

# Numerical study on 2D Riemann problems using state of the art solvers

Ferre Van Assche, Vergauwen Bob

KU Leuven

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# Outline

Introduction

Numerical schemes

Software and computations

Numerical results

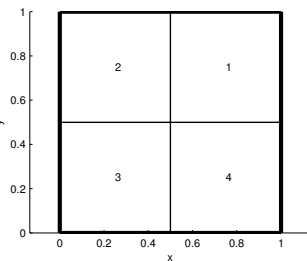
# Introduction

## Riemann problem in 2D

A Riemann problem consists of a system of conservation equation together with a piecewise constant initial condition.

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

$$U_0(x, y) = \begin{cases} u_1 & (x, y) \in [0.5, 1]^2 \\ u_2 & (x, y) \in [0, 0.5] \times [0.5, 1] \\ u_3 & (x, y) \in [0, 0.5]^2 \\ u_4 & (x, y) \in [0.5, 1] \times [0, 0.5] \end{cases}$$



# The equations

## Euler equation for compressible fluids

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

with

$$U = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ e \end{pmatrix} \quad F = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(e + p) \end{pmatrix} \quad G = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(e + p) \end{pmatrix}$$

Equation describing the dynamics of a compressible fluid.

Conserved quantities are:  $\rho$  density,  $\rho u$  momentum in  $x$ ,  $\rho v$  momentum in  $y$  and the total energy  $e$ .

# Numerical methods

5 different numerical schemes tested:

- ▶ TVDLF
- ▶ HLL
- ▶ HLLC
- ▶ TVD-MUSCL
- ▶ FD

# TVDLF - Total Variation Diminishing (TVD) concept

Total variation of numerical approximation of  $u$ :

$$TV(u^n) = \sum_{i=0}^N |u_{i+1}^n - u_i^n|$$

Scheme is total variation diminishing in time if

$$TV(u^{n+1}) \leq TV(u^n) \quad \forall n$$

# TVDLF

First order Lax-Friedrichs scheme:

$$U_j^{n+1} = U_j^n - \frac{\Delta t}{\Delta x} (F_{j+1/2} - F_{j-1/2}) + \frac{1}{2} (\Phi_{j+1/2} - \Phi_{j-1/2})$$

where

$$F_{j+1/2} = \frac{F_j + F_{j+1}}{2}$$

$$\Phi_{j+1/2} = U_{j+1} - U_j$$

Scheme is TVD  $\Leftrightarrow$  CFL condition satisfied

Scheme is first order accurate

Reduce numerical diffusion (with local Courant number, maximal speed):

$$\Phi_{j+1/2} = \frac{\Delta t}{\Delta x} c_{j+1/2}^{max} (U_{j+1} - U_j)$$

## TVDLF - second order spatial accuracy

Linear approximation of  $U$  and fluxes at boundary interfaces

$U$  at  $x_{j+1/2}$ , linear interpolation:

$$U_{j+1/2}^L = U_j^n + \frac{1}{2} \Delta \bar{U}_j^n$$

$$U_{j+1/2}^R = U_{j+1}^n - \frac{1}{2} \Delta \bar{U}_{j+1}^n$$

Limited slopes  $\Delta \bar{U}$  will be defined later

$$F_{j+1/2} = \frac{F(U_{j+1/2}^L) + F(U_{j+1/2}^R)}{2}$$

$$\Phi_{j+1/2} = \frac{\Delta t}{\Delta x} c_{j+1/2}^{\max} \left( U_{j+1/2}^R - U_{j+1/2}^L \right)$$



## TVDLF - slope limiter

Required to ensure TVD property

For example *minmod* limiter

$$\bar{\Delta}U_j = \text{minmod}(\Delta U_{j-1/2}, \Delta U_{j+1/2})$$

with

$$\Delta U_{j+1/2} = U_{j+1} - U_j$$

and

$$\text{minmod}(w_1, w_2, \dots, w_n) = \\ \text{sgn}(w_1) \max[0, \min(|w_1|, \text{sgn}(w_1)w_2, \dots, \text{sgn}(w_1)w_n)]$$

The *minmod* function takes the argument with the smallest modulus when all arguments have the same signs and otherwise it is zero.

## TVDLF - Temporally second order accuracy

Use Hancock's predictor step:

$$U_j^{n+1/2} = U_j^n - \frac{1}{2} \frac{\Delta t}{\Delta x} \left[ F(U_j^n + \frac{1}{2} \Delta^- U_j^n) - F(U_j^n - \frac{1}{2} \Delta^- U_j^n) \right]$$

used for calculating linear extrapolations:

$$U_{j+1/2}^L = U_j^{n+1/2} + \frac{1}{2} \Delta^- U_j^n$$

$$U_{j+1/2}^R = U_{j+1}^{n+1/2} - \frac{1}{2} \Delta^- U_{j+1}^n$$

# TVD-MUSCL

MUSCL = Monotonic Upstream Scheme for Conservation Laws

- ▶ same Hancock predictor step and upwinding as TVDLF
- ▶ upwinding is applied for characteristic variables rather than conservative variables

Characteristic variables  $\vec{r}^k$

- ▶ linear combinations of conservative variables
- ▶ right eigenvectors of  $\partial \vec{F} / \partial \vec{U}$

$$\frac{\partial \vec{F}}{\partial \vec{U}} \vec{r}^k = c^k \vec{r}^k$$

- ▶ eigenvalues  $c^k$  are real
- ▶ eigenvectors form a complete orthogonal basis
- ▶ left eigenvectors  $\vec{l}^k$ :

$$\vec{l}^k \cdot \vec{r}^k = \delta_{k,m}$$

# TVD-MUSCL

Modify  $\vec{\Phi}$ :

$$\vec{\Phi} = \frac{\Delta t}{\Delta x} \sum_k \vec{r}^k |c^k| \vec{l}^k \cdot (\vec{U}^R - \vec{U}^L)$$

where  $\vec{r}^k$ ,  $c^k$  and  $\vec{l}^k$  are calculated for  $U_{j+1/2}$

- ▶  $\vec{l}^k \cdot (\vec{U}^R - \vec{U}^L)$  determines jump in k-th characteristic variable
- ▶ multiplication by  $\vec{r}^k$  transforms result back to conservation variables

Comparison to TVDLF

- ▶ Advantage: use of eigenvalue  $c^k$  instead of largest eigenvalue  $c^{max} \Rightarrow$  upwinding is accurate for each characteristic variable  $\Rightarrow$  less numerical diffusion
- ▶ Disadvantage: left and right eigenvectors must be calculated for each cell interface (can be very expensive)

# FD

## Finite Differences

The flow variables are given as point-wise values  $U_j$  at locations  $x_j$  as:

$$U_j(t) = U(x_j, t)$$

Difference formulae of a given order of accuracy can be derived from Taylor expansion around the grid points

## FD

Example, 1D, grid spacing  $\Delta x$ :

→ a first order spatial derivative can be approximated by the centered finite difference formula:

$$\begin{aligned} & \frac{U_{j+1} - U_{j-1}}{2\Delta x} \\ &= \frac{1}{2\Delta x} \left[ U_j + \Delta x \partial_x U + \frac{(\Delta x)^2}{2!} \partial_{xx} U + \dots \right] \\ & \quad - \frac{1}{2\Delta x} \left[ U_j - \Delta x \partial_x U + \frac{(\Delta x)^2}{2!} \partial_{xx} U + \dots \right] \\ &= \partial_x U + O((\Delta x)^2) \end{aligned}$$

# HLL

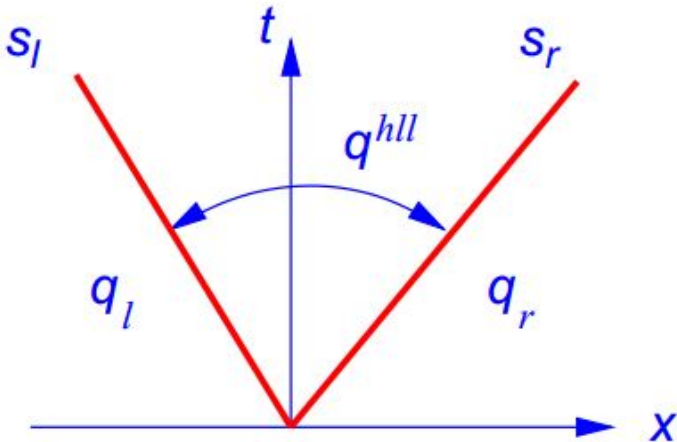
Riemann solver of Harten, Lax and van Leer  
System of one-dimensional conservation laws:

$$q_t + f(q)_x = 0$$

with

$$q(x, 0) = \begin{cases} q_l & \text{if } x < 0 \\ q_r & \text{if } x > 0 \end{cases}$$

## Overview of different numerical methods





# HLL

Integrating over control volume:

$$q^{hll} = \frac{s_r q_r - s_l q_l + f_l - f_r}{s_r - s_l}$$

Following approximation is proposed:

$$\tilde{q}(x, t) = \begin{cases} q_l & \text{if } \frac{x}{t} \leq s_l \\ q^{hll} & \text{if } s_l \leq \frac{x}{t} \leq s_r \\ q_r & \text{if } \frac{x}{t} \geq s_r \end{cases}$$

Corresponding flux:

$$f_{i+1/2}^{hll} = \begin{cases} f_l & \text{if } 0 \leq s_l \\ \frac{s_r f_l - s_l f_r + s_l s_r (q_r - q_l)}{s_r - s_l} & \text{if } s_l \leq 0 \leq s_r \\ f_r & \text{if } 0 \geq s_r \end{cases}$$

# HLL

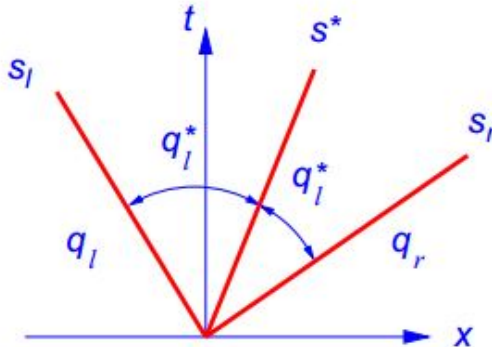
These formulas can be used in the explicit conservative formula:

$$q_i^{n+1} = q_i^n + \frac{\Delta t}{\Delta x} [f_{i-1/2} - f_{i+1/2}]$$

Wave speeds  $s_l$  and  $s_r$  must be estimated.

# HLLC

Modification of HLL scheme in which the missing contact and shear waves are restored.



# HLLC

$$\tilde{q}(x, t) = \begin{cases} q_l & \text{if } \frac{x}{t} \leq s_l \\ q_l^* & \text{if } s_l \leq \frac{x}{t} \leq s^* \\ q_r^* & \text{if } s^* \leq \frac{x}{t} \leq s_r \\ q_r & \text{if } \frac{x}{t} \geq s_r \end{cases}$$

$$f_{i+1/2}^{hllc} = \begin{cases} f_l & \text{if } 0 \leq s_l \\ f_l + s_l(q_l^* - q_l) & \text{if } s_l \leq 0 \leq s^* \\ f_r + s_r(q_r^* - q_r) & \text{if } s^* \leq 0 \leq s_r \\ f_r & \text{if } 0 \geq s_r \end{cases}$$

Intermediate states  $q_l^*$  and  $q_r^*$  can be determined.

Wave speeds  $s_l$ ,  $s_r$  and  $s^*$  need to be estimated.

# MPI-AMRVAC and HPC



## Server interaction

A script can do this better than we do!

- ▶ No need to ssh
- ▶ All changes can be made locally
- ▶ Bulk submitting
- ▶ No need to wait on the compilation
- ▶ Compresses and downloads all automatic

Less than 10 minutes to compare 5 methods on a new problem.

# Some problems

- ▶ Compiler error: segmentation problem
- ▶ Some of the problems ran only on one node
- ▶ The visualisation software crashed a lot

# Configuration 1 - Results from paper

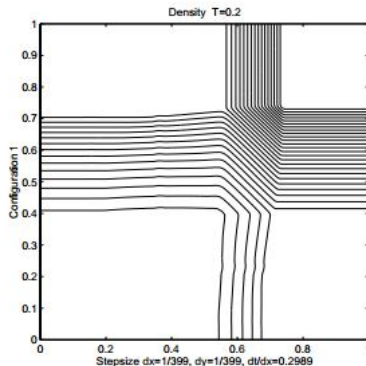
CONFIGURATION 1.  $\overrightarrow{R_{32}}$   $\overrightarrow{R_{21}}$   $\overrightarrow{R_{34}}$   $\overrightarrow{R_{41}}$  : the initial data are

$$\begin{aligned} p_2 &= 0.4 \\ u_2 &= -0.7259 \\ p_3 &= 0.0439 \\ u_3 &= -0.7259 \end{aligned}$$

$$\begin{aligned} \rho_2 &= 0.5197 \\ v_2 &= 0 \\ \rho_3 &= 0.1072 \\ v_3 &= -1.4045 \end{aligned}$$

$$\begin{aligned} p_1 &= 1 \\ u_1 &= 0 \\ p_4 &= 0.15 \\ u_4 &= 0 \end{aligned}$$

$$\begin{aligned} \rho_1 &= 1 \\ v_1 &= 0 \\ \rho_4 &= 0.2579 \\ v_4 &= -1.4045 \end{aligned}$$





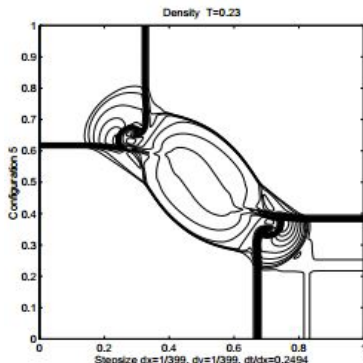
# Configuration 1 - Own results

movie

# Configuration 5 - Results from paper

CONFIGURATION 5.  $J_{32}^-$   $J_{21}^-$   $J_{41}^-$  : the initial data are

$p_2 = 1$	$p_2 = 2$	$p_1 = 1$	$p_1 = 1$
$u_2 = -0.75$	$v_2 = 0.5$	$u_1 = -0.75$	$v_1 = -0.5$
$p_3 = 1$	$p_3 = 1$	$p_4 = 1$	$p_4 = 3$
$u_3 = 0.75$	$v_3 = 0.5$	$u_4 = 0.75$	$v_4 = -0.5$

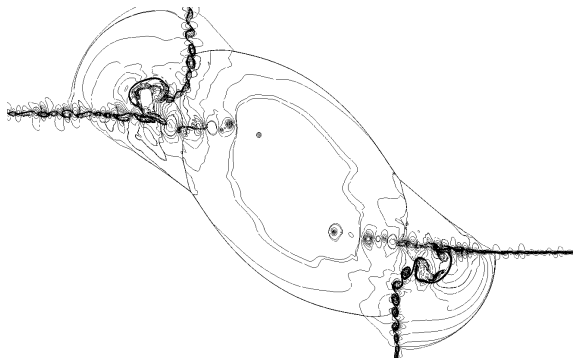


# Configuration 5 - Own results

movie

# Configuration 5 - Own results

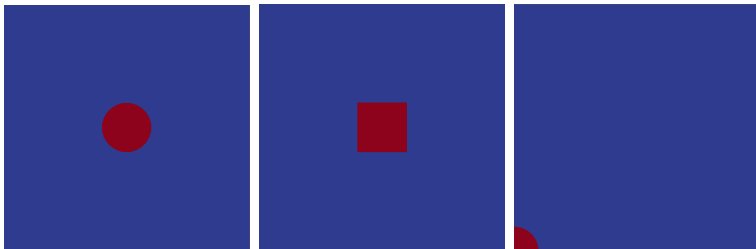
High Resolution - HLLC



## Setup for the explosion

We tried several parameters

- ▶ Size of the explosion centre
- ▶ Pressure difference
- ▶ Location of the explosion



# Comparing two explosions

## Movie

# 3d rayleigh taylor

