Second Law.

4. The Euler Equations for Fluid Flow

The Euler equations for compressible inviscid flow may be viewed to model a very large collection of "fluid particles" following Newton's Second Law subject to a pressure force given by the state equation of a perfect gas. This is a Hamiltonian reversible system, which may formally be obtained by taking moments (averages) of Boltzmann's equation of a gas (with no contribution from the collision term). As a special case we have the Euler equations for an incompressible fluid describing a special flow regime including turbulence but not shocks.

It is known that the compressible Euler equations in general lack pointwise solutions, in particular because shocks develop but also because of turbulence. Neither do the incompressible Euler equations in general have pointwise solutions because of turbulence. Thus, both computation and Nature will have to go for suitable approximate solutions of the Euler equations. Computation will then rely on G2, with presumably Nature resorting to something similar, which inevitable (because of the least squares residual control in G2) will introduce a dissipative effect implying irreversibility.

We thus have a situation, where the equations we want to solve have no exact pointwise solutions (or if they have, then they are unstable), while the turbulent/shock solutions which do exist in fact only are approximate weak solutions and not pointwise solutions, and moreover these approximate solutions necessarily have a dissipative character resulting in irreversibility. The paradox of irreversibility in a formally reversible Hamiltonian system is thus a consequence of the non-existence of stable laminar/shock-free pointwise (strong) solutions to the Euler equations, which would have been reversible if they had only existed, and the dissipative nature of the turbulent/shock approximate weak solutions, which do exist computationally and and for which mean value outputs can be accurately computed.

We note that the non-existence of exact solutions, strong or weak, changes the way mathematics for the Euler equations can be presented: With non-existent exact solutions, the attention has to move to existing approximate solutions, and thus the computational aspect takes a prime position before analytical mathematics.

The non-existence of pointwise solutions to the Euler equations, which may be viewed as a failure of mathematics, in fact may be turned around into an advantage from a computational point of view: If there were an exact solution, one could always ask for more precision in computing this solution requiring finer resolution and higher computational cost, but if there is no exact solution, then we could be relieved from this demand beyond a certain point. A key feature in this situation is that the absolute size of the fine scales no longer are important, and this could save computational work. We know that there are around 10^{23} molecules in a mole of gas, but it is likely that we can computationally model gas dynamics with instead say 10^6 degrees of freedom.

We will also see that the pointwise non-solvability of the inviscid Euler equations reflect the presence of small scale turbulence/shocks in slightly viscous flow, with a passage to the limit of vanishing viscosity being impossible.

In order for a Hamiltonian system to develop turbulence, it has to be rich enough in degrees of freedom. In particular, the incompressible or compressible Euler equations in less than three space dimensions are not rich enough, even if the mesh is very fine. On the other hand, turbulence invariably develops in three dimensions if the viscosity is small or zero. Our experience with turbulent solutions of the incompressible Navier-Stokes equations indicates that a mesh with 100.000 mesh points in space may suffice in simple geometries, while in more complex geometries millions, but not billions, of mesh points may be needed.

5. Compressible Euler Equations in 1d

The Euler equations in one space dimension (1d) modeling the flow of a compressible inviscid perfect gas in an infinite tube along the real axis $\mathbb{R}$, take the following form: Find $u = (\rho, m, e)$ depending on (x, t) such that

$$\begin{array}{rcl} \dot\rho + (w\rho)' &=& 0, \quad x \in \mathbb{R},\ t \in \mathbb{R}_+, \\ \dot m + (wm + p)' &=& 0, \quad x \in \mathbb{R},\ t \in \mathbb{R}_+, \\ \dot e + (we + pw)' &=& 0, \quad x \in \mathbb{R},\ t \in \mathbb{R}_+, \\ u(x, 0) &=& u^0(x) \quad x \in \mathbb{R}, \end{array} \tag{5.1}$$

where $u^0(x)$ is a given initial condition, $\mathbb{R}_+ = \{t \in \mathbb{R} : t > 0\}$, ρ is the density, $m = \rho w$ the momentum with w the velocity, e the total energy being the sum of the kinetic energy $\rho w^2/2$ and the internal energy in the form of heat measured by temperature, and p is the pressure given by the state equations for a perfect gas $p = (\gamma - 1)(e - m^2/(2\rho))$, where $\gamma > 1$ is a constant. Further, $\dot v = \frac{\partial v}{\partial t}$ and $v' = \frac{\partial v}{\partial x}$. We assume that $u(x, t)$ tends to zero as $|x|$ tends to infinity.

The system of equations (5.1) may be written in vector form as

$$\begin{array}{rcl} \dot u + (f(u))' &=& 0, \quad x \in \mathbb{R},\ t \in \mathbb{R}_+, \\ u(x, 0) &=& u^0(x) \quad x \in \mathbb{R}, \end{array} \tag{5.2}$$

where $f(u) = (w\rho, wm + p, we + pw)$ is the flux vector, which expresses conservation of mass, momentum and energy, where the momentum equation corresponds to Newton's Second Law with p' representing the net force on a fluid element from the pressure, and in the energy equation $(pw)'$ represents the work from the pressure acting on a fluid element. Here $w\rho$, wm and we are the convective fluxes of the mass, momentum and energy, and p' and $(pw)'$ are fluxes related to the pressure. We also refer to an equation of the form (5.2) as a conservation law.

The Euler equations (5.2) express conservation in pointwise (strong) form as $R(u) \equiv \dot u + (f(u))' = 0$ in $\mathbb{R} \times \mathbb{R}_+$, asking u to be a differentiable and in particular continuous pointwise solution with residual $R(u)$ vanishing pointwise. The Euler equations are Hamiltonian and formally reversible in the sense that a change of sign of time t and velocity w leave the equations unchanged.

The Euler equations have conservation form, since they express conservation, which means that a notion of weak solution can be introduced as follows: Multiply $R(u) = 0$ with a smooth test function $\varphi = (\varphi_1, \varphi_2, \varphi_3)$ vanishing for $t = 0$ and large (x, t), integrate in space/time, and then integrate by parts to move all space and time derivatives onto the smooth test function φ. We can then express the Euler equations in weak form as $(R(u), \varphi) = 0$ for all smooth test functions φ, where $(\cdot, \cdot)$ indicates integration in space-time, and φ carries the derivatives. For example, mass conservation takes the weak form $-(\rho, \dot\varphi_1) - (w\rho, \varphi_1') = 0$ for all smooth test functions φ_1. Accordingly, we say that a bounded function $u(x, t)$, which thus may be discontinuous, is a a weak solution if $(R(u), \varphi) = 0$ for all smooth test functions φ, and it suitably satisfies the initial condition.

The function $\eta = \eta(u) = \rho \log(p\rho^{-\gamma})$ is a mathematical entropy for the Euler equations, which means that $\eta(u)$ is a convex function of u, and there is a corresponding entropy flux $q(u) = w\eta$ such that if u is a pointwise (strong) solutions, then

$$\dot\eta + (w\eta)' = 0 \qquad \text{in } \mathbb{R} \times \mathbb{R}_+.$$

This equation follows by multiplying the residual equation $R(u) = 0$ by the Jacobian $D\eta(u)$ of $\eta(u)$ with respect to u, and using the compatibility relation $Dq(u) = D\eta(u)Df(u)$. More generally, weak solutions of the Euler equations corresponding to physically admissible solutions, satisfy the entropy inequality

$$\dot\eta + (w\eta)' \le 0 \qquad \text{in } \mathbb{R} \times \mathbb{R}_+,$$

in weak form, which expresses the Second Law of Thermodynamics. Here $-\eta$ corresponds to the physical entropy. The important feature to notice here is that pointwise solutions satisfy the entropy inequality with equality, and they correspond to reversible solutions with constant entropy, while weak solutions with strictly decreasing entropy correspond to irreversible solutions.

It is well known that compressible inviscid flow in general develops shocks, which in 1d correspond to discontinuous weak solutions of the Euler equations with sudden sharp jumps from one state to another, and which in 3d probably also has a turbulent region around the jump. Shock solutions satisfy the entropy inequality with strict inequality, and thus shocks are irreversible.

We conclude that the compressible Euler equations offer an example of a system which is formally reversible, but nevertheless has irreversible solutions. Clearly, it is the existence of shocks/turbulence, which are not pointwise solutions to the Euler equations, which open for this scenario. Thus, it is the non-existence of pointwise solutions, which causes the irreversibility. We note that the irreversibility is unavoidable because shocks are unavoidable. The compressible Euler equations in 1d offer a model of irreversibility in the form of shocks without the presence of turbulence. We use this model in Part I to expose the principal ideas, and consider the real case with turbulence in 3d in Part II-III.

Now we approach this phenomenon of irreversibility in a formally reversible system from a purely computational point of view. We will show that if we use G2 to compute solutions to the Euler equations, then G2 will automatically single out physically admissible entropy solutions, without explicitely enforcing the entropy condition. We shall see that this is a result of the least squares control of the pointwise residual and the coupling of residual control to the entropy inequality.

We may interprete these G2 results in physical terms as follows: Nature seeks to satisfy the conservation laws expressesd by the Euler equations. When shocks appear, which is inevitable, the equations can no longer be satisfied pointwise, because shocks are discontinuous, and Nature then seeks to handle this situation by resorting to something like G2 involving a weak satisfaction of the conservation laws combined with a certain control of the pointwise residual. The result is that Nature produces a solution which satisfies the entropy condition or the Second Law of Thermodynamics, which follows from what we show for G2 below. Of course the key point here is that Nature in this way achieves to satisfy the Second Law, not by explicitly seeking to do so, but as a result only of solving the original conservation equations by G2.

Again, Nature may be supposed to directly react to the conservation laws, but it is not likely that Nature has any direct sensor of entropy. Thus, from a scientific point of view the crucial point is to explain how Nature can be forced to satisfy the entropy inequality, without knowing anything about it. We show that this is achieved automatically by solving the conservation laws by something like G2.

It is known that adding a small viscous term in the Euler Equations to get the Navier-Stokes equations, is a way to automatically satisfy the entropy inequality in the limit of vanishing viscosity, as a consequence of the conservation laws. As indicated above, we do not consisder this approach scientifically satisfying, since the nature of such a viscosity in fact is the essence of the mystery of irreversibility in reversible systems.

We have noted that a key point is the automatic satisfaction of the entropy inequality by G2. In particular, it means that G2 will never compute a weak solution which corresponds to a physically non-admissible shock violating the entropy inequality. Another way of expressing the non-physical nature of a shock violating the entropy condition would be to say that it is unstable, and that G2 will prefer to compute stable entropy satisfying weak solutions before unstable entropy violating weak solutions. Computing a shock backwards in time would correspond to computing an entropy violating shock, and this computation would be unstable, because the stabilizing term is destabilizing when computing backwards. Thus we may express the entropy inequality satisfaction built into G2 as a result of the stabilizing least squares term which, by its stabilizing nature, will choose a stable solution satisfying the entropy condition before an unstable solution violating the entropy condition. There is thus a close connection between stability and the entropy inequality.

The impossibility of solving a shock problem backwards, which corresponds to the impossibility to recover all the heat generated in a shock and irreversibility, thus may be viewed as a reflection of instability. If the instability could be controled, complete recovery and reversibility would be possible, but such a minute control (corresponding to the Maxwell Demon) seems impossible, with the simple reason is that heat is a small scale phenomenon.

6. A Scenario of Irreversibility

The compressible Euler equations offer a scenario of irreversibility in a formally reversible system in the form of discontinuous shock solutions, which have been studied intensively since the 1940s when von Neumann during the war initiated a study of the mathematics and numerics of high speed gas dynamics. A shock solution satisfies the Euler equations in a weak sense, but not in a pointwise sense, while it also satisfies an entropy inequality corresponding to the Second Law of Thermodynamics stating that the mathematical entropy of a (physical) solution can never increase (with the mathematical entropy being equal to minus the physical entropy). Smooth solutions have constant (mathematical) entropy, while the entropy for shocks is strictly decreasing, which effectively makes a shock irreversible, since time reversal would correspond to a shock solution with increasing entropy. Thus, shock solutions for the Euler equations represent a well studied phenomenon of irreversibility in a formally reversible system.

However, one may ask how in fact Nature succeds to satisfy the entropy condition, which is a direct consequence of the conservation laws for smooth solutions, but not for weak solutions. In fact, there are so called unphysical shocks, which are weak solutions of the Euler equations violating the entropy condition, and one may ask what Natures mechanism of preferring shocks satisfying the entropy inequality may be? The standard answer to this question is to add a small amount of viscosity to the Euler equations and show that limits of viscous solutions as the viscosity tends to zero, satisfy the entropy inequality. The argument would then be that Nature always has some viscosity, although very small, and the presence of this viscosity would be the mechanism choosing the entropy solution. However, again the physical origin of this viscosity would then have to be explained, and we would again have to deal with some small (mysterious) friction or viscosity in some Aether filling empty space, which we seek to avoid.

We give in this note instead an alternative answer to this question using the basic property of G2 by showing that G2 solutions of the Euler equations automatically satisfy the entropy inequality (approximately). We thus show that for G2 the satisfaction of the entropy inequality is a consequence of the weak satisfaction of the conservation laws combined with the weighted least squares control of the residual. G2 would thus not be capable of computing an unphysical entropy-violating solution. This puts the entropy inequality and the Second Law of Thermodynamics in new light: Specifically we show that the Second Law may be viewed as a consequence of the First Law expressing the conservation law combined with finite precision G2 computation. This indicates that Nature would satisfy the entropy inequality automatically by using an analog computation similar to G2, thus without explicit presence of viscosity as in the standard argument. Altogether, we show that the Second Law is a consequence of the First Law combined with G2 finite precision computation.

7. Imperfect Nature and Mathematics?

How are we to handle the fact that the Euler equations do not have pointwise solutions in general? Does this express an imperfection of mathematics? And what is the consequence in physics? Is Nature simply unable to satisfy the basic laws laid down in the form of e.g. Newton's Second Law? Does this mean that also Nature is imperfect? And if now both mathematics and Nature indeed are imperfect, what is the degree of imperfection and how does it show up?

We may make a parallel with the squareroot of two $\sqrt{2}$, which is the length of the diagonal in a square with side length 1. We know that the Pythagoreans discovered that $\sqrt{2}$ is not a rational number. This knowledge had to be kept secret, since it indicated an imperfection in the creation by God formed as relations between natural numbers according the basic belief of the Pythagoreans. Eventually this unsovable conflict ruined their philosophical school and gave room for the Euclidean school based on geometry instead of natural numbers. Civilization did not recover until Descartes resurrected numbers and gave geometry an algebraic form, which opened for Calculus and the scientific revolution.

But how is the Pythagorean paradox of non-existence of $\sqrt{2}$ as a rational number handled today? Well, we know that the accepted mathematical solution since Cantor and Dedekind is to extend the rational numbers to the real numbers, some of which like $\sqrt{2}$ are called irrational, and which can only be described approximately using rational numbers. We may say that this solution in fact is a kind of non-solution, since it acknowledges the fact that the equation $x^2 = 2$ cannot be solved exacly using rational numbers, and since the existence of irrational numbers (as infinite decimal expansions or Cauchy sequences of rational numbers) has a different nature than the existence of natural numbers or rational numbers. The non-existence is thus handled by expanding the solution concept until existence can be assured.

We handle the non-existence of pointwise solutions to the Euler equations similarly, that is, by extending the solution concept to approximate solutions in a weak sense combined with some control of pointwise residuals. Doing so we necessarily introduce a dissipation causing irreversibility. In this case, the non-existence of solutions thus has a cost: irreversibility. In the perfect World, pointwise solutions would exist, but this World cannot be constructed neither mathematically nor physically, and in a constructible World necessarily there will exist irreversible phenomena as a consequence of the non-existence of pointwise solutions. The non-existence of pointwise solutions reflects the development of complex solutions with small scales, and thus the non-existence also relects a complexity of the constructible World. The perfect World would lack this complexity, so in addition to being non-existent it would also probably be pretty non-interesting. The World we live in thus does not seem to be perfect, but it surely is complex and interesting.

What is the reason that the resolution of the paradox we are proposing has not been presented before, if it indeed uncovers the mystery? We believe it can be explained by the Ideal Worlds that both mathematicians and physicists assume as basis of their science. In the Ideal World of mathematics, exact solutions to differential equations exist as well as infinite sets, not just approximate solutions and finite sets, and the World of physics is supposed to follow laws of physics exactly, not just approximately, unless a resort to statistics is made (which is a very strong medication with severe side effects). It thus appears that an imperfect World of mathematics or physics, where equations cannot be solved exactly or laws of physics cannot be exactly satisfied, classically is unthinkable at least as a deterministic World, and thus has recieved little attention by mathematicians and physicists with little background in computational mathematics. Yet, such an imperfect World seems to be a reality in both mathematics and physics, and thus should be studied.

8. A New Paradigm?

From a philosophical point of view, we may say that the traditional paradigm of both mathematics and physics is Platonistic in the sense that it assumes the existence of an Ideal World, where equations/laws are satisfied exactly. We may say that this is an Ideal World of infinities because exact satisfaction of e.g. the equation $x^2 = 2$ requires infinitely many decimals. This is the mathematical Ideal World of Cantor, which represents a formalist/logicist school. In strong opposition to this school of infinities, is the constructivist school, which only deals with mathematicial objects that can be constructed in a finite number of steps. In the constructivists Constructible World, the set of natural numbers does not exist as a completed mathematical object as in Cantors Ideal World, but only as a never-ending project where always a next natural number can be constructed if needed, which follows the suggestions of e.g. Aristotle and Gauss. The Constructible World is finitary and thus inherently computational, while Cantors Ideal World is non-finitary and non-computational. In the educational project [10] and the pamphlett [11], we compare the two schools, and give our vote to the Constructible World, which today can be explored using the computer, and we question the existence of an Ideal World as a scientifically meaningful concept.

9. Physics vs Computation

The mechanism making G2 irreversible when applied to a sufficiently complex formally reversible Hamiltonian system, is the least squares control of the pointwise residual introducing a dissipative effect when pointwise solutions do not exist. It is natural to believe that Nature resorts to something similar, but the more precise physics of this effect is of course up to debate and study. In general, one may view the physics/mechanics of a system of interacting particles as some kind of analog computation, where during each little time step the particles exchange data concerning (relative) positions and forces determining accelerations and then update velocities, positions and forces for the next time step. But the more exact nature of the exchange process is largely unknown, and it is conceivable that a careful study of a computational model may open doors to understanding, as suggested by the famous computer scientist Dijkstra: *Originallly I viewed it as the function of the abstract machine to provide a truthful picture of the physical reality. Later, however, I learned to consider the abstract machine as the "true" one, because that is the only one we can "think"; it is the physical machine's purpose to supply a "working model", a (hopefully) sufficiently accurate physical simulation of the true, abstract machine.*

10. Burgers' Equation

We now proceed to fill in the details of the scenario scetched above in the setting of the compressible Euler equations. To simplify the discussion we consider the simplest model of compressible flow in the form of Burgers' equation. We will return to the compressible Euler equations in 1d below and to the real case of 3d in [8].

Burgers' equation reads: Find the scalar function $u = u(x,t)$ such that

$$\begin{aligned} \dot{u} + (f(u))' &= 0, \quad x \in \mathbb{R},\ t \in \mathbb{R}_+, \\ u(x,0) &= u^0(x), \quad x \in \mathbb{R}. \end{aligned} \tag{10.1}$$

where $f(u) = u^2/2$, and we assume that $u(t,x)$ tends to zero as $x \to \pm\infty$. Obviously, Burgers' equation takes the pointwise form $\dot{u} + uu' = 0$ for a smooth solution u.

A pointwise solution $u(x,t)$ is constant with values $u^0(\bar{x})$ along straight line characteristics $x = st + \bar{x}$, where $s = f'(u^0(\bar{x}))$. If $u^0(x)$ is increasing with increasing x and is smooth, then there is a smooth solution $u(t,x)$ for all time given by this formula. However, if the initial data $u^0(x)$ is strictly decreasing, then characteristics cross in finite time, and then a shock solution necessarily develops, which is discontinuous in x.

A discontinuous shock solution $u(x,t)$ satisfies Burgers' equation in the following weak sense:

$$\int_{\mathbb{R}\times\mathbb{R}_+} (-u\dot{\varphi} - f(u)\varphi')dx\,dt - \int_{\mathbb{R}} u^0(x)\varphi(x,0)\,dx = 0 \tag{10.2}$$

for all differentiable test functions φ such that $\varphi(x,t)$ vanishes for large (x,t). Here the initial condition appears in weak form together with the conservation law in the form of Burgers' equation. This equation is obtained from (10.1) by multiplication by φ and integration by parts.

A discontinuous function $u(x,t)$ defined by $u(x,t) = u_+$ if $x > st$ and $u(x,t) = u_-$ if $x < st$, where u_+ and u_- are two constant states and s is a constant, corresponding to a discontinuity propagating with speed s, is a weak solution to Burgers' equation if the shock speed satisfies the Rankine-Hugoniot condition

$$s = \frac{[f(u)]}{[u]}, \tag{10.3}$$

where $[u] = u_+ - u_-$ and $[f(u)] = f(u_+) - f(u_-)$. With $f(u) = u^2/2$ as in Burgers' equation, we have

$$s = (u_+ + u_-)/2. \tag{10.4}$$

The Rankine-Hugoniot condition expresses the conservation law in weak form for a piecewise constant discontinuous u.

10.1. Rarefaction wave.

The solution to Burgers' equation with the increasing discontinuous initial data $u^0(x) = 0$ for $x < 0$, and $u^0(x) = 1$ for $x > 0$, is a rarefaction wave given by

$$\begin{array}{rcll} u(x,t) & = & 0 & \text{for} \quad x < 0, \\ u(x,t) & = & \frac{x}{t} & \text{for} \quad 0 \le \frac{x}{t} \le 1, \\ u(x,t) & = & 1 & \text{for} \quad 1 < \frac{x}{t}. \end{array} \tag{10.5}$$

This is a continuous function for $t > 0$, differentiable off the lines $x = 0$ and $x = t$, which satisfies (10.1) pointwise for $t > 0$. In a rarefaction wave, an initial discontinuity separating two constant states develops into a continuous linear transition from one state to the other of width t in space, corresponding to "fan-like" level curves in space-time, see Fig 10.1:

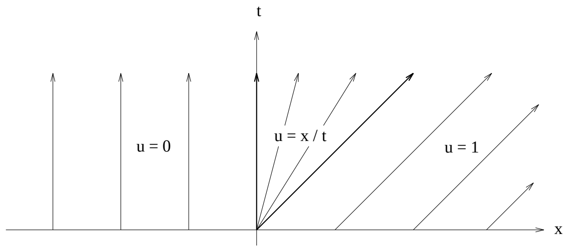

FIGURE 1. Characteristics of a rarefaction wave.

The stability of a rarefaction wave $u(x,t)$ is governed by the linearized equation

$$\dot{w} + (uw)' = 0 \quad \text{in } \mathbb{R} \times \mathbb{R}_+ \tag{10.6}$$

where w represents a (small) perturbation (tending to zero for $|x|$ tending to infinity). Multiplying by w and integrating in space, we obtain by a simple computation using the fact that $u'(x,t) = 1/t$ for $0 \le x \le t$ and $u'(x,t) = 0$ else,

$$\frac{d}{dt}\int_{\mathbb{R}} w^2(x,t)\,dx + \int_0^t w^2(x,t)\frac{1}{t}\,dx = 0, \quad \text{for } t > 0,$$

from which follows that

$$\int_{\mathbb{R}} w^2(x,t)\,dx \le \int_{\mathbb{R}} w^2(x,0)\,dx \quad \text{for } t > 0. \tag{10.7}$$

This inequality shows that the L_2-norm in space of a perturbation of initial data does not grow with time, which proves stability of a rarefaction wave. Note that this argument builds on the fact that the rarefaction wave $u(x,t)$ is increasing in x so that u' is non-negative.

10.2. **Shock.** The solution with decreasing discontinuous initial data $u^0(x) = 1$ for $x < 0$, and $u^0(x) = 0$ for $x > 0$, is a discontinuous shock wave moving with speed $\frac{1}{2}$:

$$\begin{array}{rcll} u(x,t) & = & 1 & \text{for} \quad x < \frac{t}{2}, \\ u(x,t) & = & 0 & \text{for} \quad x > \frac{t}{2}, \end{array} \tag{10.8}$$

see Fig 2. The stability proof used above to prove stability of a rarefaction wave, does not work the same way for a shock, since in this case $u(x,t)$ is decreasing with x. In fact a

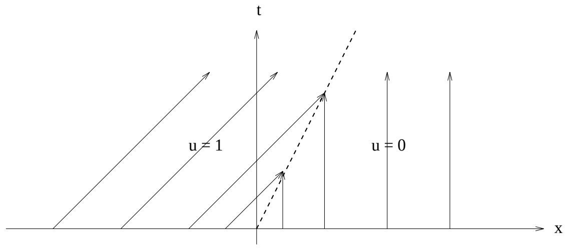

FIGURE 2. Characteristics of a shock

shock does not satisfy an L_2 stability estimate of the form (10.7). However, one may prove instead an L_1-bound of the form

$$\int_{\mathbb{R}} |w(x,t)|\, dx \leq \int_{\mathbb{R}} |w(x,0)|\, dx \quad \text{for } t > 0. \tag{10.9}$$

This follows by multiplying (10.6) by $sgn(w) = +1$ if $w > 0$ and -1 if $w < 0$, to get by integration by parts:

$$\frac{d}{dt}\int_{\mathbb{R}} |w(x,t)|\, dx + (u_- - u_+)|w(\frac{t}{2},t)| = 0, \tag{10.10}$$

and using the fact that for a shock $u_+ < u_-$. Moreover, we will below with a different type of stability estimate show that a shock is stable from a computational G2 point of view. Thus, a shock is a stable phenomenon from both physical and computational point of view.

In one space dimension, shocks exist as piecewise constant (discontinuous) solutions. In three space dimensions such sharp discontinous shocks are probably not stable, and instead a shock will be surrounded by a turbulent transition region. We will return to this issue in further studies.

10.3. **Weak solutions may be non-unique.** The rarefaction wave initial data $u^0(x) = 0$ for $x < 0$ and $u^0(x) = 1$ for $x > 0$, also admits the alternative discontinuous weak solution

$$\begin{aligned} u(x,t) &= 0 \quad \text{for} \quad x < \tfrac{t}{2}, \\ u(x,t) &= 1 \quad \text{for} \quad x > \tfrac{t}{2}, \end{aligned} \tag{10.11}$$

corresponding to a discontinuity $\{(x,t) : x = st\}$ moving with speed $s = \frac{1}{2}$. This solution is obviously different from the rarefaction wave solution (10.5), which since it is a classical solution, also is a weak solution. Thus, we have in this case two different weak solutions, and thus we have an example of non-uniqueness of weak solutions.

We saw above that the rarefaction wave solution is stable, and we now study the stability of the alternative weak solution (10.11). By the same argument as used to prove (10.10) we obtain

$$\frac{d}{dt}\int_{\mathbb{R}} |w(x,t)|\, dx = (u_+ - u_-)|w(\frac{t}{2},t)|, \tag{10.12}$$

where now $u_+ > u_-$. In this case, $\int_{\mathbb{R}} |w(x,t)|\, dx$ can grow arbitrarily fast, since the positive right hand side in (10.12) in no way can be controled by the left hand side, and we thus conclude that the alternative weak solution is unstable. We may thus discard the alternative weak solution on the ground that it is unstable and thus not physical, because physics would of course prefer to realize a stable solution before an unstable. We may refer to the alternative unstable weak solution, as a non-physical shock.

We shall now disqualify the alternative weak solution as a physical solution also because it violates a certain entropy inequality satisfied by physical solutions. We thus have two methods to single out physical weak solutions, one based on stability, and the other on an entropy inequality.

10.4. **The entropy inequality.** A pointwise solution of Burgers' equation $\dot{u} + (\frac{u^2}{2})' = 0$ also satisfies the entropy equality

$$\frac{\partial}{\partial t}(\frac{u^2}{2}) + (\frac{u^3}{3})' = 0, \tag{10.13}$$

which is obtained by multiplying $\dot{u} + (\frac{u^2}{2})' = 0$ by u and rearranging terms. The quantity $\eta(u) = \frac{u^2}{2}$ is a mathematical entropy for Burgers' equation with corresponding entropy flux $q(u) = \frac{u^3}{3}$. The entropy equality is thus obtained by multiplying Burgers'equation with $\eta'(u) = u$, where here the prime indicates differentiation with respect to u. More generally, as an entropy $\eta(u)$ for Burgers' equation $\dot{u} + (f(u))' = 0$, we may choose any convex function $\eta(u)$ of u since in the present case it is always possible to find a corresponding entropy flux $q(u)$ satisfyig the compatibility relation $q'(u) = \eta'(u)f'(u)$. The situation is different for the Euler equations in 3d, where only one type of entropy is known to exist.

We shall motivate below that a weak solution u which is physically admissible, will satisfy in a weak sense the following entropy inequality:

$$\frac{\partial}{\partial t}(\frac{u^2}{2}) + (\frac{u^3}{3})' \leq 0, \tag{10.14}$$

which we will see corresponds to the Second Law of Thermodynamics. The entropy inequality shows upon integration in space and time that

$$\int_{\mathbb{R}} \eta(u(x,t))\, dx \leq \int_{\mathbb{R}} \eta(u^0(x))\, dx,$$

which states that the total entropy cannot increase with time. The entropy $\eta(u) = \frac{u^2}{2}$ corresponds to the kinetic energy, and the entropy inequality states that the kinetic energy of a Burgers solution cannot increase. We shall see that a shock has a substantial loss of kinetic energy as a result of strict entropy inequality, where the lost kinetic energy is dissipated into heat.

For a discontinuous solution consisting of two constant states u_+ and u_- separated by the line $\{x = st\}$, the entropy inequality takes the form

$$s[\frac{u^2}{2}] - [\frac{u^3}{3}] \geq 0, \tag{10.15}$$

from which by a simple computation, we get

$$0 \leq \frac{1}{2}(u_- + u_+)\frac{1}{2}[u^2] - \frac{1}{3}[u^3] = (u_- - u_+)\frac{1}{12}(u_- - u_+)^2. \tag{10.16}$$

We conclude that the entropy inequality for a discontinuous weak solution can be stated as $u_- \geq u_+$, that is,

$$u_- \geq s \geq u_+. \tag{10.17}$$

A physical shock solution is thus characterized by the condition $u_- > u_+$ with shock speed $(u_- + u_+)/2$, in which case the entropy inequality is satisfied with strict inequality. We conclude that a shock dissipates kinetic energy into heat.

The entropy inequality states that the characteristics of a physically admissible discontinuous weak solution of the inviscid Burgers equation "converge into" the shock, corresponding to $u_- > u_+$. This eliminates the discontinuous weak solution to the rarefaction initial data as an unphysical weak solution violating the entropy condition, since in this case $u_- < u_+$, and the characteristics appear to "emerge from" the discontinuity. This reflects that the entropy inequality states that in a closed system information may get destroyed (as in a shock with converging characteristics), but not created (as in an unphysical rarefaction with diverging characteristis).

10.5. **Motivation of the entropy inequality.** We shall now motivate the entropy inequality (10.14) by using a vanishing viscosity argument. This does not mean that we resurrect viscosity as explaining irreversibility. Below we shall present an analog of this argument for G2, where instead the role of viscosity is taken over by least squares stabilization, which is thus different from artificially introducing viscosity, something we want to avoid. However, in motivating the entropy inequality, an approach using vanishing artificial viscosity is mathematically and physically sound.

We thus change Burgers'equation into $\dot{u} + uu' - \epsilon u'' = 0$, where ϵ is a small positive viscosity, which we refer to as the viscid Burgers' equation. Multiplying this equation by u, integrating in time and space, we obtain the basic energy estimate:

$$\int_{\mathbb{R}} |u(x,t)|^2\, dx + D_\epsilon(u) = \int_{\mathbb{R}} |u(x,0)|^2\, dx, \tag{10.18}$$

where the dissipation

$$D_\epsilon(u) = 2\int_0^t \int_{\mathbb{R}} \epsilon (u')^2\, dx\, ds, \tag{10.19}$$

represents the kinetic energy turned into heat. Clearly, it follows that for $t > 0$

$$\|u(\cdot,t)\| \leq \|u_0\|, \tag{10.20}$$

with $\|\cdot\|$ denoting the $L_2(\mathbb{R})$-norm.

We now compare the size of the dissipation $D_\epsilon(u)$ in the case of a rarefaction wave and a shock wave. We find that $D_\epsilon(u) \propto \epsilon$ in the case of a rarefaction wave and $D_\epsilon(u) \propto |[u]|$ in the case of a shock wave with jump $[u]$. Thus, in the case of a rarefaction wave, $D_\epsilon(u) \to 0$ as $\epsilon \to 0$, while in the shock case we have $D_\epsilon(u) \to |[u]| \neq 0$ as $\epsilon \to 0$. Thus, in a limit of vanishing viscosity ϵ, we will have equality in (10.20) in the case of a rarefaction wave, and strict inequality in the case of a shock wave expressing a "loss of information" or "(physical) entropy production" corresponding to generation of heat in the case of a shock wave.

To justify (10.14) we now assume that solutions u of the viscid Burgers' equation are bounded for $\epsilon > 0$, and tend pointwise to some bounded limit, again denoted by u, as ϵ tends to zero. Multiplying the viscid Burgers' equation first by a smooth test function φ vanishing for $t = 0$, and integrating by parts, we obtain

$$\begin{aligned} -\int_0^t\int_{\mathbb{R}} u\dot{\varphi}\,dx\,ds &- \tfrac{1}{2}\int_0^t\int_{\mathbb{R}} u^2\varphi'\,dx\,ds \\ &= -\int_0^t\int_{\mathbb{R}} \epsilon u'\varphi'\,dx\,ds. \end{aligned}$$

Since by (10.18)

$$2\int_0^t\int_{\mathbb{R}} \epsilon(u')^2\,dx\,ds \le \|u_0\|^2, \tag{10.21}$$

we have using Cauchy's inequality and the smoothness of φ,

$$\int_0^t\int_{\mathbb{R}} \epsilon u'\varphi'\,dx\,ds \le \|u_0\|\sqrt{\epsilon}(\int_0^t\int_{\mathbb{R}}(\varphi')^2dx\,ds)^{1/2} \to 0 \quad \text{as } \epsilon \to 0. \tag{10.22}$$

Thus, we conclude that the limit u satisfies (10.2) with $f(u) = u^2/2$ and hence is a weak solution of the (inviscid) Burgers' equation.

Next, multiplying by $u\varphi$, where φ is a smooth test function now assumed to be also non-negative, we obtain integrating by parts

$$\begin{aligned} -\int_0^t\int_{\mathbb{R}} \tfrac{u^2}{2}\dot{\varphi}\,dx\,ds &- \int_0^t\int_{\mathbb{R}} \tfrac{u^3}{3}\varphi'\,dx\,ds \\ +\int_0^t\int_{\mathbb{R}} \epsilon(u')^2\varphi\,dx\,ds &= -\int_0^t\int_{\mathbb{R}} \epsilon uu'\varphi'\,dx\,ds. \end{aligned}$$

Arguing as above, using also the boundedness of u, we see that the right hand side tends to zero. Using also the positivity of φ to see that the third term on the right hand side is positive, we conclude that the limit u satisfies

$$-\int_0^t\int_{\mathbb{R}} \frac{u^2}{2}\dot{\varphi}\,dx\,ds - \int_0^t\int_{\mathbb{R}} \frac{u^3}{3}\varphi'\,dx\,ds \le 0, \tag{10.23}$$

for all smooth non-negative test functions ϕ, with strict inequality if $D_\epsilon(u)$ tends to some non-zero limit. This is the entropy inequality (10.14) stated in weak form.

We have now shown that a limit of solutions of the viscid Burgers' equation as the viscosity tends to zero satisfies the entropy inequality (10.14). We have also seen that for a shock the inequality is strict. It follows that a shock solution to Burgers' equation is irreversible since effectively the mathematical entropy decreases, and reversing time would correspond to strictly increasing mathematical entropy violating the entropy inequality.

10.6. **Sum up Burgers.** We have shown that the mathematical entropy of a shock solution to Burgers' equation is strictly decreasing, which shows that a shock solution to the formally reversible Burgers'equation, is irreversible. Letting time pass backwards in a shock problem with converging characteristics in forward time, would correspond to an unphysical rarefaction initial data solution with diverging charcteristics in backward time. We may thus say that the irreversibility of a shock in the inviscid Burgers' equation, is reflected by instability when seeking to recover the initial data by computing backwards in time from final data. We may thus phraze the irreversibility as reflecting forward stability and backward instability, just as in the heat equation, although formally we are dealing with an inviscid equation.

We have presented a very simple concrete (well known) example of irreversibility in a formally reversible problem, and we have seen that the irreversibility requires non-existence of pointwise solutions in order to occur. We have thus presented a key basic example of the scenario of irreversibility in reversible systems, which we are seeking to uncover in the more general setting of incompressible and compressible flow, particle dynamics and hopefully eventually for quantuum mechanics.

We now proceed to the computational version of the scenario. The key here will be the G2 method and its property of automatically satisfying the entropy inequality, without explicitely being required to do so, which is a parallel of Natures ability to satisfy the Second Law of Thermodynamics again without knowing anything about it. This is made possible by computing, in a situtation where pointwise solution is impossible because of non-existence of pointwise solutions, an approximate solution which satisfies the basic conservation laws in a weak sense combined with a weighted least squares control of the pointwise residual. It is this combination which automatically builds the entropy inequality into a weak solution. We may say that by the combination of Galerkin and least squares stabilization, G2 will automatically prefer to compute stable (physical) weak solutions before unstable (non-physical) weak solutions.

11. G2 for Burgers' equation

We now turn to the G2-method which is Galerkin's method combined with a weighted least-squares control of the residual. G2 is based on piecewise polynomial approximation in space-time and offers a spectrum of computational methods depending on the choice of the space-time mesh. G2 uses piecewise polynomials in space-time. We refer to these variants as cG(p)cG(q), cG(p)dG(q) et cet, with cG(p)/dG(p) referring to continuous/discontinuous piecewise approximation of degree p in space, and cG(q)/dG(q) referring to continuous/discontinuous approximation in time of degree q. G2 is Eulerian if the space-time mesh is oriented along the space and time coordinate axis, Lagrangean if the space-time mesh is oriented along particle paths in space-time, and Arbitrary Lagrangean-Eulerian or ALE if the space-time mesh is oriented according to some other feature such as space-time gradients of the solution. We also refer to Lagrangean variants as characteristic Galerkin, ALE-methods as oriented Galerkin, and Eulerian variants as SUPG and Streamline Diffusion-methods. In all these variants the space-time mesh is usually organized in space-time slabs between discrete time levels, and the space mesh may be changed across the discrete time levels to avoid mesh distortion and allow mesh adaption. In dG(q) the approximation is discontinuous in time and the space mesh may vary from one slab to the next. If the space mesh is changed across a discrete time level in cG(q), then a projection from the previous mesh to the new mesh is performed. The projection is built into the Galerkin method through a jump term corresponding to a L_2 projection. The discrete solution between the discrete time levels may be viewed as an approximate *transport* step, and the whole process may be viewed as a method of the basic form projection-transport.

The traditional finite difference methods are of Eulerian type with the first order Lax-Friedrichs' scheme from the 50s as a prototype on conservation form and with artificial viscosity proportional to the mesh size. The next generation of classical schemes originates from Godunov's method in 1d, which is of the form projection-transport with a piecewise constant (discontinuous) approximation and a Riemann solver for the transport step. The multi-dimensional finite volume schemes developed in recent decades, use discontinuous polynomial approximation with numerical fluxes often constructed using 1d Riemann solvers. All these methods may alternatively be viewed as particular G2 methods.

Galerkin/least squares methods were pionereed in the early 1980s by Hughes followed by Johnson in the form of SUPG and Streamline Diffusion methods, see [12, 4, 5].

11.1. **G2 in the form cG(1)dG(1).** We now define G2 in the form of cG(1)dG(1) on an Eulerian mesh for Burgers' equation. Let then $0 = t_0 < t_1 < ... < t_N = T$ with T a final time, be an increasing sequence of time levels with corresponding time steps $k_n = t_n - t_{n-1}$, and let $S_n = \mathbb{R} \times I_n$ where $I_n = (t_{n-1}, t_n]$, be the corresponding space-time slabs. Associate to each slab S_n a set V_n of continuous piecewise linear functions $v(x,t)$ on S_n, typically of the form $v(x,t) = v_0(x) + tv_1(x)$, where $v_0(x)$ and $v_1(x)$ are continuous piecewise linear on a mesh of mesh size h_n on $\mathbb{R}$. Then define $V_h = \prod_{n=1}^N V_n$, where h is a measure of the mesh size in space-time. Thus, V_h consists of piecewise linear functions in space-time, which are continuous in space and discontinuous in time (and in addition vanish for $|x|$ large). For simplicity, we assume that the time step k_n and mesh size in space h_n one each slab V_n are of constant size h.

A function $v \in V_h$ is discontinuous in time across a discrete time level t_n with limits $v_n^+(x) = \lim_{s\to 0, s>0} v(x, t_n + s)$ and $v_n^-(x) = \lim_{s\to 0, s<0} v(x, t_n + s)$, and with jump $[v_n] = v_n^+ - v_n^-$.

We can now formulate G2 in the form cG(1)dG(1) as follows: Find $U \in V_h$, such that for $n = 1, 2, ...,$,

$$(R(U), v)_{S_n} + (hR(U), \dot{v} + Uv')_{S_n} + ([U_{n-1}], v_{n-1}^+)_{\mathbb{R}} = 0, \quad \forall v \in V_n, \tag{11.1}$$

where $R(U) = \dot{U} + UU'$ is the residual, $U_0^- = u^0$, $(v,w)_{S_n} = \int_{S_n} vw\, dxdt$, and $(v,w)_{\mathbb{R}} = \int_{\mathbb{R}} vw\, dx$.

11.2. **The basic energy estimate for G2.** Choosing $v = U$ in (11.1), we obtain by integration by parts and summation over $n = 1, ..., N$:

$$\frac{1}{2}\int_{\mathbb{R}} U_N^-(x)^2\, dx + \frac{1}{2}\sum_{n=1}^N \|[U_{n-1}]\|_{\mathbb{R}}^2 + \int_0^{t_N}\int_{\mathbb{R}} hR(U)^2\, dxdt = \frac{1}{2}\int_{\mathbb{R}} u^0(x)^2\, dx,$$

that is,

$$\frac{1}{2}\|U_N\|^2_{\mathbb{R}} + \frac{1}{2}\sum_{n=1}^{N}\|[U_{n-1}]\|^2_{\mathbb{R}} + \|\sqrt{h}R(U)\|^2_{Q_N} = \frac{1}{2}\|u^0\|^2_{\mathbb{R}},$$

where $\|\cdot\|_D$ is the $L_2(D)$-norm with $D = \mathbb{R}$ and $D = Q_N \equiv \mathbb{R}\times(0, t_N)$. This is the basic energy estimate for G2 for Burgers'equation, which also represents an entropy inequality for the mathematical entropy $\eta(u) = u^2/2$. We see that the least squares term $\|\sqrt{h}R(U)\|^2_{Q_N}$ and the jump term acts as dissipative terms, effectively causing the mathematical entropy to decrease significantly in a situation when the slab residual $R(U)$ and jumps cannot be pointwise small, which will happen in the case of a shock. We may view the jump $[u]$ as being part of the residual, with the jump being zero for an exact solution as well as the residual on each slab.

11.3. **G2 is entropy consistent.** We shall now prove as a major observation of this note that G2 automatically satisfies the entropy inequality (10.14) in a weak sense, and thus automatically computes a physical solution without explicitely enforcing the entropy inequality. The key point is thus that the construction of G2 as a weak satisfaction of the conservation law combined with weighted least squares constrol of the pointwise residual, assures that a G2 solution also satisfies the entropy inequality characterizing physical solutions. In particular, there is no chance that G2 will produce a non-physical solution violating the entropy condition significantly.

To see this, we choose a smooth non-negative test function φ, write $w = \varphi U$ and then choose in G2 the finite element test function $v = w_h$, where $w_h \in V_h$ is a nodal interpolant of w, noting that w does not belong to V_h in G2 in general. We then have with $\tilde{U}_n = \frac{1}{2}(U_n^+ + U_n^-)$, by integration by parts in space and time,

$$-(\frac{1}{2}U^2, \dot{\varphi})_{Q_N} - (\frac{1}{3}U^3, \varphi')_{Q_N}$$

$$= \sum_{n=1}^{N}\big((R(U), w)_{S_n} + ([U_{n-1}], \tilde{U}_{n-1}\varphi^+_{n-1})_{\mathbb{R}}\big)$$

$$= \sum_{n=1}^{N}\big(R(U), \hat{w}_h)_{S_n} - (hR(U), \dot{w}_h + Uw_h')_{S_n} + ([U_{n-1}], \tilde{U}_{n-1}\varphi^+_{n-1} - w^+_{h,n-1})_{\mathbb{R}}\big)$$

$$\equiv I + II + III,$$

where $\hat{w}_h = w - w_h$, and we used (11.1) with $v = w_h$. We now estimate the interpolation error $\hat{w}_h$ as follows:

$$\|\hat{w}_h\|_{S_n} \le \|h^2D^2w\|_{S_n} \le Ch\|U\|_\infty,$$

where D represents first order derivation in space or time, C depends on first and second derivatives of φ and $\|U\|_\infty = \max_{Q_N}|U| \equiv M$. This type of estimate is referred to as super-approximation since it contains the factor h without paying the price of first derivatives of

U, which results from the special form of $w = \varphi U$ as a product of a finite element function U and a smooth function. We conclude that

$$I \leq CM\|hR(U)\|_{Q_N} \leq CM\sqrt{h},$$

where we used the basic energy estimate assuming $\|u^0\| \sim 1$. Further

$$II = \sum_{n=1}^{N}(hR(U), \frac{\partial}{\partial t}\hat{w}_h + U\hat{w}_h')_{S_n} - \sum_{n=1}^{N}(hR(U), \dot{w} + Uw')_{S_n} = II_a + II_b.$$

We have again by super-approximation and the energy estimate that $II_a \leq CM\sqrt{h}$, and

$$II_b = -\sum_{n=1}^{N}(hR(U), \dot{U}\varphi + UU'\varphi)_{S_n} - \sum_{n=1}^{N}(hR(U), U\dot{\varphi} + UU\varphi')_{S_n}$$

$$\leq -\sum_{n=1}^{N}(hR(U), R(U)\varphi)_{S_n} + CM\sqrt{h} \leq CM\sqrt{h},$$

where we used the non-negativity of φ. The term III is estimated similarly. We conclude that for all non-negative test functions φ, we have

$$-(\frac{1}{2}U^2, \dot{\varphi})_{Q_N} - (\frac{1}{3}U^3, \varphi')_{Q_N} \leq CM\sqrt{h},$$

where M is a bound for U and C depends on up to second derivatives of φ. This expresses that the G2 solution U approximately satisfies the entropy inequality in weak form and the approximation improves as h gets smaller. We refer to this property of G2 as entropy consistency. In particular G2 cannot compute a non-physical solution significantly violating the entropy inequality. Note that the M-bound on U is natural and can be proved by a maximum principle if G2 is suitably modified by introducing residual-dependent shock-capturing, [5].

We have now established the key feature of G2 to automatically satisfy the entropy inequality approximately, as a consequence of the least squares stabilization. The key to the proof is the super-approximation making it effectively possible to choose $U\varphi$ as a test function in G2, from which entropy consistency follows using the positivity of the least squares term, which reflects that the entropy inequality is obtained by multiplication of the viscid Burgers' equation by $\eta'(u)\varphi = u\varphi$. Note that choosing U as a test function gives the basic energy estimate, which is the integrated form of the entropy inequality, and the step to choose instead $(U\phi)_h$ is not large, but requires the least squares stabilization to work out.

11.4. **A posteriori error estimation.** Applying the general technique of a posteriori error estimation for G2 presented in detail in [5] and [6], we may obtain an estimate of the form

$$\|u - U\|_{Q_N} \leq S\|hR(U)\|_{Q_N}, \tag{11.2}$$

where u is an exact Burgers solution, U is a G2 solution with mesh size h, and

$$S = \frac{\|h\phi''\|_{Q_N}}{\|e\|_{Q_N}}, \tag{11.3}$$

where $e = u - U$, is a normalized stability factor defined by the solution ϕ of the following linearized dual problem:

$$\begin{aligned} -\dot{\phi} - a\phi' - h\phi'' = e, &\quad x \in R,\ 0 < t < t_N, \\ \phi(x,t) \to 0, &\quad x \to \pm\infty,\ 0 < t < t_N, \\ \phi(x,T) = 0, &\quad x \in \mathbb{R}, \end{aligned} \tag{11.4}$$

where $a = (u + U)/2$. We notice that the dual problem has a viscous term with viscosity coefficient h.

We first note that by the basic energy stability estimate, we have that $\|hR(U)\|_{Q_N} \leq \sqrt{h}$ if $\|u^0\|_{\mathbb{R}} = 1$, and thus

$$\|u - U\|_{Q_N} \leq S\sqrt{h}. \tag{11.5}$$

Clearly the size of the stability factor S determines the quality of the error bound. We shall now prove that for a shock $S \sim 1$, which shows that a shock is safely computable with G2, with a $L_2(Q_N)$ error of size $\sqrt{h}$ which is optimal from approximation point of view, since the exact solution u is discontinuous and U is continuous in x.

The a posteriori error estimate (11.2) follows by multiplying (11.4) by $u - U$ and integrating in space and time to get the error representation

$$\|u - U\|_{Q_N}^2 = (R(U), \phi)_{Q_N},$$

where the jump term is included in $R(U)$ to simplify the reading. We now use the Galerkin equation (11.1) with $v = \phi_h \in V_h$ an interpolant of the dual solution ϕ, to get

$$\|u - U\|_{Q_N}^2 = (R(U), \phi - \phi_h)_{Q_N} - (hR(U), \dot{\phi}_h + U\phi_h')_{Q_N},$$

which combined with an interpolation error bound of the form $\|\phi - \phi_h\|_{Q_N} \leq \|h^2\phi''\|_{Q_N}$, shows that

$$\|u - U\|_{Q_N}^2 \leq \|hR(U)\|_{Q_N}\|h\phi''\|_{Q_N},$$

from which the desired result directly follows. Here, for simplicity we only accounted for approximation in space. We also used the dual equation to bound $\|\dot{\phi}_h + U\phi_h'\|_{Q_N}$ by $\|h\phi''\|_{Q_N}$ replacing $a = (u+U)/2$ by U and ϕ_h by ϕ. We also regularized the exact solution u leaving a very small regularizing term. For details, we refer to [6]. We note the simple form of (11.2), which holds in a wide generality.

11.5. **Stability estimate for a shock.** We shall now investigate the stability properties of the dual problem (11.4) and bound $h\phi''$ in terms of the right hand side e. For simplicity we linearize at the exact solution $u(x,t)$ (instead of the mean value $(u + U)/2$) and thus consider the dual problem

$$\begin{aligned} -\dot{\phi} - u\phi' - h\phi'' = e, &\quad x \in \mathbb{R},\ 0 < t < t_N, \\ \phi(x,T) = 0, &\quad x \in \mathbb{R}. \end{aligned} \tag{11.6}$$

The stability properties are largely determined by the sign of u', which reflects the change of the direction u of the characteristics. If $u' \leq 0$, then the characteristics converge with increasing t, which typically occurs in the case of a shock. If $u' \geq 0$, then the characteristics diverge, which typically occurs in the case of a rarefaction. If u' is bounded below by a moderate constant, e.g. $u' \geq 0$, then we may estimate $\|\phi\|_{L_\infty(L_2(\mathbb{R}))}$ and $\|\sqrt{h}\phi'\|_Q$ in terms of a moderate constant times $\|e\|_Q$, which we refer to as *weak stability*. If u' is bounded above by a moderate constant, e.g. $u' \leq 0$, then we may estimate $\|h\phi''\|_Q$ in terms of a moderate constant times $\|e\|_Q$, which we refer to as *strong stability*, because we estimate second derivatives of ϕ, cf. (11.3). These estimates are proved by multiplying by ϕ and $-h\phi''$, respectively, bringing in the positive stabilizing terms $\frac{1}{2}u'\phi^2$ and $-\frac{1}{2}hu'(\phi')^2$, respectively.

We now give the details in the case of a shock with $u' \leq 0$, where we assume u is differentiable with a very large negative x-derivative close to the shock. We indicate the general nature of the characteristics of the dual problem in Fig 11.5. We shall prove that the solution ϕ of (11.6) satisfies

$$\|h\phi''\|_{Q_N} + \|\dot{\phi} + u\phi'\|_{Q_N} + \sup_{0<t<T} \|h^{1/2}\phi'(\cdot,t)\|_R \leq 3\|e\|_{Q_N}. \tag{11.7}$$

To see this we multiply the first equation in (11.6) by $-h\phi''$, integrating by parts with respect to x, and integrating in time over (τ, T) with $0 < \tau < T$, we get with $Q_\tau = \mathbb{R}\times(\tau, T)$

$$\begin{aligned} &\tfrac{1}{2}\int_{\mathbb{R}} h\left(\phi'(\cdot,\tau)\right)^2 dx + \int_{Q_\tau} (h\phi'')^2\, dxdt + \int_{Q_\tau} \tfrac{1}{2}\left(uh\left(\phi'\right)^2\right)'\, dxdt \\ &\leq \tfrac{1}{2}\int_{Q_\tau} \left(hu'\left(\phi'\right)^2 + e^2 + (h\phi'')^2\right)\, \mathrm{d}x\mathrm{d}t, \end{aligned} \tag{11.8}$$

which proves the desired result stating that $S \sim 1$ for a shock.

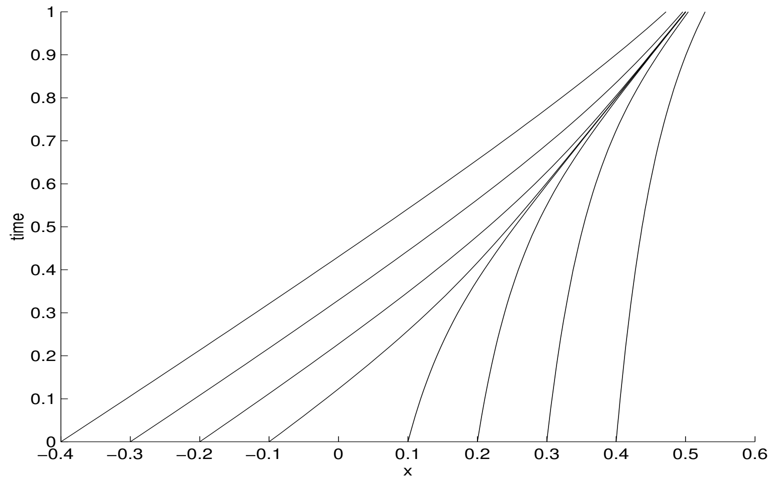

FIGURE 3. Characteristics of the dual problem for a regularized shock solution.

As comparison, let us now attempt to derive a weak stability estimate for (11.6) in the case u is a shock. Multiplication by ϕ and integration over Q_τ gives

$$\frac{1}{2}\int_R \phi^2(x,\tau)\ dx + h\int_{Q_\tau} (\phi'(x,t))^2\ dxdt$$
$$= -\frac{1}{2}\int_{Q_\tau} u'\phi^2(x,t)\ dx + \int_R e(x,t)\phi(x,t)\ dx.$$

Since u' is large negative in the case of a shock, we have a large positive term of the right hand side, and using a Grönwall's inequality would results in a very large stability factor. The situation is more favorable concerning weak stability estimates for a rarefaction wave solution with $u' \geq 0$, as we demonstrate below.

Summing up, we see that for a shock, the linearized dual problem satisfies a strong stability estimate with a stability factor of moderat size, while a corresponding weak stability estimate appears to have a very large stability factor. These stability features may be understood in a qualitative sense, by pondering the directionality of the characteristics and the nature of the L_2-norm.

11.6. **Stability estimates for a rarefaction wave.** We now consider the linearized dual Burgers' equation (11.6), linearized at the exact solution $u(x,t) = x/t$, corresponding to a rarefaction wave. Multiplying now (11.6) by $-ht\phi''$, and using standard manipulations, we obtain the following weighted norm strong stability estimate for $0 < \tau < T$,

$$\|\tau^{1/2}h^{1/2}\phi'\| + \|\omega h\phi''\|_{Q_\tau} \leq \|\omega e\|_{Q_\tau}, \tag{11.9}$$

where $\omega(t) = t^{1/2}$ acts as a weight.

A weighted norm analog of the a posteriori error estimate (11.2) takes the form

$$\|\omega^{-1}e\|_{Q_N} \leq S_\omega\|\omega^{-1}hR(U)\|_{Q_N} \tag{11.10}$$

with S_ω defined by the direct weighted norm analog of (11.3). The estimate (11.9) then shows that $S_\omega \sim 1$, and thus a rarefaction wave solution is computable in the weighted norm with a computational work corresponding to interpolation. Note that the presence of the weight $t^{-1/2}$ will force more stringent demands on the mesh for t close to zero, which will force an accurate resolution of the initial phase of the rarefaction. This is intuitively reasonable and corresponds to the fact that an initial error in the computation of a rarefaction will get amplified as time goes, because characteristics diverge forward in time. On the other hand, in the case of a shock, an initial error may be eliminated at later times, because of converging characteristics, Thus, a rarefaction is more delicate to compute than a shock, which we will see in the computational results we now present.

11.7. **Dual solution and stability factors for Burgers' equation.** In [5, 3] an approximate solution is computed consisting of a combination of a rarefaction wave and a shock using the cG(1)dG(0)- method on a uniform space mesh with $h = 10^{-3}$ and time step 10^{-4}. We plot the computed solution at t=0, t=0.3, t=0.8, t=1 in Fig 4. We see that the initial discontinuity develops into a rarefaction and that a shock is formed for $t \approx 0.5$.

The dual problem is solved using the following different approximations of the coefficient $a = (u+U)/2$ and the error e, with $\bar{u}$ the analytical, inviscid solution, and $U(h)$ the finite

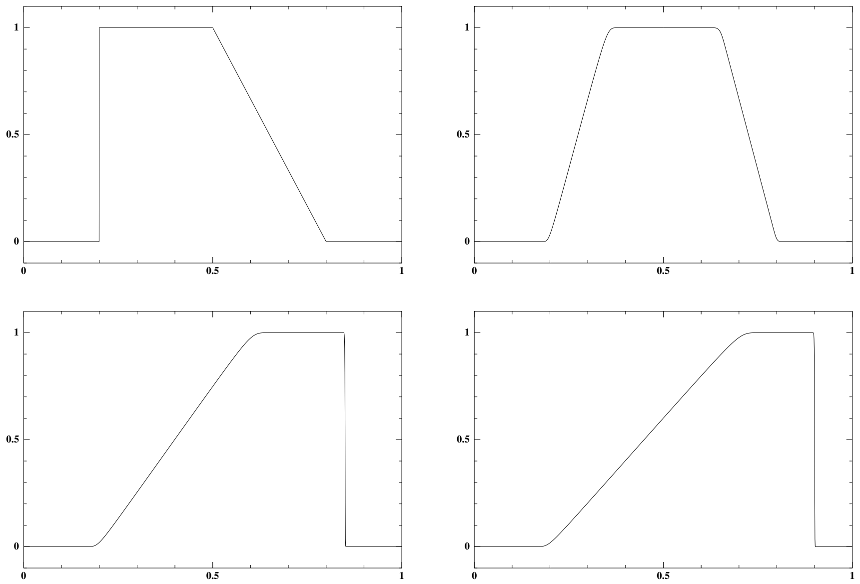

FIGURE 4. A combined rarefaction and shock wave (computations by Burman [3]).

element solution on a mesh of size h: (i) $a = (\bar{u} + U(h))$ and $e = \bar{u} - U(h)$, (ii) $a = U(h)$ and $e = \bar{u} - U(h)$, (iii) $a = (U(h/4) + U(h))/2$ and $e = U(h/4) - U(h)$. We plot the corresponding dual solutions ϕ at the same time levels as above, but in reverse order (t=1, t=0.8, t=0.3 , t=0) in Fig 11.7. We also plot in Fig. 6 the corresponding second derivatives ϕ''. We note the change of $|\phi''|$, which may be viewed as a weight in the a posteriori error estimate, from being large close to the shock at final time towards being large close to the initial discontinuity at $(x, t) = (0.2, 0)$ initiating the rarefaction. We see that it is the data from the rarefaction at final time which generates the large values of ϕ'' at $t = 0$, and not those from the shock. This indicates that a rarefaction is more delicate to compute than a shock.

We plot in Fig. 7 the strong stability factor S defined by (11.3) for (i)-(iii) and $h = 0.0001$, $h = 0.00005$, $h = 0.00001$. We see that $S \sim 1$, which shows that the Burgers' solution consisting of a rarefaction and shock wave is computable in $L_2(Q_N)$ with work comparable to interpolation.

12. THE EULER EQUATIONS FOR COMPRESSIBLE FLOW

We now extend to the Euler equations for an inviscid perfect gas, including details on the formulation of the G2-method. The a posteriori error estimation generalizes in a direct way. G2 has the entropy consistency automatically built in if we compute in entropy variables. If we compute using the standard conservation variables, we need to add a residual dependent artificial viscosity, to ensure entropy consistency. The computational results

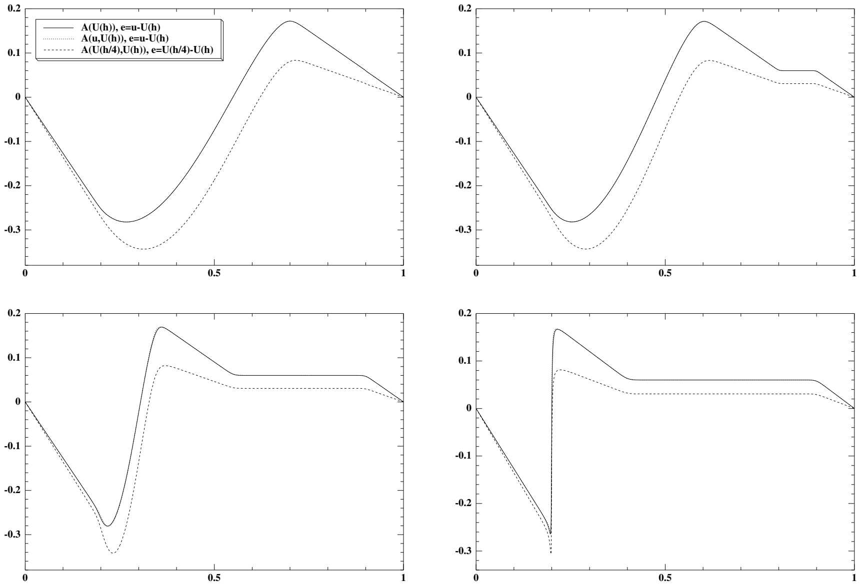

FIGURE 5. Dual solution in reverse time (computations by Burman [3]).

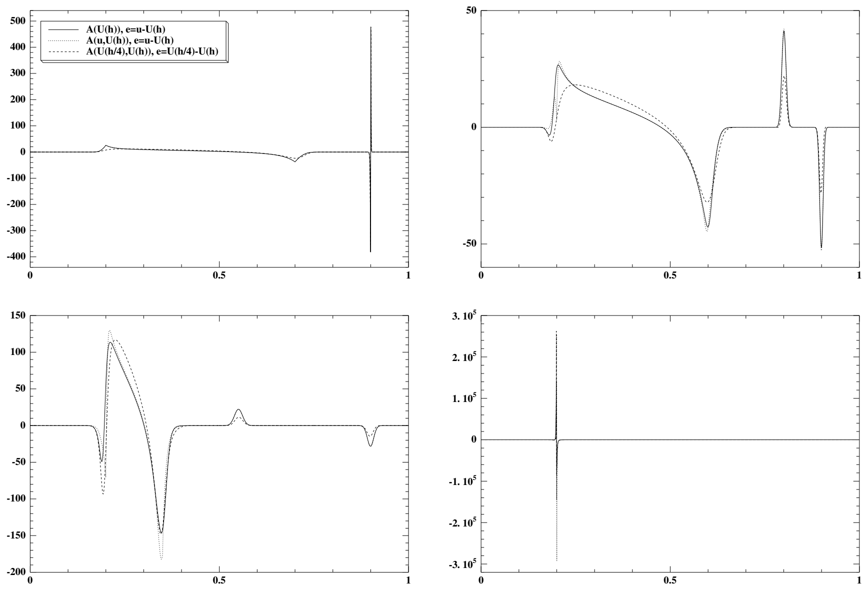

FIGURE 6. Second deriatives of the dual solution in reverse time (computations by Burman [3]).

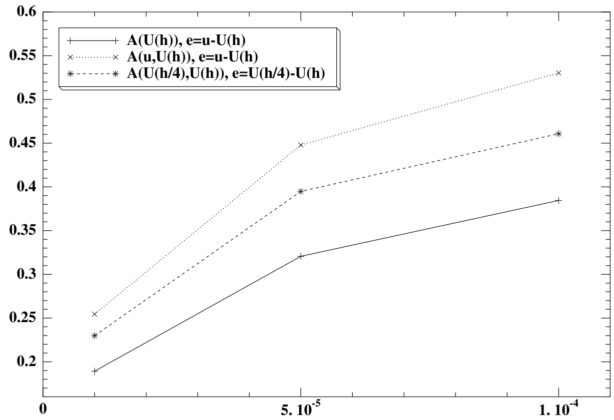

FIGURE 7. Strong stability factor for different h (computations by Burman [3]).

in 1d are entirely analogous to those presented for Burgers' equation, with in particular strong stability factors being of unit size. We present computaions in 3d in Part III.

The Euler equations for a compressible inviscid perfect gas in $\mathbb{R}^3$ read on conservation form: find $u(x,t)$ such that

$$\begin{array}{rcll}\dot{u}+\sum_{i=1}^3 f_i(u)_{,i} & = & 0 & x\in\mathbb{R}^3,\ t>0,\\ u(x,0) & = & u_0(x) & x\in\mathbb{R}^3,\end{array} \tag{12.1}$$

where u_0 is given initial data,

$$u=\rho\begin{bmatrix}1\\ w_1\\ w_2\\ w_3\\ e\end{bmatrix},\quad f_i=w_iu+p\begin{bmatrix}0\\ \delta_{1i}\\ \delta_{2i}\\ \delta_{3i}\\ w_i\end{bmatrix},$$

ρ is the density, $w=(w_1,w_2,w_3)$ is the particle velocity, e is the total energy density, $p=(\gamma-1)(\rho e-\rho|w|^2)/2)$ is the pressure, δ_{ij} the Kronecker delta, $\gamma>1$ is a constant, and $v_{,i}=\partial v/\partial x_i$. These equations generalize the one-dimensional equations (5.1) and express conservation of mass, momentum and energy. For smooth solutions the conservation law (12.1) can be written as a generalized convection problem of the form

$$\dot{u}+\sum_{i=1}^{3}A_i(u)u_{,i}=0, \tag{12.2}$$

where the $A_i=\frac{\partial f_i}{\partial u}$ are the Jacobians of the $f_i(u)$.

The function $\eta(u)=\rho\log(p\rho^{-\gamma})$ is a mathematical entropy for (12.1) corresponding to the negative of the physical entropy, which up to trivial modfications is the only known entropy for (12.1). The function $\eta(u)$ is a convex function of u, with symmetric positive definite Hessian η''. Smooth solutions of (12.1) or equivalently (12.2), satisfy the equation

$$\frac{\partial}{\partial t}\eta(u) + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(q_i(u)) = 0.$$

where $q(u) = (q_i(u)) = \eta w = (\eta w_i)$ is the entropy flux. This equation follows by multiplying (12.2) by the gradient $\eta'(u)$ of $\eta(u)$ and using the compatibility relation

$$\eta'(u)^* A_i(u) = q_i'(u)^*, \tag{12.3}$$

with $*$ denoting the transpose. The compatibility condition (12.3) is equivalent to the relation

$$\eta'' A_i = A_i^* \eta'', \quad i = 1, 2, 3, \tag{12.4}$$

stating that the Hessian η'' simultaneously symmetrizes all the A_i. The entropy inequality characterizing physical weak solutions reads in strong form

$$\frac{\partial}{\partial t}\eta(u) + \sum_{i} \frac{\partial}{\partial x_i}(q_i(u)) \leq 0. \tag{12.5}$$

12.1. **G2 for the Euler equations.** Let V_h be as above and set $W_h = [V_h]^3$. G2 for (12.1) can then be formulated as follows: Find $U \in W_h$ such that for $n = 1, 2, ...,$

$$\begin{aligned} &(R(U), v)_{Q_N} + (R(U), \delta(\dot{v} + \textstyle\sum_i A_i^*(U) v_{,i}))_{S_n} \\ &+([U_{n-1}], v_{n-1}^+)_{\mathbb{R}} = 0 \quad \forall v \in W_n = [V_n]^3, \end{aligned} \tag{12.6}$$

where $*$ denotes transpose,

$$\delta^* = \delta(U)^* = \frac{h}{2}(I + \sum_{i=1}^{3} A_i(U)^2)^{-\frac{1}{2}} \quad \text{on } S_n, \tag{12.7}$$

$$R(U) = \dot{U} + \sum_i A_i(U) U_{x_i} \quad \text{on} \quad S_n.$$

To see that the square root in (12.7) is well defined, we note that (12.4) implies that $A_0 = (\eta'')^{-1}$ symmetrizes the A_i, so that $\bar{A}_i \equiv A_i A_0$ is symmetric, $i = 1, 2, 3$. Therefore

$$A_0^{-\frac{1}{2}} A_i A_0^{\frac{1}{2}} = A_0^{-\frac{1}{2}} \bar{A}_i A_0^{-\frac{1}{2}}$$

is symmetric, and thus the similarity transform induced by $A_0^{\frac{1}{2}}$ transforms the matrix $M \equiv (k_n^{-2} I + h^{-2} \sum_i A_i^2)$ to an obviously positive definite symmetric matrix. It follows that M has positive eigenvalues and a full set of eigenvectors which shows that $M^{-\frac{1}{2}}$ can be computed.

One can prove as above that G2 augumented by a residual dependent artificial viscosity of the form $\hat{\epsilon} = h^2 |R(U)|$, is entropy consistent.

12.2. **G2 in entropy variables.** The change of variables $\bar{u} = \eta'(u)$, which is one-to-one since η'' is positive definite, transforms (12.2) into

$$\bar{A}_0\dot{\bar{u}} + \sum \bar{A}_i\bar{u}_{,i} = 0 \tag{12.8}$$

where $\bar{A}_0(\bar{u}) = (\eta'')^{-1}(\bar{u})$ is positive definite symmetric, and $\bar{A}_i = A_i\bar{A}_0$ are symmetric because of (12.4). We refer to $\bar{u} = \eta'(u)$ as the *entropy varibles.*

In the entropy variables $\bar{u} = \eta'(u)$, the conservation law (12.2) takes the form of the symmetric hyperbolic system (12.8) with the $\bar{A}_i$ symmetric and $\bar{A}_0$ positive definite. The entropy inequality is obtained multiplying a viscous variant of (12.8) by $\bar{u}\phi$, with ϕ a non-negative test function, and letting the viscosity tend to zero, as for Burgers equation, since $\bar{u} = \eta'(u)$.

We may now apply the G^2 method to (12.8), and we may as in the case of Burgers'equation prove entropy consistency by choosing the test function to be an interpolant of $\bar{U}\phi$. Thus G2 in entropy variables is entropy consistent without the residual dependent artificial viscosity. The use of G2 in entropy variables was pioneered by Hughes in [12].

We continue our study of irreversibility in the compressible Euler equations in [8].

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