Three-dimensional Shock Propagation Using Kinematical Conservation Laws (KCL)

Phoolan Prasad

DEPARTMENT OF MATHEMATICS
INDIAN INSTITUTE OF SCIENCE, BANGALORE

(Based on the joint work with K. R. Arun)

Conference on New Perspectives in Nonlinear PDE's
In celebration of Blake Temples 60th birthday
The University of Michigan, Ann Arbor

May 2 - 6, 2011

Outline

1. Introduction
   - Motivation
   - Two-dimensional problem

Outline

1. Introduction
   - Motivation
   - Two-dimensional problem
2. 3-D Kinematical conservation laws
   - Derivation
   - Properties

Outline

Outline

1. Introduction
   - Motivation
   - Two-dimensional problem
2. 3-D Kinematical conservation laws
   - Derivation
   - Properties
3. Closure relations for 3-D KCL
   - Weakly nonlinear ray theory in a polytropic gas
   - Shock ray theory
4. Numerical approximation
   - Numerical scheme
   - Constrained transport

Outline

1. Introduction
   - Motivation
   - Two-dimensional problem
2. 3-D Kinematical conservation laws
   - Derivation
   - Properties
3. Closure relations for 3-D KCL
   - Weakly nonlinear ray theory in a polytropic gas
   - Shock ray theory
4. Numerical approximation
   - Numerical scheme
   - Constrained transport
5. Numerical case studies

Motivation

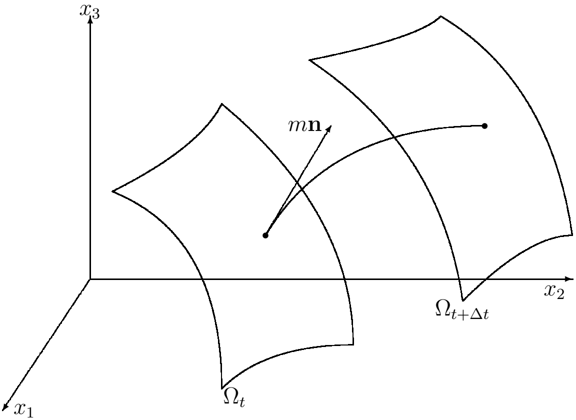


Figure: Evolution of a surface Ω_t in a ray velocity field $\boldsymbol{\chi} = m\mathbf{n}$

Different methods used in computation of successive positions of Ω_t

1. Ray tracing method
    - One of the earliest methods
    - Rays are obtained by Fermat's principle of least time
2. Level set method
    - Developed by Stanley Osher and James Sethian
    - Based on solving eikonal equations
    - It very easy to follow shapes that change the topology
    - Very popular in image processing, computer graphics, computational geometry, optimisation, computational fluid dynamics,...
3. There are many other powerful methods such as front tracking method of James Glimm and collaborators

Formation of singularities on shock fronts

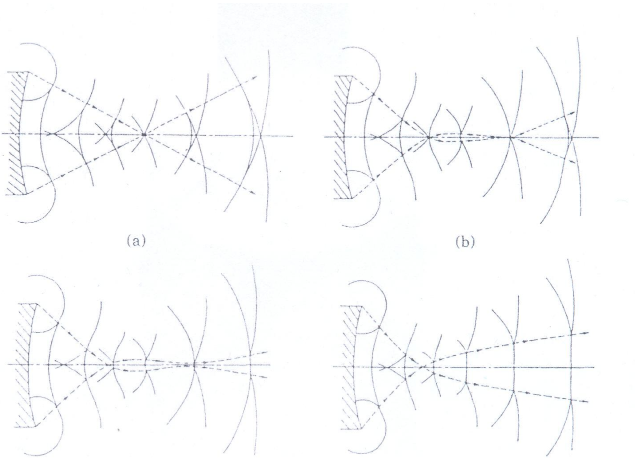
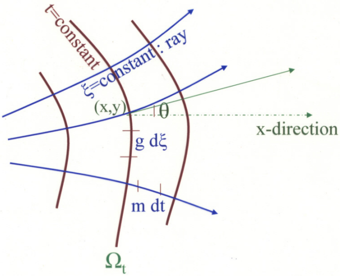


Figure: Self focusing of shock fronts (Sturtevant and Kulkarny, 1976)

- Experimental results (Sturtevant and Kulkarny, 1976) and analytical studies (Whitham, 1957, 1959) show that converging shock fronts do develop singularities.
- Evolution of wavefronts and shock fronts can be described using a ray theory.
- These governing equations of a ray theory in a differential form are not valid when singularities appear on the fronts.
- It necessitates the need for a conservative formulation of ray theories.
- Lead to the development of 2-D kinematical conservation laws (KCL) (Morton, Prasad and Ravindran, 1992).

Two-dimensional Kinematical Conservation Laws: 2-D KCL

Ray coordinate system associated with $\Omega_t : (\xi, t)$



(x, y) is a point on the moving curve Ω_t at time t.

θ= angle which the ray at (x, y) makes with x-direction.

12

- Isotropic case: rays associated with Ω_t are orthogonal to Ω_t
- m is a suitably non-dimensionalised normal velocity of propagation of Ω_t, i.e. the Mach number of Ω_t
- $\xi =$ const are rays
- $t =$ const are successive positions of Ω_t
- $g\mathrm{d}\xi$ is an element of distance along the front Ω_t
- $m\mathrm{d}t$ is an element of length along a ray.

2-D KCL

Simple geometrical considerations gives the 2-D KCL

$$(g\sin\theta)_t + (m\cos\theta)_\xi = 0, \quad (1)$$

$$(g\cos\theta)_t - (m\sin\theta)_\xi = 0. \quad (2)$$

Here m is a properly non-dimensionalised front velocity of Ω_t.

- *A pair of conservation laws in one space variable.*
- *Under-determined: two equations in three unknowns m, θ and g.*
- *Additional closure relations depending on the dynamics of Ω_t yield a completely determined system.*
- *Weak solutions can have shocks in (ξ, t)-plane.*
- *The mapping between (ξ, t)-plane and (x_1, x_2)-plane is given by the ray equations*

$$(x_{1t}, x_{2t}) = m(\cos\theta, \sin\theta). \quad (3)$$

- *Shocks are mapped onto kinks on Ω_t.*

1. Weakly nonlinear ray theory (WNLRT) for a nonlinear wavefront (Prasad and Sangeeta, 1999)

$$\left((m-1)^2 e^{2(m-1)} g\right)_t = 0. \qquad (4)$$

2. Motion of the crest line of a curved solitary wave on the surface of shallow water (Baskar and Prasad, 2003)

$$\left((m-1)^{\frac{3}{2}} e^{\frac{3}{2}(m-1)} g\right)_t = 0. \qquad (5)$$

3. Shock ray theory (SRT) for a curved weak shock (Monica and Prasad, 2001)

$$\left(G(M-1)^2 e^{2(M-1)}\right)_t + 2M(M-1)^2 e^{2(M-1)} G\mathcal{V} = 0, \qquad (6)$$

$$\left(G\mathcal{V}^2 e^{2(M-1)}\right)_t + G\mathcal{V}^3 (M+1) e^{2(M-1)} = 0. \qquad (7)$$

Here $m = M$ for a shock front and $\mathcal{V}$ is a measure of the gradient of the flow variables.

Remark

1. *The conservative formulations of many ray theories using 2-D KCL give rise to hyperbolic systems of balance laws for* $m > 1$.
2. *Analytical and numerical investigations reveal many fascinating geometrical features of the fronts (Prasad, 2001).*
3. *Very successful in modelling several physical problems:*
   - *Propagation of a weakly nonlinear wavefront in a polytropic gas.*
   - *Propagation of a curved weak shock front.*
   - *Motion of the crest line of a curved solitary wave in shallow water.*
   - *A new formulation of sonic boom produced by a manoeuvring aerofoil as a one parameter family of Cauchy problems (Baskar and Prasad, 2006).*

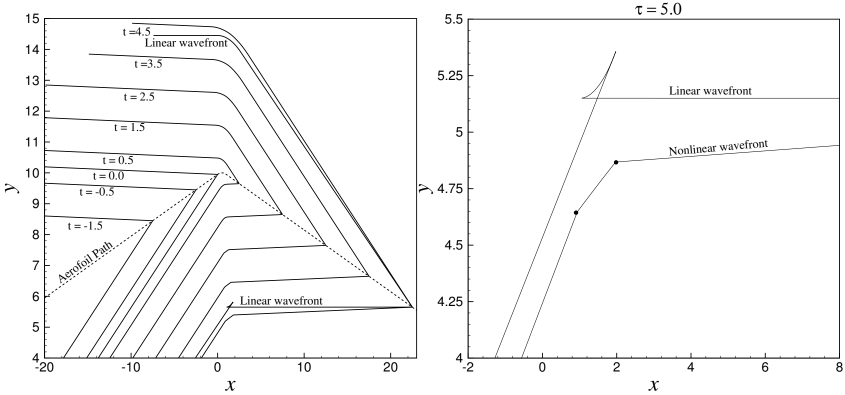


Figure: Application of 2-D KCL to the sonic boom problem

Derivation

Isotropically evolving surface Ω_t - ray equations

- Consider isotropic evolution of surface $\Omega_t \colon \varphi(\mathbf{x}, t) = 0$ in $\mathbb{R}^3$ in a ray velocity field $\boldsymbol{\chi} = m\mathbf{n}$.
- Evolution equation is the eikonal or the level set equation

$$\varphi_t + m||\nabla\varphi|| = 0, \tag{8}$$

  where m denotes the normal velocity.
- Let

$$\mathbf{n} = \frac{\nabla\varphi}{||\nabla\varphi||} \tag{9}$$

  be a unit unit normal to Ω_t.
- The Charpit's equations of (8) give the rays

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = m\mathbf{n}, \ ||\mathbf{n}|| = 1, \tag{10}$$

$$\frac{\mathrm{d}\mathbf{n}}{\mathrm{d}t} = -\mathbf{L}m := -\{\nabla - \mathbf{n}\langle\mathbf{n}, \nabla\rangle\}m \tag{11}$$

  where $\mathbf{L}$ is a tangential derivative.
- Additional equations involving $\mathbf{x}, \mathbf{n}$ and m give a complete system.

1. We introduce a ray coordinate system (ξ_1, ξ_2, t) in such a way that
   - $t = \text{const}$ is the surface Ω_t.
   - ξ_1 and ξ_2 are surface coordinates on $\mathbb{R}^3$.
2. Both $(\xi_2 = \text{const}, t = \text{const})$ and $(\xi_1 = \text{const}, t = \text{const})$ are two families of curves on Ω_t.
3. Let $\mathbf{u}$ and $\mathbf{v}$ be respectively unit tangent vectors along these curves on Ω_t so that $(\mathbf{u}, \mathbf{v}, \mathbf{n})$ forms a right handed system with

$$\mathbf{n} = \frac{\mathbf{u} \times \mathbf{v}}{||\mathbf{u} \times \mathbf{v}||}. \tag{12}$$

4. Let g_1 and g_2 be the metrics associated with the coordinates ξ_1 and ξ_2.
5. The normal velocity m serves the role of the metric associated with time t.

3-D ray coordinates

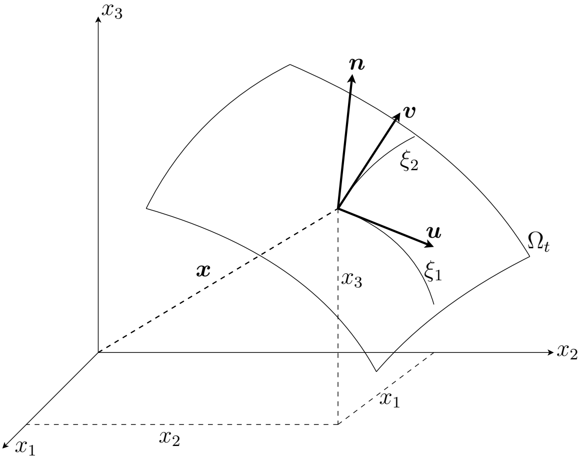


Figure: A ray coordinate system of a surface Ω_t

The displacement of a point P in $\mathbf{x}$-space due to an arbitrary displacement in (ξ_1, ξ_2, t)-space is

$$\mathrm{d}\mathbf{x} = g_1 \mathbf{u} \mathrm{d}\xi_1 + g_2 \mathbf{v} \mathrm{d}\xi_2 + m \mathbf{n} \mathrm{d}t \tag{13}$$

The integrability conditions yields the 3-D KCL

$$(g_1 \mathbf{u})_t - (m\mathbf{n})_{\xi_1} = 0, \tag{14}$$
$$(g_2 \mathbf{v})_t - (m\mathbf{n})_{\xi_2} = 0 \tag{15}$$

and

$$(g_2 \mathbf{v})_{\xi_1} - (g_1 \mathbf{u})_{\xi_2} = 0. \tag{16}$$

Remark

If the third equation is satisfied at $t = 0$, then the first two equations imply that it is satisfied for $t > 0$.

Finally, the 3-D KCL is obtained as (Giles, Prasad and Ravindran, 1996, analysed by Arun and Prasad 2009)

$$(g_1\mathbf{u})_t - (m\mathbf{n})_{\xi_1} = 0, \quad (17)$$
$$(g_2\mathbf{v})_t - (m\mathbf{n})_{\xi_2} = 0, \quad (18)$$

with ξ_1 *and* ξ_2 *so chosen that*

$$(g_2\mathbf{v})_{\xi_1} - (g_1\mathbf{u})_{\xi_2} = 0 \textit{ at } t = 0. \quad (19)$$

The number of dependent variables in 6 KCL equations	
$\mathbf{u} = (u_1, u_2, u_3)$	only 2
$\mathbf{v} = (v_1, v_2, v_3)$	only 2
(g_1, g_2)	2
m	1
Total	7, Hence under-determined system

The derivation of 3-D KCL led to an additional relation

$$(g_2\mathbf{v})_{\xi_1} - (g_1\mathbf{u})_{\xi_2} = 0. \tag{20}$$

If (20) is satisfied at $t = 0$, 3-D KCL shows that it is satisfied for all times. Let us introduce three vectors $\mathfrak{B}_k, k = 1, 2, 3$ in $\mathbb{R}^2$ via

$$\mathfrak{B}_k := (g_2 v_k, -g_1 u_k). \tag{21}$$

We rewrite (20) as

$$\text{div}(\mathfrak{B}_k) = 0, \; k = 1, 2, 3. \tag{22}$$

Thus, we have a constraint analogous to the solenoidal constraint in the equations of ideal magnetohydrodynamics. The constraint (22) is termed as 'geometric solenoidal constraint'.

Properties

Theorem

Given m *as a smooth function of* $\mathbf{x}$ *and* t*, the ray equations*

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = m\mathbf{n}, \ ||\mathbf{n}|| = 1, \tag{23}$$

$$\frac{\mathrm{d}\mathbf{n}}{\mathrm{d}t} = -\mathbf{L}m := -\{\nabla - \mathbf{n}\langle\mathbf{n}, \nabla\rangle\}m \tag{24}$$

are equivalent to the 3-D KCL

$$(g_1\mathbf{u})_t - (m\mathbf{n})_{\xi_1} = 0, \tag{25}$$

$$(g_2\mathbf{v})_t - (m\mathbf{n})_{\xi_2} = 0, \tag{26}$$

with

$$(g_2\mathbf{v})_{\xi_1} - (g_1\mathbf{u})_{\xi_2} = 0 \text{ at } t = 0. \tag{27}$$

The derivation of 3-D KCL from ray equations.

1. Assume Ω_0 to be given. Solution of ray equations give successive positions of Ω_t.
2. On Ω_t we choose the coordinates (ξ_1, ξ_2). Let the metrics be g_1, g_2 and unit tangent fields be $\mathbf{u}$ and $\mathbf{v}$ respectively.
3. Previous derivation implies 3-D KCL.

Remark

A direct derivation of the differential form of the 3-D KCL

$$g_{1t} = -m\langle \mathbf{n}, \mathbf{u}_{\xi_1} \rangle, \tag{28}$$

$$g_{2t} = -m\langle \mathbf{n}, \mathbf{v}_{\xi_2} \rangle, \tag{29}$$

$$g_1 \mathbf{u}_t = m_{\xi_1} \mathbf{n} + m\langle \mathbf{n}, \mathbf{u}_{\xi_1} \rangle \mathbf{u} + m\mathbf{n}_{\xi_1}, \tag{30}$$

$$g_2 \mathbf{v}_t = m_{\xi_2} \mathbf{n} + m\langle \mathbf{n}, \mathbf{v}_{\xi_2} \rangle \mathbf{v} + m\mathbf{n}_{\xi_2} \tag{31}$$

from the ray equations is also possible.

The derivation of ray equations from KCL.

1. Let three smooth vector functions $\mathbf{u}, \mathbf{v}$ and $\mathbf{n}$ and three smooth scalar functions m, g_1, g_2 in (ξ_1, ξ_2, t)-space, satisfying $\langle \mathbf{n}, \mathbf{u} \rangle = \langle \mathbf{n}, \mathbf{v} \rangle = 0$ and KCL be given.
2. The 3-D KCL and the geometric solenoidal constraints imply that there exists $\mathbf{x}$ such that
$$(\mathbf{x}_t, \mathbf{x}_{\xi_1}, \mathbf{x}_{\xi_2}) = (m\mathbf{n}, g_1\mathbf{u}, g_2\mathbf{v}). \tag{32}$$
3. The $t =$ const in (ξ_1, ξ_2, t)-space is mapped on to a surface Ω_t in (x_1, x_2, t)-space with ξ_1 and ξ_2 as coordinates on Ω_t and $\mathbf{u}, \mathbf{v}$ as tangent vectors. The first equation of (32) is the first part of ray equations.
4. Let Ω_t be represented by $\varphi(\mathbf{x}, t) = 0$, then the first set of ray equations shows φ satisfies the eikonal
$$\varphi_t + m||\nabla\varphi|| = 0 \tag{33}$$
This leads to the second part of ray equations.

Shock jump conditions in (ξ_1, ξ_2, t)-space

- 3-D KCL is a system of conservation laws and the Rankine-Hugoniot jump conditions across a shock give

$$K[\![g_1\mathbf{u}]\!] + E_1[\![m\mathbf{n}]\!] = 0, \ K[\![g_2\mathbf{v}]\!] + E_2[\![m\mathbf{n}]\!] = 0, \qquad (34)$$

  where K is the shock speed and (E_1, E_2) is the unit normal to a shock front in (ξ_1, ξ_2)-plane.

- Multiply the first relation in (34) by E_1 and the second relation by E_2, adding and using $E_1^2 + E_2^2 = 1,$ we get

$$E_1K[\![g_1\mathbf{u}]\!] + E_2K[\![g_2\mathbf{v}]\!] + [\![m\mathbf{n}]\!] = 0. \qquad (35)$$

- The above equation (35) also gives an expression for the shock speed K.

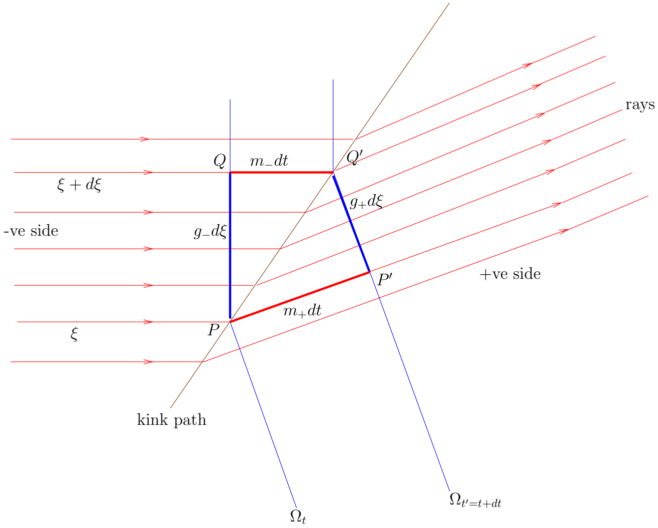


Figure: The kink path is PQ'

A kink curve on Ω_t in 3-D

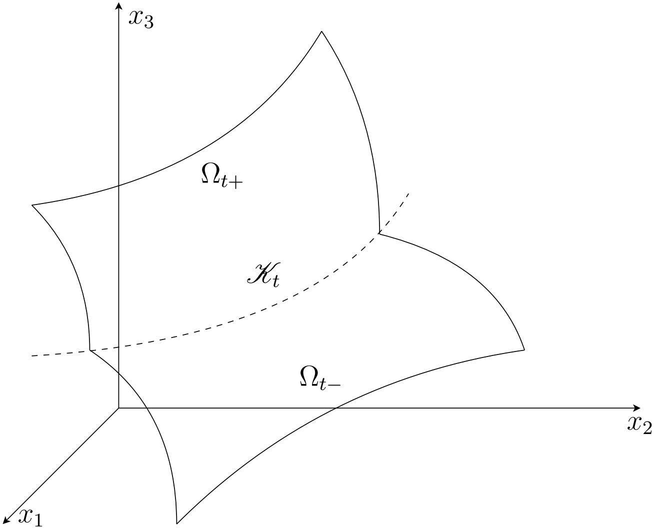


Figure: A kink curve $\mathscr{K}_t$ on Ω_t in 3-D. As Ω_t evolves, $\mathscr{K}_t$ generates a kink surface.

- We take a point $P(\mathbf{x})$ on Ω_t and another $Q'(\mathbf{x}+\mathrm{d}\mathbf{x})$ on $\Omega_{t+\mathrm{d}t}$ such that P and Q' lie on a kink surface.
- Equating the expressions for $\mathrm{d}\mathbf{x}$ on both sides of a kink surface gives $(\mathrm{d}\mathbf{x})_- = (\mathrm{d}\mathbf{x})_+$, i.e.

$$g_{1+}\mathrm{d}\xi_1\mathbf{u}_+ + g_{2+}\mathrm{d}\xi_2\mathbf{v}_+ + m_+\mathrm{d}t\mathbf{n}_+ = g_{1-}\mathrm{d}\xi_1\mathbf{u}_- + g_{2-}\mathrm{d}\xi_2\mathbf{v}_- + m_-\mathrm{d}t\mathbf{n}_-. \tag{36}$$

- Take the direction of the line element PQ' in the direction of the normal to the shock curve in (ξ_1, ξ_2)-plane, then

$$\frac{\mathrm{d}\xi_1}{\mathrm{d}t} = E_1K, \ \frac{\mathrm{d}\xi_2}{\mathrm{d}t} = E_2K. \tag{37}$$

and (35) gives

$$(g_{1+}E_1\mathbf{u}_+ + g_{2+}E_2\mathbf{v}_+)K + m_+\mathbf{n}_+ = (g_{1-}E_1\mathbf{u}_- + g_{2-}E_2\mathbf{v}_-)K + m_-\mathbf{n}_-. \tag{38}$$

- The equation (38) is same as (35) obtained from the R-H conditions!

Theorem

The six jump relations (34) imply conservation of distance in x_1, x_2 *and* x_3 *directions (and hence in any arbitrary direction in* $\mathbf{x}$*-space) in the sense that the expressions for a vector displacement* $(\mathrm{d}\mathbf{x})_{\mathscr{K}_t}$ *of a point of the kink line* $\mathscr{K}_t$ *in an infinitesimal time interval* $\mathrm{d}t$*, when computed in terms of variables on the two sides of a kink surface, have the same value. This displacement of the point is assumed to take place on the kink surface and that of its image in* (ξ_1, ξ_2, t)*-space takes place on the shock surface such that the corresponding displacement in* (ξ_1, ξ_2)*-plane is with the shock front, i.e. it is in the direction*

$$\frac{\mathrm{d}}{\mathrm{d}t}(\xi_1, \xi_2) = (E_1, E_2)K \tag{39}$$

Remark

As an implication of the above theorem we have

- *Conservation of distance on the two sides of a kink surface implies the R-H conditions.*
- *R-H conditions imply conservation of distance for a displacement along a shock ray.*

For Weakly nonlinear ray theory (WNLRT) in a polytropic gas

- So far we discussed results from 3-D KCL without closure relations.
- Now we consider the 3-D Euler equations of a polytropic gas, state represented by $(\varrho, \mathbf{q}, p)$.
- We look for its solutions which are small perturbations of a steady state $(\varrho_0, \mathbf{0}, p_0)$ with $\varrho_0 = p_0 =$ const.
- We also make a single mode approximation, i.e. solution is localised in a neighbourhood of an upstream propagating wave corresponding to the characteristic speed $\lambda = \langle \mathbf{n}, \mathbf{q} \rangle + a$.
- In the so-called high frequency approximation, the solution can be represented in terms of an amplitude w and a phase function φ.
- The disturbed region can be represented by means of a one-parameter family of wavefronts given by $\varphi =$ const and the amplitude w satisfies a transport equation along the rays.

- A perturbation of the steady state on the wavefront can be represented in terms the amplitude w via

$$\varrho - \varrho_0 = \frac{\varrho_0}{a_0} w, \ \mathbf{q} = w\mathbf{n}, \ p - p_0 = \varrho_0 a_0 w. \tag{40}$$

- The evolution of any of the wavefronts Ω_t is governed by (Prasad 1975)
  1. ray equations

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = a_0 \left(1 + \frac{\gamma+1}{2} \frac{w}{a_0}\right) n_i, \tag{41}$$

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = -a_0 \{\nabla - \mathbf{n}\langle \mathbf{n}, \nabla \rangle\} \left(1 + \frac{\gamma+1}{2} \frac{w}{a_0}\right), \tag{42}$$

  2. **coupled to** a transport equation for the amplitude

$$\left(\frac{\partial}{\partial t} + a_0 \left(1 + \frac{\gamma+1}{2} \frac{w}{a_0}\right) \langle \mathbf{n}, \nabla \rangle \right) w = a_0 \mathit{\Omega} w, \tag{43}$$

  where $\mathit{\Omega}$ is the mean curvature of Ω_t.

- The ray equations of Ω_t are equivalent to 3-D KCL. We need to get a conservation form the transport equation.
- We introduce the non-dimensional normal velocity m via

$$m := 1 + \frac{\gamma + 1}{2} \frac{w}{a_0} \tag{44}$$

- The mean curvature Ω is related to the ray tube area $\mathcal{A} = g_1 g_2 \sin\chi$, where $0 < \chi < \pi$ is the angle between the vectors $\mathbf{u}$ and $\mathbf{v}$.
- The operator $\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + m\langle \mathbf{n}, \nabla \rangle$ in space-time becomes simply the partial derivative $\frac{\partial}{\partial t}$ in the ray coordinate system (ξ_1, ξ_2, t).
- The energy transport equation becomes $\frac{2m_t}{m-1} = -\frac{1}{m\mathcal{A}}\mathcal{A}_t$.

Conservation form of the energy transport equation is obtained as

$$\left((m-1)^2 e^{2(m-1)} g_1 g_2 \sin\chi\right)_t = 0, \tag{45}$$

Complete system of conservation laws of 3-D WNLRT is given by

$$(g_1\mathbf{u})_t - (m\mathbf{n})_{\xi_1} = 0, \quad (46)$$

$$(g_1\mathbf{v})_t - (m\mathbf{n})_{\xi_2} = 0, \quad (47)$$

$$\left((m-1)^2 e^{2(m-1)} g_1 g_2 \sin\chi\right)_t = 0. \quad (48)$$

with the constraint

$$(g_2\mathbf{v})_{\xi_1} - (g_1\mathbf{u})_{\xi_2} = 0 \ \textit{at} \ t = 0. \quad (49)$$

Eigen-structure of the equations of 3-D KCL based WNLRT

- Differential form of the conservation laws for the variable $V = (u_1, u_2, v_1, v_2, m, g_1, g_2)$ can be written

$$AV_t + B^{(1)} V_{\xi_1} + B^{(2)} V_{\xi_2} = 0. \tag{50}$$

Here $A, B^{(1)}$ and $B^{(2)}$ are 7×7 matrices.

- The hyperbolicity of the system (50) depends on whether the roots of the characteristic equation

$$\det(e_1 B^{(1)} + e_2 B^{(2)} - \lambda A) = 0 \tag{51}$$

are real or not.

- The expressions for $A, B^{(1)}$ and $B^{(2)}$ are so complicated that we could not solve (51) directly.
- Main difficulty is how to check the hyperbolicity?

Transformation of coordinates to get eigenvalues from **frozen** orthogonal coordinates **at a point** to the general case

- Frozen orthogonal coordinates (η_1, η_2) with $\langle \mathbf{u}', \mathbf{v}' \rangle = 0$. Expressions for the eigenvalues have been obtained in this case.
- General coordinates (ξ_1, ξ_2) with $\mathbf{u}$ and $\mathbf{v}$.
- Suppose

$$\mathbf{u}\prime = \gamma_1 \mathbf{u} + \delta_1 \mathbf{v}, \;\; \mathbf{v}\prime = \gamma_2 \mathbf{u} + \delta_2 \mathbf{v}. \tag{52}$$

Theorem

Let λ' be an expression for an eigenvalue of equations in frozen orthogonal coordinates in terms of e_1'/g_1' and e_2'/g_2'. Then the expression for the same eigenvalue in the coordinates (ξ_1, ξ_2) in terms of e_1/g_1 and e_2/g_2 can be obtained from it by replacing e_1'/g_1' and e_2'/g_2' by

$$\lambda' = \lambda, \;\; \frac{e_1'}{g_1'} = \gamma_1 \frac{e_1}{g_1} + \delta_1 \frac{e_2}{g_2}, \;\; \frac{e_2'}{g_2'} = \gamma_2 \frac{e_1}{g_1} + \delta_2 \frac{e_2}{g_2}. \tag{53}$$

- Let (ξ_1, ξ_2) be the given surface coordinates at a point P_0 on Ω_t with unit vectors $(\mathbf{u}, \mathbf{v})$.
- We choose an orthogonal coordinates at P_0 with unit vectors $(\mathbf{u}', \mathbf{v}')$ as $\mathbf{u}' = \mathbf{u},\ \mathbf{v}' = \gamma_2 \mathbf{u} + \delta_2 \mathbf{v}$ so that $\langle \mathbf{u}', \mathbf{v}' \rangle = 0$ and $||\mathbf{v}'|| = 1$.
- The unknown coefficients can be obtained as

$$\gamma_1 = 1,\ \delta_1 = 0, \gamma_2 = -\frac{\cos\chi}{\sin\chi},\ \delta_2 = \frac{1}{\sin\chi}. \tag{54}$$

- The signs of γ_2 and δ_2 are so chosen that vectors $(\mathbf{u}', \mathbf{v}', \mathbf{n}')$ form a right handed system.
- Expressions for the eigenvalues in orthogonal coordinates are known. Using the theorem, we get the eigenvalues $\lambda_1, \lambda_2 = -\lambda_1, \lambda_3 = \cdots = \lambda_7 = 0$, where

$$\lambda_1 = \left\{ \frac{m-1}{2\sin^2\chi} \left(\frac{e_1^2}{g_1^2} - \frac{2e_1e_2}{g_1g_2}\cos\chi + \frac{e_2^2}{g_2^2} \right) \right\}^{1/2}. \tag{55}$$

We summarise our results as follows.

Theorem

The 3-D WNLRT system has seven eigenvalues $\lambda_1, \lambda_2(= -\lambda_1), \lambda_3 = \lambda_4 = \cdots = \lambda_7 = 0$, *where* λ_1 *and* λ_2 *are real for* $m > 1$ *and purely imaginary for* $m < 1$. *Further, the dimension of the eigenspace corresponding to the multiple eigenvalue* 0 *is* 4.

Remark

1. *This important theorem completely describes the nature of the equations of WNLRT.*
2. *It shows that the system is degenerate and it would require considerable effort to solve it numerically even in the case* $m > 1$.
3. *We need to develop a numerical method which respects the geometric solenoidal constraint also.*

Physical interpretation of $m > 1$ and $m < 1$

1. $m > 1$ corresponds to a pulse in which the the gas pressure is greater than that in the ambient medium in which the waves are moving. In this case the WNLRT equations form a weakly hyperbolic system.
2. $m < 1$ corresponds to a pulse in which the the gas pressure is less than that in the ambient medium in which the waves are moving. In this case the WNLRT equations form a system, in which two eigenvalues are imaginary and the multiple eigenvalue of multiplicity five is real but with incomplete eigenspace.
3. We have tried to solve a Cauchy problem for $m < 1$ for the much simpler case of 2-D KCL. This involved solving an ill posed nonlinear Cauchy problem but we succeeded in solving only some model problems and not the original problem.

For shock ray theory (SRT) in a polytropic gas

- From the R-H conditions for the Euler equations we can obtain an evolution equation for a shock surface $\Omega_t \colon s(\mathbf{x}, t) = 0$

$$s_t + \langle \mathbf{q}_r, \nabla \rangle s + A||\nabla s|| = 0, \quad (56)$$

where $\mathbf{q}_r$ is the fluid velocity ahead of the shock, $\mathbf{N}$ the unit normal to the shock front and A is the normal speed of the shock relative to the gas ahead of it.

- Using (56) we can define the shock ray velocity (Prasad, 1982)

$$\boldsymbol{\chi} = \mathbf{q}_r + A\mathbf{N}, \quad (57)$$

- Given the velocity $\boldsymbol{\chi}$ the evolution equations for the shock rays can be obtained.
- How to get a transport equation for the shock amplitude?

Weak shock theory

- Grinfel'd (1978) and Maslov (1980) have independently shown that there is an infinity of transport equations for the amplitude and its normal derivatives behind the shock.
- Dealing with this infinite system is very difficult even in the 1-D case.
- For a weak shock the infinite system can be truncated at the second stage (Prasad and Ravindran, 1990).
- A weak shock theory can also be deduced from the weakly nonlinear ray theory (Prasad, 1982).

Theorem

For a weak shock, the shock ray velocity components are equal to the mean of the bicharacteristic velocity components just ahead and just behind the the shock, provided we take the wavefronts generating the characteristic surface ahead and behind to be instantaneously coincident with the shock surface. Similarly, the rate of turning of the shock front is also equal to the mean of the rates of turning of such wavefronts just ahead and just behind the shock.

Equations of a 3-D shock ray theory (SRT) for a weak shock

Evolution of the shock front is governed by

1. Shock ray equations

$$\frac{\mathrm{d}\mathbf{X}}{\mathrm{d}T} = a_0\left(1 + \epsilon\frac{\gamma+1}{4}\mu\right)\mathbf{N}, \tag{58}$$

$$\frac{\mathrm{d}\mathbf{N}}{\mathrm{d}T} = -\epsilon\frac{\gamma+1}{4}a_0\mathbf{L}\mu, \tag{59}$$

   where $\epsilon\mu$ is a measure of the shock amplitude $\mathbf{L} = \{\nabla - \mathbf{N}\langle\mathbf{N},\nabla\rangle\}$ is a tangential derivative along the shock front and $\frac{\mathrm{d}}{\mathrm{d}T} = \frac{\partial}{\partial t} + a_0 M\langle\mathbf{N},\nabla\rangle$.

2. An infinite system of transport equations

$$\frac{\mathrm{d}\mu}{\mathrm{d}T} = a_0\Omega_s\mu - \frac{\gamma+1}{4}\mu\mu_1, \tag{60}$$

$$\frac{\mathrm{d}\mu_1}{\mathrm{d}T} = a_0\Omega_s\mu_1 - \frac{\gamma+1}{2}\mu_1^2 - \frac{\gamma+1}{4}\mu\mu_2, \tag{61}$$

$$\frac{\mathrm{d}\mu_2}{\mathrm{d}T} = \cdots \tag{62}$$

- We truncate the infinite system by removing the term containing μ_2 in the second equation.
- Let us define two non-dimensional variables

$$M := 1 + \epsilon \frac{\gamma + 1}{4} \mu, \ \mathcal{V} := \frac{\gamma + 1}{4} \mu_1. \tag{63}$$

We also take T as a non-dimensional time measured while moving along a shock ray.

- The truncated system in the variables M and $\mathcal{V}$ reads

$$\frac{\mathrm{d}M}{\mathrm{d}T} = \Omega_s (M - 1) - \mathcal{V}(M - 1), \tag{64}$$

$$\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}T} = \Omega_s \mathcal{V} - 2\mathcal{V}^2 \tag{65}$$

Here Ω_s is the non-dimensional mean curvature of the shock front.

As in the case of WNLRT we derive the conservation form of last two equations.

The complete system of conservation form of 3-D shock ray theory (SRT)

$$(G_1\mathbf{U})_t - (M\mathbf{N})_{\xi_1} = 0, \quad (66)$$

$$(G_2\mathbf{V})_t - (M\mathbf{N})_{\xi_2} = 0. \quad (67)$$

$$\left\{(M-1)^2 e^{2(M-1)} G_1 G_2 \sin\chi\right\}_t = -2M(M-1)^2 e^{2(M-1)} G_1 G_2 \mathcal{V} \sin\chi, \quad (68)$$

$$\left\{e^{2(M-1)} G_1 G_2 \mathcal{V}^2 \sin\chi\right\}_t = -(M+1) e^{2(M-1)} G_1 G_2 \mathcal{V}^3 \sin\chi. \quad (69)$$

with the constraint

$$(G_2\mathbf{V})_{\xi_1} - (G_1\mathbf{U})_{\xi_2} = 0 \text{ at } t = 0. \quad (70)$$

Eigen-structure of the equations of 3-D KCL based SRT

Theorem

The system (66)-(69) has eight eigenvalues
$\lambda_1, \lambda_2\ (= -\lambda_1), \lambda_3 = \lambda_4 = \cdots = \lambda_8 = 0$,
where

$$\lambda_1 = \left\{ \frac{M-1}{2\sin^2\chi} \left(\frac{e_1^2}{G_1^2} - \frac{2e_1e_2}{G_1G_2}\cos\chi + \frac{e_2^2}{G_2^2} \right) \right\}^{\frac{1}{2}} \tag{71}$$

Here λ_1 *and* λ_2 *are real for* $M > 1$ *and pure imaginary for* $M < 1$*. Further, the dimension of the eigenspace corresponding to the multiple eigenvalue zero is five.*

Numerical scheme

Conservation forms of 3-D WNLRT and 3-D SRT can be recast in the usual divergence form

$$W_t + F_1(W)_{\xi_1} + F_2(W)_{\xi_2} = S(W). \tag{72}$$

For 3-D WNLRT:

$$\begin{aligned} W &= \left(g_1\mathbf{u}, g_2\mathbf{v}, (m-1)^2 e^{2(m-1)} g_1 g_2 \sin\chi\right)^T, \\ F_1(W) &= (m\mathbf{n}, \mathbf{0}, 0,)^T, \\ F_2(W) &= (\mathbf{0}, m\mathbf{n}, 0,)^T, \\ S(W) &= (\mathbf{0}, \mathbf{0}, 0)^T. \end{aligned} \tag{73}$$

For 3-D SRT:

$$\begin{aligned} W &= \left(G_1\mathbf{U}, G_2\mathbf{V}, (M-1)^2 e^{2(M-1)} G_1 G_2 \sin\chi, e^{2(M-1)} G_1 G_2 \mathcal{V}^2 \sin\chi\right)^T, \\ F_1(W) &= (M\mathbf{N}, \mathbf{0}, 0, 0)^T, \\ F_2(W) &= (\mathbf{0}, M\mathbf{N}, 0, 0)^T, \\ S(W) &= \left(\mathbf{0}, \mathbf{0}, -2M(M-1)^2 e^{2(M-1)} G_1 G_2 \mathcal{V} \sin\chi, -(M+1) e^{2(M-1)} G_1 G_2 \mathcal{V}^3 \sin\chi\right)^T. \end{aligned} \tag{74}$$

- Numerical modelling of weakly hyperbolic systems is quite difficult.
- They are known to be more sensitive to numerical schemes than strictly hyperbolic systems.
- Due to lack of hyperbolicity, upwind schemes are not applicable.
- Central finite volume schemes are less dependent on the hyperbolic structure.
- Central schemes also avoid the solution of complex Riemann problems and characteristic decompositions.
- This is particularly important in multi-dimensional problems, where there are no exact Riemann solvers.
- High order accuracy can be easily achieved by standard recovery procedures and Runge-Kutta time stepping.
- The 'geometric solenoidal constraint' has also to be enforced.

We use rectangular mesh cells with mesh sizes h_1 and h_2. Let us denote by $\overline{W}_{i,j}$, the cell average of W at time t taken over a mesh cell $C_{i,j}$, i.e.

$$\overline{W}_{i,j}(t) := \frac{1}{h_1 h_2} \int_{C_{i,j}} W(\xi_1, \xi_2, t) \mathrm{d}\xi_1 \mathrm{d}\xi_2. \tag{75}$$

First, a piecewise linear interpolant is reconstructed from the given cell averages $\overline{W}^n_{i,j}$ at time $t^n = n\Delta t$,

$$W(\xi_1, \xi_2, t^n) = \sum_{i,j} \left(\overline{W}^n_{i,j} + W'_{i,j} \left(\xi_1 - \xi_{1i}\right) + W^{\backprime}_{i,j} \left(\xi_2 - \xi_{2j}\right) \right) \mathbb{1}_{i,j}(\xi_1, \xi_2), \tag{76}$$

where $\mathbb{1}_{i,j}$ is the characteristic function of the cell $C_{i,j}$ and $W'_{i,j}$ and $W^{\backprime}_{i,j}$ are respectively the discrete slopes in ξ_1- and ξ_2- directions.

The slopes can be computed by the central weighted essentially non-oscillatory (CWENO) limiter (Jiang and Shu, 1996)

$$\begin{aligned} W'_{i,j} &= \text{CWENO}\left(\frac{\overline{W}^n_{i+1,j} - \overline{W}^n_{i,j}}{h_1}, \frac{\overline{W}^n_{i,j} - \overline{W}^n_{i-1,j}}{h_1}\right), \\ W^{\backprime}_{i,j} &= \text{CWENO}\left(\frac{\overline{W}^n_{i,j+1} - \overline{W}^n_{i,j}}{h_2}, \frac{\overline{W}^n_{i,j} - \overline{W}^n_{i,j-1}}{h_2}\right), \end{aligned} \tag{77}$$

where the CWENO function is defined by

$$\text{CWENO}(a,b) = \frac{\omega(a)\cdot a + \omega(b)\cdot b}{\omega(a)+\omega(b)}, \; \omega(a) = \left(\epsilon + a^2\right)^{-2}, \; \epsilon = 10^{-6}. \tag{78}$$

A semi-discrete approximation of the system of balance laws reads

$$\frac{\mathrm{d}\overline{W}_{i,j}}{\mathrm{d}t} = -\frac{\mathcal{F}1_{i+\frac{1}{2},j} - \mathcal{F}1_{i-\frac{1}{2},j}}{h_1} - \frac{\mathcal{F}2_{i,j+\frac{1}{2}} - \mathcal{F}2_{i,j-\frac{1}{2}}}{h_2} + S(\overline{W}_{i,j}). \quad (79)$$

We use the Kurganov-Tadmor high resolution numerical fluxes

$$\mathcal{F}1_{i+\frac{1}{2},j}\left(W^R_{i,j}, W^L_{i+1,j}\right) = \frac{1}{2}\left(F_1\left(W^L_{i+1,j}\right) + F_1\left(W^R_{i,j}\right)\right) - \frac{a_{i+\frac{1}{2},j}}{2}\left(W^L_{i+1,j} - W^R_{i,j}\right),$$
$$\mathcal{F}2_{i,j+\frac{1}{2}}\left(W^T_{i,j}, W^B_{i,j+1}\right) = \frac{1}{2}\left(F_2\left(W^B_{i,j+1}\right) + F_2\left(W^T_{i,j}\right)\right) - \frac{a_{i,j+\frac{1}{2}}}{2}\left(W^B_{i,j+1} - W^T_{i,j}\right). \quad (80)$$

Here the maximal propagation speed at the right hand vertical edge of the cell $C_{i,j}$ is given by

$$a_{i+\frac{1}{2},j} := \max\left\{\rho\left(\frac{\partial F_1}{\partial W}\left(W^R_{i,j}\right)\right), \rho\left(\frac{\partial F_1}{\partial W}\left(W^L_{i+1,j}\right)\right)\right\} \quad (81)$$

Let us denote

$$\mathcal{L}_{i,j}(W) = -\frac{\mathcal{F}_{1_{i+\frac{1}{2},j}} - \mathcal{F}_{1_{i-\frac{1}{2},j}}}{h_1} - \frac{\mathcal{F}_{2_{i,j+\frac{1}{2}}} - \mathcal{F}_{2_{i,j-\frac{1}{2}}}}{h_2} + S(\overline{W}_{i,j}) \quad (82)$$

To improve the temporal accuracy and to gain second order accuracy in time we use a TVD Runge-Kutta scheme consisting of two stages

$$\begin{aligned} W_{i,j}^{(1)} &= \overline{W}_{i,j}^{n} + \Delta t \mathcal{L}_{i,j}\left(W^{n}\right), \\ \overline{W}_{i,j}^{n+1} &= \frac{1}{2}\overline{W}_{i,j}^{n} + \frac{1}{2}W_{i,j}^{(1)} + \frac{1}{2}\Delta t \mathcal{L}_{i,j}\left(W^{(1)}\right). \end{aligned} \quad (83)$$

Constrained transport

- A discrete analogue of the geometric solenoidal constraint has to be satisfied by the numerical solution.
- This is important particularly at discontinuities, where the discretisation errors can produce very large divergences.
- This can lead to oscillatory or even unphysical solutions.
- Therefore we use a constrained transport to enforce the constraints as in the case of MHD.
- The conditions $\text{div}(\mathfrak{B}_k) = 0$, implies the existence of three potentials $\mathbb{A}_k, k = 1, 2, 3$ such that

$$g_1 u_k = \mathbb{A}_{k\xi_1}, \; g_2 v_k = \mathbb{A}_{k\xi_2}. \tag{84}$$

- The 3-D KCL system can be converted into three evolution equations

$$\mathbb{A}_{kt} - m n_k = 0. \tag{85}$$

Grid staggering

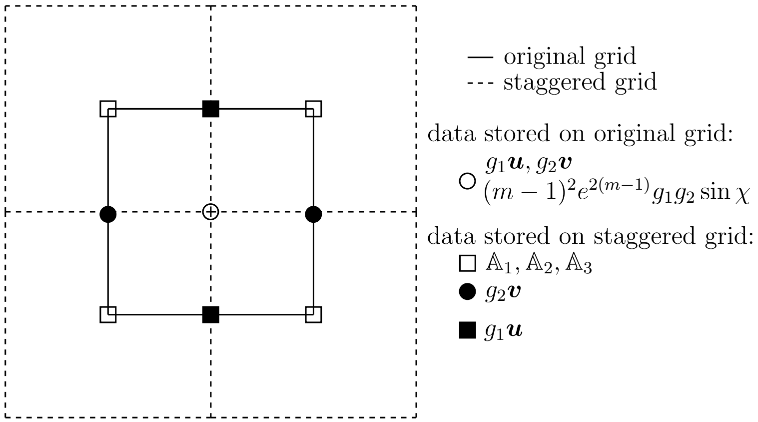


Figure: Arrangement of the variables in the grids.

The corrected values of the vectors $g_1\mathbf{u}$ and $g_2\mathbf{v}$ are obtained as

$$\begin{aligned} [g_1 u_k]^{n+1}_{i,j+\frac{1}{2}} &= \frac{1}{h_1}\left(\mathbb{A}_{k\,i+\frac{1}{2},j+\frac{1}{2}} - \mathbb{A}_{k\,i-\frac{1}{2},j+\frac{1}{2}}\right), \\ [g_2 v_k]^{n+1}_{i+\frac{1}{2},j} &= \frac{1}{h_2}\left(\mathbb{A}_{k\,i+\frac{1}{2},j+\frac{1}{2}} - \mathbb{A}_{k\,i+\frac{1}{2},j-\frac{1}{2}}\right). \end{aligned} \tag{86}$$

The discrete divergence is now zero:

$$\begin{aligned} [\text{div}(\mathfrak{B}_k)]^{n+1}_{i,j} &= \frac{[g_2 v_k]^{n+1}_{i+\frac{1}{2},j} - [g_2 v_k]^{n+1}_{i-\frac{1}{2},j}}{h_1} - \frac{[g_1 u_k]^{n+1}_{i,j+\frac{1}{2}} - [g_1 u_k]^{n+1}_{i,j-\frac{1}{2}}}{h_2} \\ &= 0, \quad \text{using (86).} \end{aligned} \tag{87}$$

- Integrating $\mathbb{A}_{kt} = mn_k$ over a staggered grid gives the update formula

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\mathbb{A}_k\right]_{i+\frac{1}{2},j+\frac{1}{2}} = \left[mn_k\right]_{i+\frac{1}{2},j+\frac{1}{2}} \tag{88}$$

- How to evaluate the term on the RHS?
- Note that the factor mn_k appears in the flux functions F_1 and F_2.
- The numerical flux functions $\mathcal{F}_1$ and $\mathcal{F}_2$ at the interfaces are already available from the central scheme.
- Following the approach of Ryu et.al (1998) we take

$$\left[mn_k\right]_{i+\frac{1}{2},j+\frac{1}{2}} = \frac{1}{4}\left(\left[mn_k\right]_{i+\frac{1}{2},j} + \left[mn_k\right]_{i+\frac{1}{2},j+1} + \left[mn_k\right]_{i,j+\frac{1}{2}} + \left[mn_k\right]_{i+1,j+\frac{1}{2}}\right). \tag{89}$$

Formulation of the initial data for the conservation laws

- Let the initial position of a weakly nonlinear wavefront or a shock front Ω_t be given as

$$\Omega_0 \colon \mathbf{x} = \mathbf{x}_0(\xi_1, \xi_2). \tag{90}$$

- On Ω_0 we choose

$$g_{10} = ||\mathbf{x}_{0\xi_1}||, \;\; g_{20} = ||\mathbf{x}_{0\xi_2}||, \tag{91}$$

$$\mathbf{u}_0 = \frac{\mathbf{x}_{0\xi_1}}{||\mathbf{x}_{0\xi_1}||}, \;\; \mathbf{v}_0 = \frac{\mathbf{x}_{0\xi_2}}{||\mathbf{x}_{0\xi_2}||}. \tag{92}$$

- The geometric solenoidal constraint is satisfied by the initial values at time $t = 0$.

- Let the distribution of the front velocity be given by

$$m = m_0(\xi_1, \xi_2). \tag{93}$$

- For a shock front, let us assume that $\mathcal{V} = \mathcal{V}_0(\xi_1, \xi_2)$ is given.
- The potentials $\mathbb{A}_k$s need to be initialised on the staggered grids so that

$$g_1 u_k = \mathbb{A}_{k\xi_1}, \ g_2 v_k = \mathbb{A}_{k\xi_2}. \tag{94}$$

- The choice

$$\mathbb{A}_{k0}(\xi_1, \xi_2) = \mathbf{x}_{k0}(\xi_1, \xi_2) \tag{95}$$

will serve the purpose.

Boundary conditions

Boundary conditions

- The potentials on the staggered grid needs a boundary condition.
- Depending on the problem, a ghost layer BC or periodic BC can applied.
- Ghost cell BC gives zero values for $g_1\mathbf{u}$ and $g_2\mathbf{v}$ due to the spatial derivatives.
- This can cause oscillations at the boundary cells.
- We can safely neglect the boundary values of the potentials and implement a boundary condition directly for conservative variables.

Remark

- *Solution to the Cauchy problem for a weakly hyperbolic system contains a Jordan mode which grows polynomially in time.*
- *Systems of conservation laws with a strictly convex entropy can be symmetrised (Friedrichs and Lax, 1971).*
- *Any system of conservation laws admitting a convex extension can be symmetrised by integrating the stationary differential constraints.*
- *The symmetrisation hyperbolises even degenerate systems with constraints (Boillat, 1982).*
- *Examples: Landau's superfluid equations, Lundquist equations.*
- *We could not make use of these results as we have not been able to get a convex entropy.*

Analysis of linearised 3-D WNLRT showing control of the Jordan mode

We linearised the 3-D WNLRT or 3-D SRT systems about a planar front and solved the general initial value problem to derive

Theorem

The solution of the Cauchy problem for the linearised systems

$$AW_t + B^{(1)}W_{\xi_1} + B^{(1)}W_{\xi_2} = 0, \quad (96)$$

$$W(\xi_1, \xi_2, 0) = W_0(\xi_1, \xi_2) \quad (97)$$

does not contain any Jordan mode under the constraint

$$(g_2\mathbf{v})_{\xi_1} - (g_1\mathbf{u})_{\xi_2} = 0 \text{ at } t = 0. \quad (98)$$

Remark

- *Due to the nonlinearity, the result could not be obtained for the full nonlinear system.*
- *We strongly believe it to be true also for the original system.*
- *The numerical results do not exhibit instability or any growth of the Jordan mode.*

Numerical case studies with the 3-D KCL based shock ray theory

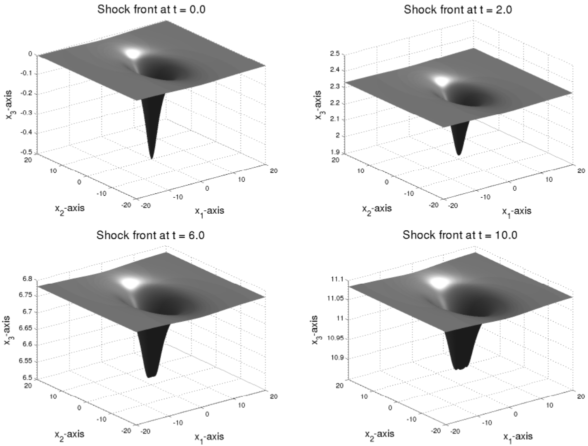


Figure: The successive positions of a shock front Ω_t with an initial smooth dip which is not axisymmetric.

Smooth dip results: SRT

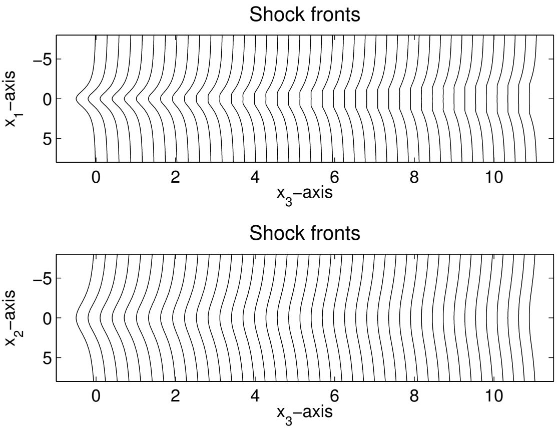


Figure: The sections of the shock fronts at times $t = 0.0, \ldots, 10.0$ with a time step 0.5. On the top: in $x_2 = 0$ plane. Bottom: in $x_1 = 0$ plane.

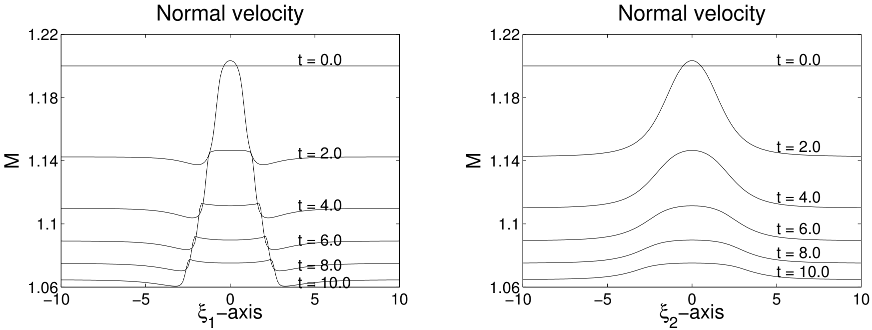


Figure: The time evolution of the normal velocity m. Left: along ξ_1-direction in the section $\xi_2 = 0$. Right: along ξ_2-direction in the section $\xi_1 = 0$.

Our numerical approximation preserves the geometric solenoidal condition almost to machine accuracy. This is true for all the numerical results we obtained.

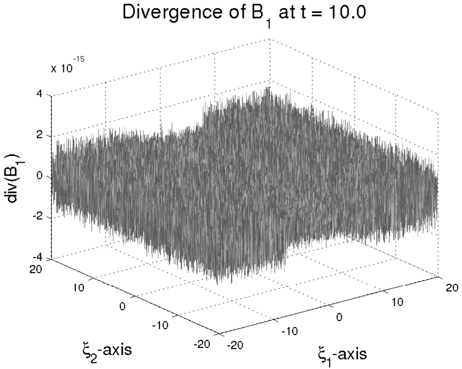


Figure: The divergence of $\mathfrak{B}_1$ at $t = 10.0$. The error is of the order of 10^{-15}.

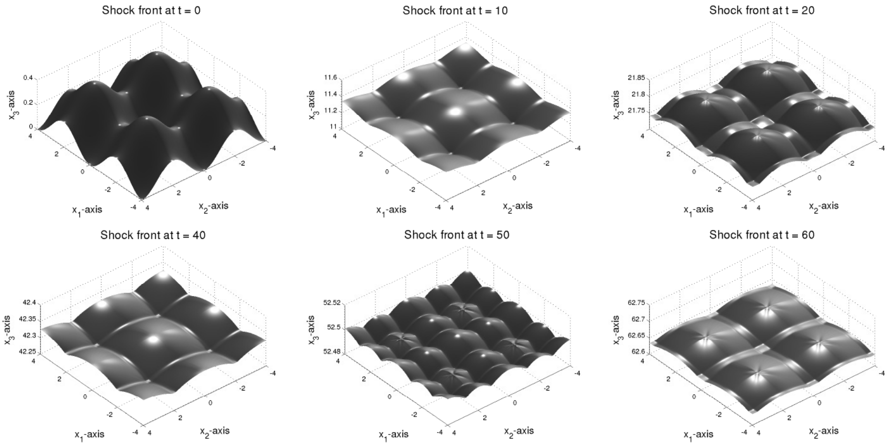


Figure: Shock front Ω_t starting initially in a periodic shape with $m_0 = 1.2$. The front develops a complex pattern of kinks and ultimately becomes planar.

Corrugation stability: SRT

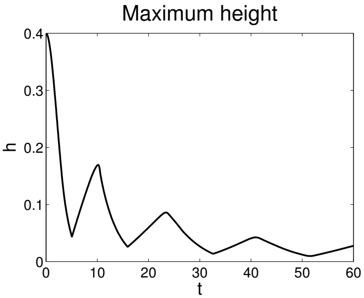


Figure: Left: variation of front height with time from from $t = 0$ to $t = 60$. Right: variation of $M_{\max}(t)$ and $M_{\min}(t)$.

Converging shock front: initial shape circular cylinder with nonuniform m

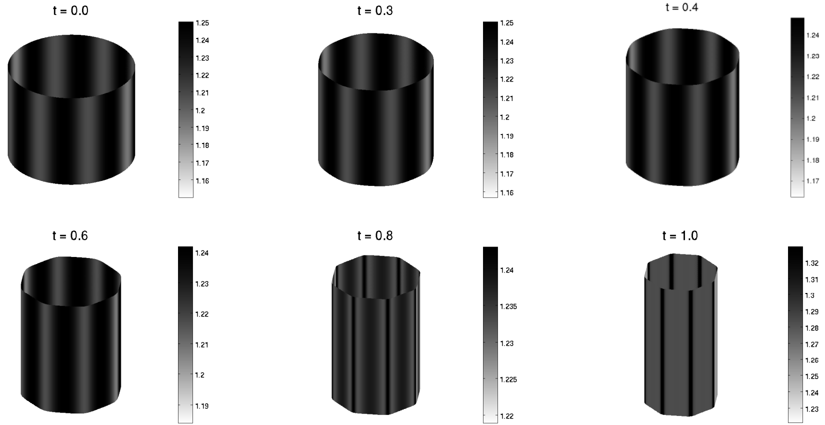


Figure: Cylindrically converging shock fronts at times $t = 0.0, 0.2, 0.6, 0.8, 1.0$. The initial front is in the shape of a circular cylinder. The colour bar on the right hand side indicates the intensity of the normal velocity m.

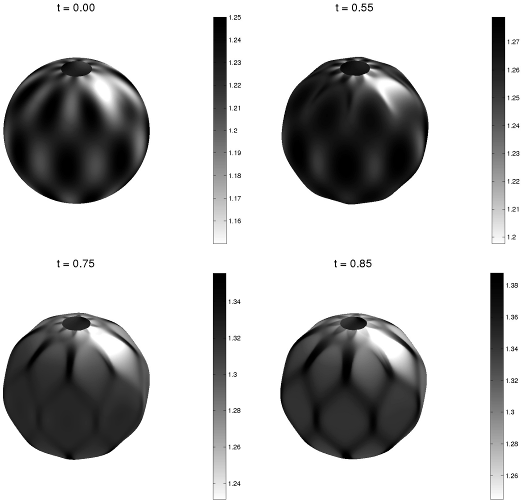


Figure: Spherically focusing shock fronts at times $t = 0.0, 0.5, 0.75, 0.85$. The colour bar on the right represents the distribution of m.

K. R. Arun and P. Prasad.
3-D kinematical conservation laws (KCL): evolution of a surface in $\mathbb{R}^3$-in particular propagation of a nonlinear wavefront.
Wave Motion, 46:293–311, 2009.

K. R. Arun, M. Lukáčová-Medviďová, P. Prasad, and S. V. Raghurama Rao.
An application of 3-D kinematical conservation laws: propagation of a three dimensional wavefront.
SIAM. J. Appl. Math., 70:2604–2626, 2010.

K. R. Arun and P. Prasad.
Eigenvalues of kinematical conservation laws (KCL) based 3-D weakly nonlinear ray theory (WNLRT).
Appl. Math. comput., 217:2285–2288, 2010.

K. R. Arun.
A Numerical Scheme for Three-dimensional Front Propagation and Control of Jordan Mode
Technical report, Department of Mathematics, Indian Institute of Science, Bangalore, 2010.

K. R. Arun and P. Prasad.
Propagation of a three-dimensional weak shock front using kinematical conservation laws.
Technical report, Department of Mathematics, Indian Institute of Science, Bangalore, 2011.

P. Prasad.
Nonlinear Hyperbolic Waves in Multi-dimensions.
Chapman and Hall/CRC, London, 2001.

Thank You for Your Attention!