Inverse Lax-Wendroff Procedure for Numerical Boundary Conditions of Hyperbolic Equations

Chi-Wang Shu

Division of Applied Mathematics

Brown University

Joint work with Sirui Tan and Francois Vilar, Ling Huang and Mengping Zhang

Outline

- Introduction
- Time dependent conservation laws
- Compressible inviscid flows involving complex moving geometries
- Conclusions and future work

Introduction

For finite difference schemes approximating PDEs, there are two major difficulties associated with numerical boundary conditions:

- High order finite difference schemes involve a wide stencil, hence there are several points near the boundary (either as ghost points outside the computational domain or as the first few points inside the computational domain near the boundary) which need different treatment.

For example, if we have the following scheme

$$u_j^{n+1} = au_{j-2}^n + bu_{j-1}^n + cu_j^n + du_{j+1}^n$$

with suitably chosen constants a, b, c and d (which depend on $\lambda = \frac{\Delta t}{\Delta x}$), approximating the PDE

$$u_t + u_x = 0.$$

$$u(x, 0) = f(x), \qquad u(0, t) = g(t)$$

to third order accuracy, then either a ghost point u_{-1}^n is needed, or the scheme cannot be used to compute u_1^{n+1}.

- The boundary of the computational domain may not coincide with grid points.

  For example, in 1D, we may have the physical boundary $x = 0$ located anywhere between two grid points. While this seems artificial, it is unavoidable for a moving boundary computed on a fixed grid.

  This difficulty is more profound in 2D (complicated geometry computed on Cartesian meshes).

  One of the major difficulties is the small cell near the boundary and the resulting small time step required for stability.

Previous work on numerical boundary conditions:

- h-box method of Berger, Helzel and LeVeque (SINUM 2003): suitable flux computation based on cells of size h. This method can overcome the difficulty of small time step for stability, but is somewhat complicated in 2D and for high order accuracy.
- Reflecting or symmetry boundary conditions for ghost points: suitable for solid walls or symmetry lines which are straight lines but lead to large errors for curved walls not aligned with meshes.

- Extrapolation to obtain ghost point values (Kreiss et al SINUM 2002, 2004; SISC 2006; Sjögreen and Petersson CiCP 2007). A GKS stability analysis must be performed to assess its stability. Second order is fine but higher order is more complicated to analyze. It is not stable if the physical boundary is too close to a grid point.
- Converting spatial derivative near the boundary to temporal derivatives (Goldberg and Tadmor, Math Comp 1978, 1981 for one-dimensional linear hyperbolic initial-boundary value problems).

Review on the traditional Lax-Wendroff procedure for solving, e.g.

$$u_t + u_x = 0$$

- Taylor expansion in time

$$u_j^{n+1} = u_j + (u_t)_j \Delta t + \frac{1}{2}(u_{tt})_j \Delta t^2 + \ldots$$

- Replace the time derivatives by spatial derivatives by repeatedly using the PDE:

$$(u_t)_j = -(u_x)_j$$

$$(u_{tt})_j = -((u_x)_t)_j = -((u_t)_x)_j = (u_{xx})_j$$

...

- Approximate the spatial derivatives by finite differences of suitable order of accuracy.

We now look at the basic idea of the inverse Lax-Wendroff procedure, by switching the roles of x and t in the traditional Lax-Wendroff procedure. Suppose we are solving

$$u_t + u_x = 0, \qquad u(0,t) = g(t)$$

and suppose the boundary $x = 0$ is of distance $a\Delta x$ from x_1 (with a constant a), the inverse Lax-Wendroff procedure to determine u_1 is as follows:

- Taylor expansion in space

$$u_1 = u(0,t) + u_x(0,t)a\Delta x + \frac{1}{2}u_{xx}(0,t)(a\Delta x)^2 + \ldots$$

- Replace the spatial derivatives by time derivatives by repeatedly using the PDE:

$$u_x = -u_t; \qquad u_x(0,t) = -u_t(0,t) = -g'(t)$$

$$u_{xx} = (-u_t)_x = -(u_x)_t = u_{tt};$$

$$u_{xx}(0,t) = u_{tt}(0,t) = g''(t)$$

...

- Compute $g'(t)$, $g''(t)$, etc. either analytically or by finite difference.

Steady state Hamilton-Jacobi equations

We are interested in the steady state solution of the Hamilton-Jacobi equation

$$H(\phi_x, \phi_y) = f(x, y) \tag{1}$$

together with suitable boundary conditions.

We can use Runge-Kutta or other methods to march in time for the time dependent PDE

$$\phi_t + H(\phi_x, \phi_y) = f(x, y) \tag{2}$$

until steady state is reached, but that is rather slow.

One class of effective numerical methods is the fast sweeping method (Boué and Dupuis, SINUM 1999; Zhao, Math Comp 2005). For high order finite difference fast sweeping methods (Zhang, Zhao and Qian, JSC 2006), the first few points near an inflow boundary are usually prescribed to be the exact solution. This is not practical for problems with unknown exact solutions.

We can design a procedure similar to the Lax-Wendroff procedure to fix the first few points near the boundary purely by the given boundary conditions and the PDE.

References:

[1] L. Huang, C.-W. Shu and M. Zhang, *Numerical boundary conditions for the fast sweeping high order WENO methods for solving the Eikonal equation*, Journal of Computational Mathematics, v26 (2008), pp.336-346.

[2] T. Xiong, M. Zhang, Y.-T. Zhang and C.-W. Shu, *Fifth order fast sweeping WENO scheme for static Hamilton-Jacobi equations with accurate boundary treatment*, Journal of Scientific Computing, v45 (2010), pp.514-536.

[3] Y.-T. Zhang, S. Chen, F. Li, H. Zhao and C.-W. Shu, *Uniformly accurate discontinuous Galerkin fast sweeping methods for Eikonal equations*, SIAM Journal on Scientific Computing, v33 (2011), pp.1873-1896.

Time dependent conservation laws

The same idea we mentioned in the introduction can be used to strongly hyperbolic conservation laws for $\boldsymbol{U} = \boldsymbol{U}(x, y, t) \in \mathbb{R}^2$

$$\begin{cases} \boldsymbol{U}_t + \boldsymbol{F}(\boldsymbol{U})_x + \boldsymbol{G}(\boldsymbol{U})_y = 0 & (x, y) \in \Omega, \quad t > 0, \\ \boldsymbol{U}(x, y, 0) = \boldsymbol{U}_0(x, y) & (x, y) \in \bar{\Omega}. \end{cases} \tag{3}$$

on a bounded domain Ω with appropriate boundary conditions prescribed on $\partial\Omega$ at time t. We assume Ω is covered by a uniform Cartesian mesh $\Omega_h = \{(x_i, y_j) : 0 \leqslant i \leqslant N_x, 0 \leqslant j \leqslant N_y\}$ with mesh size $\Delta x = \Delta y$.

One difficulty of this procedure, especially for nonlinear systems in multiple-dimensions, is that the algebra becomes very heavy for higher order derivatives.

In (Tan, Wang, Shu and Ning, JCP 2012), a simplified version of this inverse Lax-Wendroff procedure is adopted. This procedure is used only to compute the first spatial derivative u_x, subsequent derivatives u_{xx} etc. are obtained by standard extrapolation with suitable order of accuracy.

The computational examples in (Tan, Wang, Shu and Ning, JCP 2012) are for physical boundaries aligned with the mesh points. For such cases and for fifth order WENO schemes, this simplified inverse Lax-Wendroff procedure works very well with stable results in very demanding detonation problems.

In (Vilar and Shu, M^2AN 2015), we perform a rigorous stability analysis using the GKS (Gustafsson, Kreiss and Sundström) theory, using the class of central compact schemes in (Liu, Zhang, Zhang and Shu, JCP 2013) as examples.

This analysis gives explicit guidance on how many terms of u_x, u_{xx}, ... are required to be treated by the inverse Lax-Wendroff procedure in order to maintain stability (for the fully discrete case, under the same CFL number as in the periodic case) for arbitrary location of the boundary in relation to the nearest grid point.

Scheme	Required leading terms
CCS-T4	3
CCS-T6	3
CCS-T8	5
CCS-T10	8
CCS-T12	9

Table 1: Minimum number of leading terms required by the different RK3-CCS-tridiagonal schemes to remain stable under the same CFL as that for periodic boundary conditions.

At the outflow boundary, extrapolation of appropriate order is used. Either a regular or a WENO type extrapolation is appropriate depending on whether the outflow solution is smooth or contains shocks.

For the outflow boundary condition, we can show that the scheme with the extrapolation is stable for all order s.

We remark that the time step restriction of solving the system of ODEs with our boundary treatment is not more severe than the pure initial value problem. The standard CFL conditions determined by the interior schemes are used in the numerical examples.

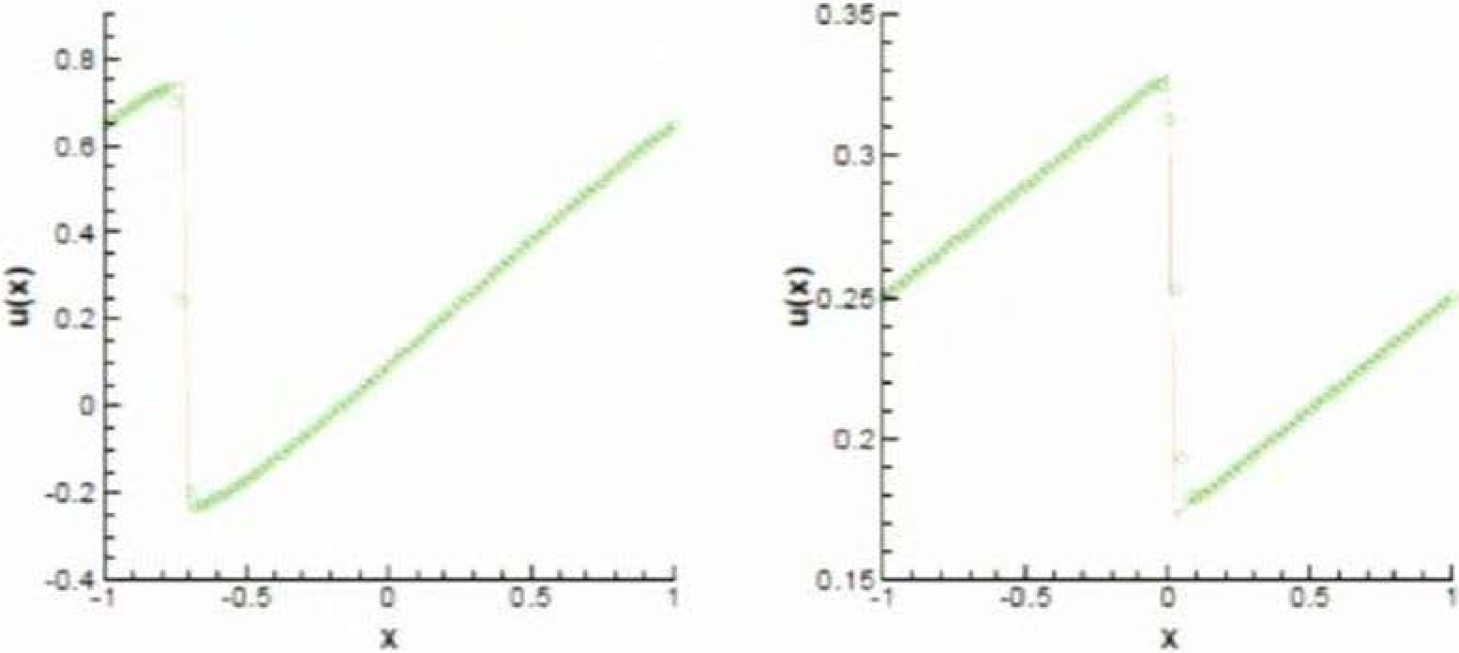
Example 1. We test the Burgers equation

$$\begin{cases} u_t + \left(\frac{1}{2}u^2\right)_x = 0 & x \in (-1,1), \quad t > 0, \\ u(x,0) = 0.25 + 0.5\sin(\pi x) & x \in [-1,1], \\ u(-1,t) = g(t) & t > 0. \end{cases} \tag{4}$$

Here $g(t) = w(-1,t)$, where $w(x,t)$ is the exact solution of the initial value problem on $(-1,1)$ with periodic boundary conditions. For all t, the left boundary $x = -1$ is an inflow boundary and the right boundary $x = 1$ is an outflow boundary.

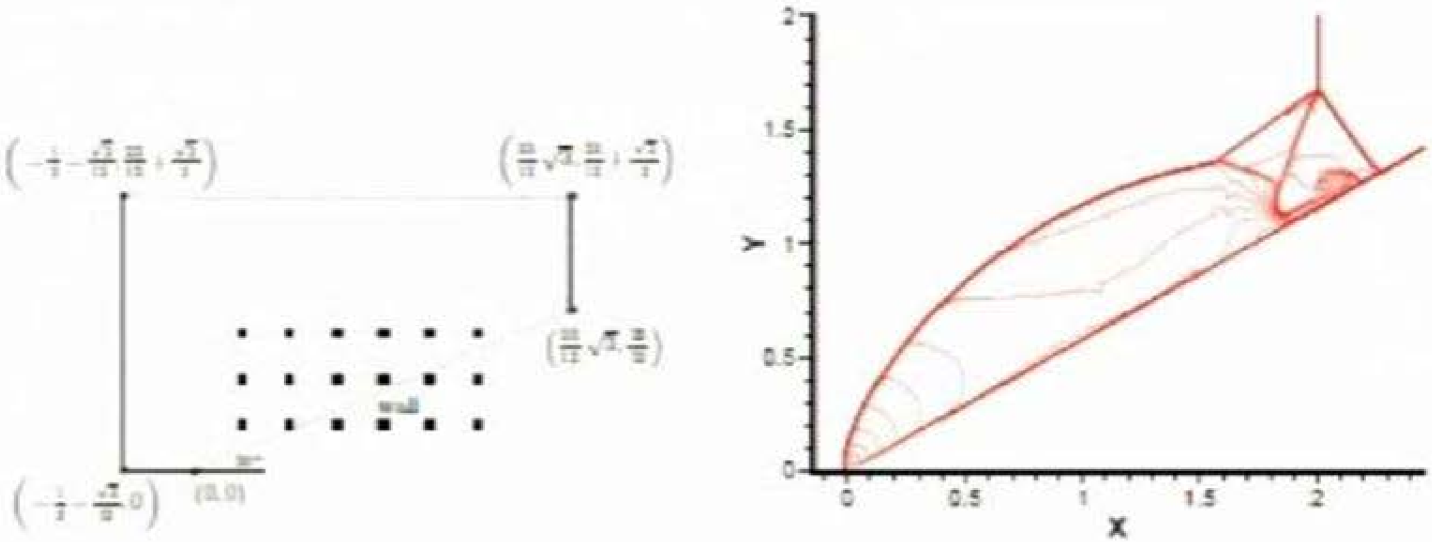
Table 2: Errors of the Burgers equation (4). $\Delta x = 2/N$ and $t = 0.3$.

N	L^1 error	order	L^∞ error	order
40	9.11E-05		3.56E-04	
80	3.10E-06	4.88	1.35E-05	4.72
160	1.31E-07	4.57	6.51E-07	4.38
320	3.97E-09	5.05	2.68E-08	4.60
640	1.02E-10	5.29	8.34E-10	5.00
1280	2.86E-12	5.15	2.62E-11	5.00



(a) $t = 1.1$ (b) $t = 12$

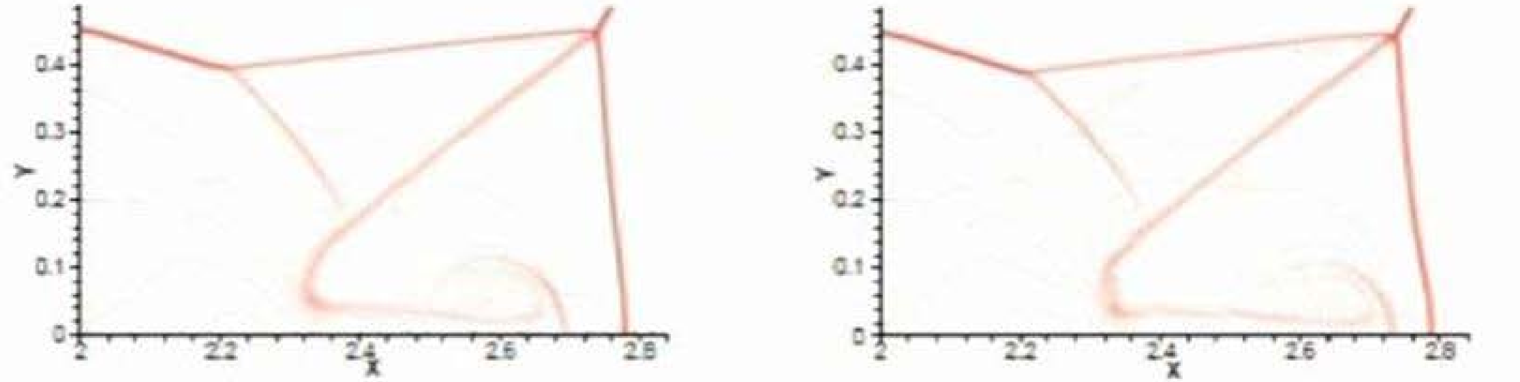
Figure 1: Burgers equation (4), $\Delta x = 1/40$. Solid line: exact solution; Symbols: numerical solution.



(a) computational domain

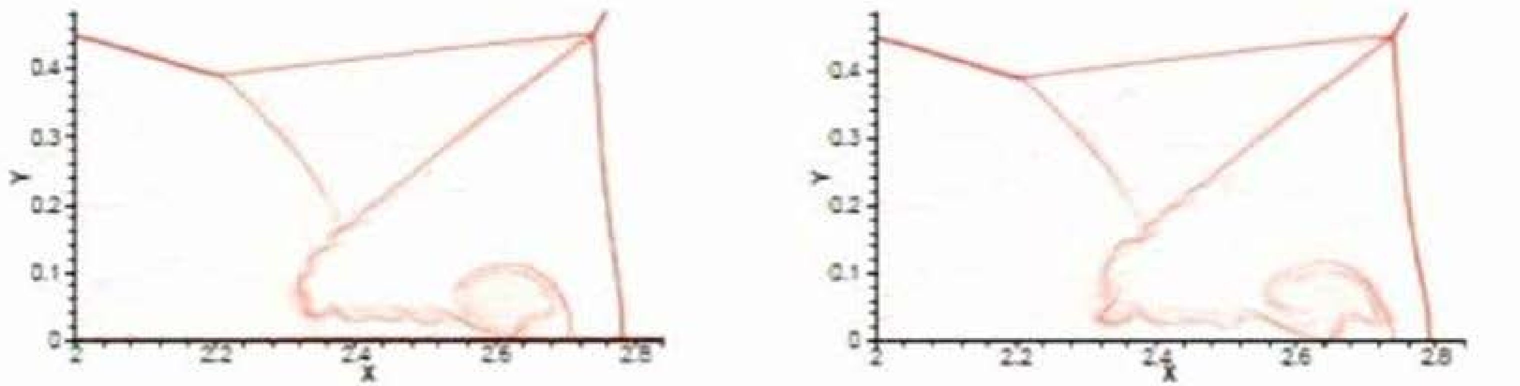
(b) density contour

Figure 2: Left: The computational domain (solid line). The dashed line indicates the computational domain used in the traditional finite difference solvers. The square points indicate some of the grid points. Right: Density contour of double Mach reflection. $\Delta x = \Delta y = \frac{1}{320}$.



(a) $\Delta x = \Delta y = \frac{1}{320}$, original problem (b) $\Delta x = \Delta y = \frac{\sqrt{3}}{480}$, equivalent problem

Figure 3: Density contours of double Mach reflection, 30 contours from 1.731 to 20.92. Zoomed-in near the double Mach stem. The plots in the left column (our computation with the new boundary condition treatment) are rotated and translated for comparison.



(a) $\Delta x = \Delta y = \frac{1}{640}$, original problem (b) $\Delta x = \Delta y = \frac{\sqrt{3}}{960}$, equivalent problem

Figure 4: Continued

Example 3. This example involves a curved wall which is a circular cylinder of unit radius positioned at the origin on a x-y plane. The problem is initialized by a Mach 3 flow moving toward the cylinder from the left. In order to impose the solid wall boundary condition at the surface of the cylinder by the reflection technique, a particular mapping from the unit square to the physical domain is usually used in traditional finite difference methods. Using our method, we are able to solve this problem directly in the physical domain.

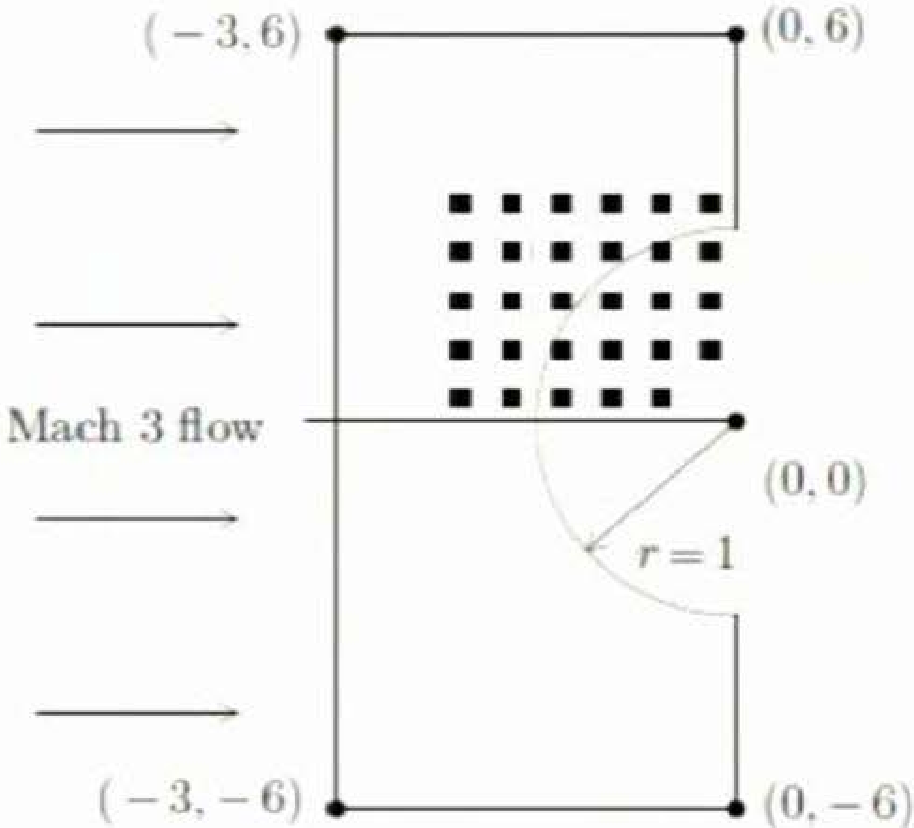
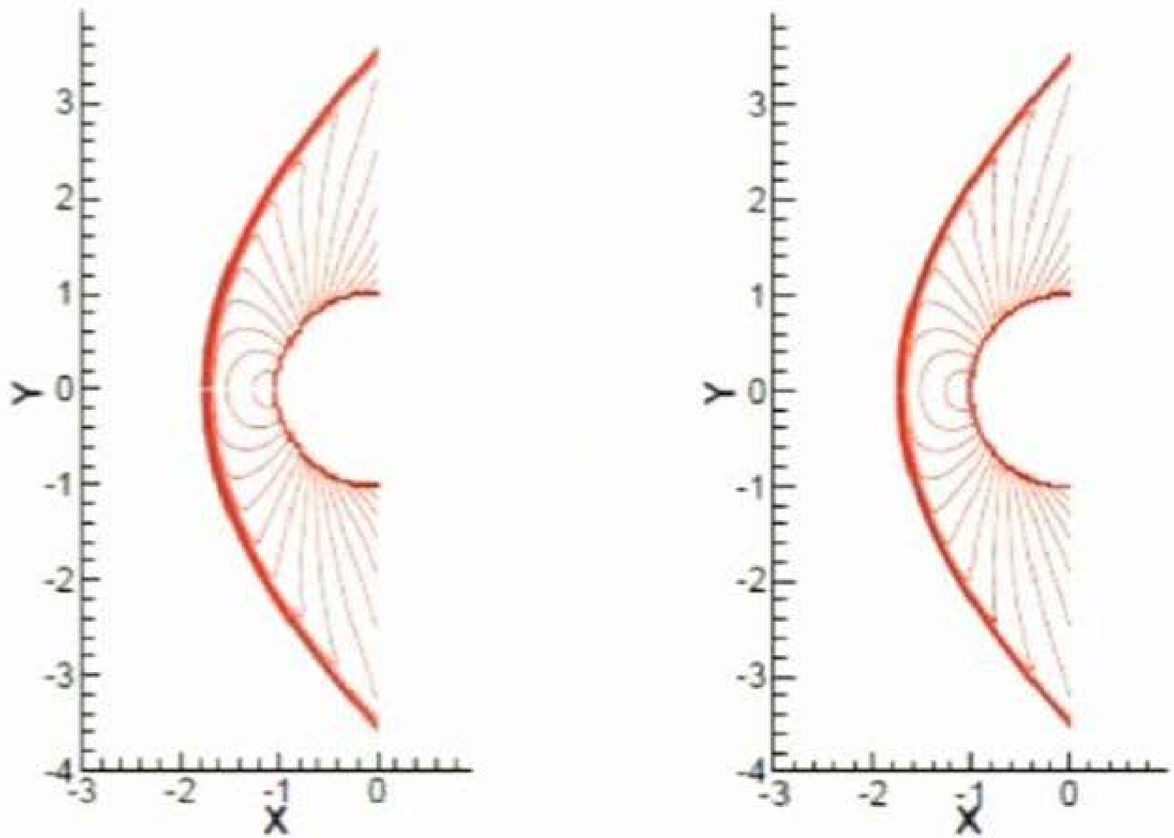


Figure 5: Physical domain of flow past a cylinder. The square points indicate some of the grid points near the cylinder. Illustrative sketch, not to scale.



(a) $\Delta x = \Delta y = \frac{1}{20}$ (b) $\Delta x = \Delta y = \frac{1}{40}$

Figure 6: Pressure contour of flow past a cylinder.

Reference:

[4] S. Tan and C.-W. Shu, *Inverse Lax-Wendroff procedure for numerical boundary conditions of conservation laws*, Journal of Computational Physics, v229 (2010), pp.8144-8166.

[5] S. Tan, C. Wang, C.-W. Shu and J. Ning, *Efficient implementation of high order inverse Lax-Wendroff boundary treatment for conservation laws*, Journal of Computational Physics, v231 (2012), pp.2510-2527.

[6] F. Vilar and C.-W. Shu, *Development and stability analysis of the inverse Lax-Wendroff boundary treatment for central compact schemes*, ESAIM: Mathematical Modelling and Numerical Analysis (M^2AN), v49 (2015), pp.39-67.

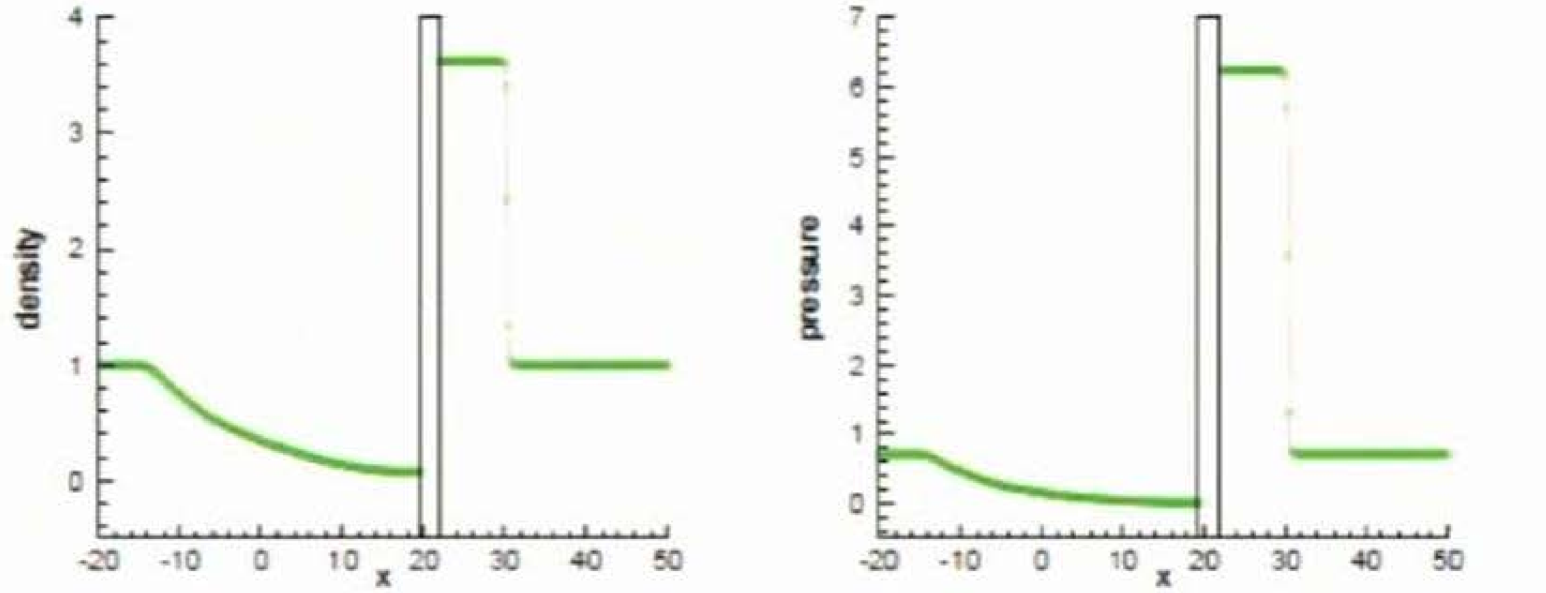
Compressible inviscid flows involving complex moving geometries

We extend the high order accurate numerical boundary condition based on finite difference methods to simulations of compressible inviscid flows involving complex moving geometries.

- For problems in such geometries, it is difficult to use body-fitted meshes which conform to the moving geometry.
- Instead, methods based on fixed Cartesian meshes have been successfully developed. For example, the immersed boundary (IB) method introduced by Peskin (JCP 1972) is widely used. One of the challenges of the IB method is the representation of the moving objects which cut through the grid lines in an arbitrary fashion.

- To solve compressible inviscid flows in complex moving geometries, most methods in the literature are based on finite volume schemes. Most of these finite volume schemes in the literature are at most second order. In particular, the errors at the boundaries sometimes often fall short of second order.
- Our inverse Lax-Wendroff procedure can be extended to such situations with moving geometries. The only change is to obtain relationships between the temporal and spatial derivatives via the PDE in moving Lagrangian framework.

Example 4. This is a 1D problem involving shocks and rarefaction waves. A piston with width $10h$ is initially centered at $x = -5h$ inside a shock tube. Here h is the mesh size. The piston instantaneously moves with a constant velocity $u_p = 2$ into an initially quiescent fluid with $\rho = 1$ and $p = 5/7$. This problem is equivalent to two independent Riemann problems and thus the exact solution can be obtained. A shock forms ahead of the piston and a rarefaction wave forms in the rear.



(a) Density (b) Pressure

Figure 7: Density and pressure profiles of Example 10. The piston is represented by the rectangle. Solid lines: exact solutions; Symbols: numerical solutions with $h = 0.25$.

Example 5. We now move on to 2D examples. A gas is confined in a rectangular region whose boundaries are rigid walls. The top and bottom walls are fixed at $y = 0$ and $y = 1$ respectively. The right wall is fixed at $x = 1$. The left moving wall is positioned at $x_l(t) = 0.5(1 - \sin t)$. The initial conditions are

$$
\begin{aligned}
\rho(x, y, 0) &= 1 + 0.2\cos\left[2\pi\,(x - 0.5)\right] + 0.1\cos\left[2\pi(y - 0.5)\right], \\
u(x, y, 0) &= x - 1, \\
v(x, y, 0) &= y(1 - y)\cos(\pi x), \\
p(x, y, 0) &= \rho(x, y, 0)^\gamma,
\end{aligned}
$$

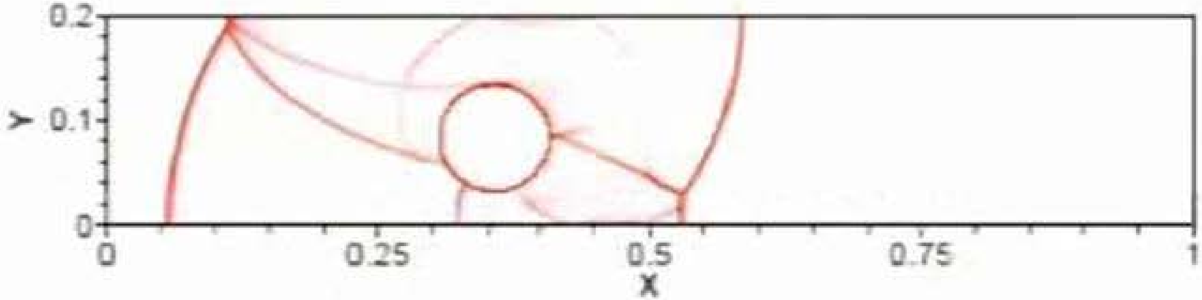
such that the initial entropy $s(x, y, 0) = 1$. We use our high order boundary treatment at the left moving wall and the reflection technique at the fixed walls.

Table 3: Entropy errors and convergence rates of Example 5.

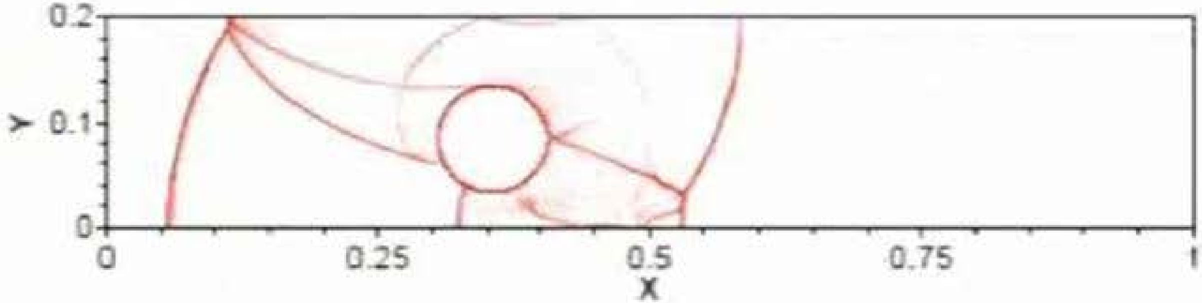
h	L^1 error	order	L^∞ error	order
1/80	2.50E-08		3.28E-07	
1/160	1.10E-09	4.50	3.06E-08	3.42
1/320	9.70E-11	3.50	6.17E-09	2.31
1/640	9.87E-12	3.30	7.06E-10	3.13

Table 4: Center of the cylinder of Example 13.

h	$t = 0.1641$		$t = 0.30085$	
	x-coordinate	y-coordinate	x-coordinate	y-coordinate
1/160	3.7058E-01	8.1140E-02	6.7178E-01	1.3759E-01
1/320	3.6153E-01	8.3219E-02	6.4959E-01	1.4444E-01
1/640	3.5706E-01	8.3680E-02	6.3895E-01	1.4517E-01
1/1280	3.5539E-01	8.4133E-02	6.3550E-01	1.4607E-01
1/2560	3.5461E-01	8.4258E-02	6.3362E-01	1.4638E-01



(a) $h = 1/640$



(b) $h = 1/1280$

Figure 8: Pressure contours at $t = 0.1641$. 53 contours from 2 to 28. $t = 0.1641$.

Reference:

[7] S. Tan and C.-W. Shu, *A high order moving boundary treatment for compressible inviscid flows*, Journal of Computational Physics, v230 (2011), pp.6023-6036.

[8] S. Tan and C.-W. Shu, *Inverse Lax-Wendroff procedure for numerical boundary conditions of hyperbolic equations: survey and new developments*, in "Advances in Applied Mathematics, Modeling and Computational Science", R. Melnik and I. Kotsireas, Editors, Fields Institute Communications 66, Springer, New York, 2013, pp.41-63.

Concluding remarks

- We have demonstrated an inverse Lax-Wendroff procedure for boundary treatment, which yields stable discretization with the same CFL number as the inner scheme and allows us to compute problems on arbitrary domains using Cartesian meshes.
- The technique can be applied to inviscid flows with complex moving geometries, yielding stable and high order accurate solutions.
- Future work would involve a generalization of this technique to other schemes such as the discontinuous Galerkin method, and to viscous problems and to problems with deformable structures.

The End

THANK YOU!