B-Sim

GUI-Based Software Package for Numerical Simulation of Nonlinear Wave Propagation Described by the Burgers Equation

User and Developer Manual

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1. Overview

The **B-Sim** is a MATLAB application designed for numerical simulation of nonlinear acoustic fields with steep shocks which appear in different applications such as air and underwater acoustics, therapeutic ultrasound, and others. The fundamental model used in this simulator is the Burgers equation accounting for nonlinearity and thermoviscous absorption. The software is developed to describe and compare the accuracy, limitations, and computational efficiency of four time-domain marching schemes: Conservative, Godunov-type, and Austin algorithms, and recently developed Intrinsic Coordinate scheme.

The MATLAB GUI (graphical user interface) application has been designed to investigate the performance of each of the four algorithms, to show a comparative analysis and make it illustrative for the user as it allows to set user-defined input parameters to the numerical model, to run simulations, and to visualize output data.

2. Software installation and launch

2.1. System requirements

The software was developed using MATLAB R2023a and App Designer. It is compatible with MATLAB versions starting from R2016a (the first version to include App Designer), but for optimal performance and to avoid potential compatibility issues, it is highly recommended to use a version close to or newer than R2023a. Users with slightly older versions might encounter minor graphical or functional discrepancies. The application is designed to work within the standard MATLAB environment. No additional toolboxes are strictly required for its core functionality.

The software is cross-platform and should run without modification on Windows, macOS, and Linux operating systems where MATLAB is supported. There are no specific hardware requirements beyond those needed to run MATLAB smoothly. Processing speed and memory will affect calculation times for high-resolution simulations or modeling up to long propagation distances.

2.2. Installation steps

The installation process is straightforward, as the software consists of a set of MATLAB files.

To download and run the software, the user must obtain the **BSim.zip** archive containing the software package. After downloading, the user should unzip the archive to a folder of their choice on their computer. This operation creates a directory containing all necessary files. The extracted folder contains several key files. It is crucial that the user does not move or rename the auxiliary files relative to the main application file.

- **BSim.mlapp** is the main application file created with App Designer. This is the file the user will run.
- Auxiliary **.m** files contain the implementations of the numerical schemes and functions for analytical solutions. These files must remain in the same directory as **BSim.mlapp**.

Before launching the application, the user must ensure that MATLAB's *Current Folder* is set to the directory containing the unzipped software files if MATLAB was already open with a different *Current Folder*. This can be done by using the *Current Folder* browser in the MATLAB desktop to navigate to the folder.

2.3. Launching the GUI

The application can be run in two ways depending on the user's goal: to run the software or to view/edit its source code.

To run the application, the user should double-click the **BSim.mlapp** file in the unzipped folder (not from MATLAB's *Current Folder* panel). MATLAB will compile and launch the graphical interface.

To view or edit the code, the user should open it in MATLAB App Designer by opening the provided **Start.m** script file. This script contains the command *appdesigner*, which will launch the App Designer environment. Another opportunity is to open the **BSim.mlapp** from MATLAB's *Current Folder* panel. Once App Designer is open, select the **BSim.mlapp** file from the folder. The project will open in App Designer, where the user can switch between:

- *Design View* option which shows the graphical layout of the interface (panels, buttons, axes, etc.) for modifying component properties.

- *Code View* option with the underlying MATLAB class definition, callbacks, helper functions, etc., that control the app's logic.

Upon successful launch, the main application window will appear (Fig. 1). The interface is organized into logical panels (see Section 3 for a detailed overview):

- A central visualization area with axes for plotting.
- Control panels for selecting the initial waveform, numerical scheme, and input physical (A, $Z_{\max}$, T) and grid parameters (h_Z, h_θ, N_{ppsh}).
- Buttons for actions like **Initial Waveform**, **Waveform at $Z_{\max}$**, **Waveform Evolution**, and **Clear All**.
- A menu bar (MENU and HELP) at the top for navigating between the software's different operational sections and accessing context-specific documentation.

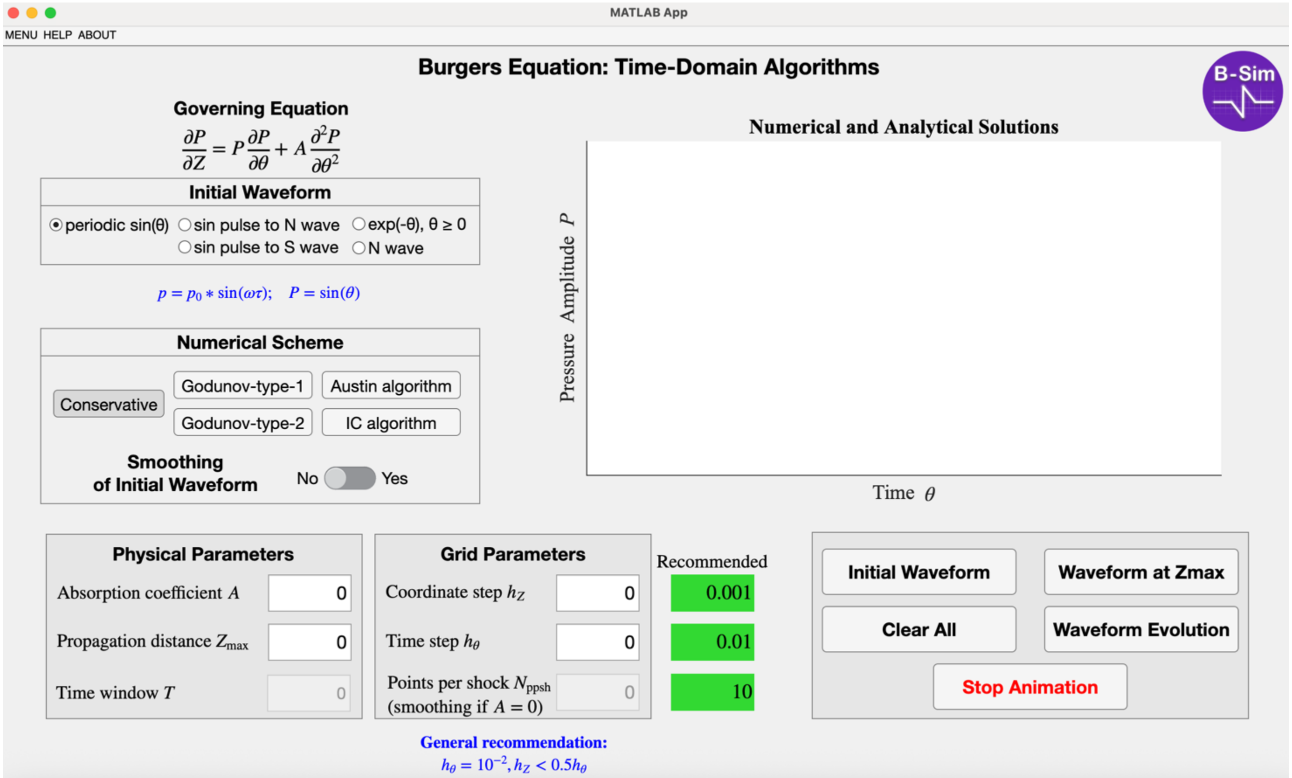

Figure 1. Main window of the B-Sim software.

3. Graphical User Interface (GUI) overview

The developed **B-Sim** software provides an interactive MATLAB-based graphical user interface (GUI) designed to facilitate the simulation and comparative analysis of nonlinear acoustic waves with shocks. The GUI is built using MATLAB App Designer and supports four distinct operating sections, each tailored to specific research or educational tasks. The interface is structured to offer intuitive access to physical parameters, numerical schemes, grid settings, and visualization tools, enabling users to explore the behavior of the waveform described by the Burgers equation under various propagation regimes.

3.1. Menu system (MENU & HELP)

The software functionality is organized through a top-level menu system (Fig. 1), providing clear navigation between its operating sections and access to guidance.

MENU Options:

- **Algorithms:** switches to the section for running and analyzing a single, user-selected numerical scheme with full parameter control.
- **IC algorithm:** activates the dedicated section for the Intrinsic Coordinates scheme, which firmly defines $A = 0$ and provides the dual-plot view (physical and intrinsic coordinates).
- **Comparison (same steps):** enters the section for comparing the results of up to five different numerical schemes, all using identical grid parameters (h_Z and h_θ).
- **Comparison (different steps):** enters the section for comparing schemes where each algorithm can be configured with its own, independently specified grid steps.

HELP Options:

- General information: provides an overview of the software, its capabilities, and basic instructions.
- Context-specific help items for each section offer concise explanations of the section's purpose, available controls and specific usage notes.

3.2. Main window layout description

The main window is organized into several functional panels that group related controls and displays.

Equation display

The governing dimensionless Burgers equation is prominently displayed as a visual reminder of the simulated physical model.

Initial waveform selection panel

A set of radio buttons allows the user to choose from five predefined initial pressure waveforms, encompassing both periodic and pulsed signals with symmetric and moving shocks (see Section 4.2 for details):

- periodic sine wave, which is labelled as **periodic sin(θ)**
- one cycle of the sine wave evolving into N wave: **sin pulse to N wave**
- one cycle of the sine wave evolving into S wave: **sin pulse to S wave**
- a shock followed by an exponential tail: **exp(-θ), $\theta \geq 0$**
- **N wave**

An expression for predefined initial waveform is given under the panel for each selected waveform in dimensional and dimensionless forms.

<u>Numerical scheme panel</u>

A central feature of this panel is the ability to choose among the five implemented time-domain algorithms and to specify the initial waveform handling, with interface details differing across operating sections. The user can select one of the following numerical schemes (see Section 5 for details):

- **Conservative:** an explicit finite-difference conservative scheme.
- **Godunov-type-1:** a shock-capturing Godunov-type scheme with weighting coefficient in derivatives $b = 1$ (enhanced stability).
- **Godunov-type-2:** a shock-capturing Godunov-type scheme with weighting coefficient in derivatives $b = 2$ (higher accuracy).
- **Austin algorithm:** an algorithm based on the exact implicit solution of the lossless Burgers equation with interpolation to the uniform grid.
- **IC algorithm:** an algorithm in the intrinsic coordinates where the waveform becomes single-valued, operating with $A = 0$ and accounting for thermoviscous absorption via equal area rule.

For initially discontinuous waveforms (a shock followed by an exponential tail and N wave) the user can also control smoothing, choosing between discontinuous and smoothed initial conditions. The availability of the smoothing parameter is dynamically linked to this choice, thermoviscous coefficient A value and the selected waveform (see Section 6.2 for details).

The specific implementation of this selection logic varies between the main operating sections:

- **Algorithms** section

A button group **Numerical Scheme** presents the five algorithms as mutually exclusive toggle buttons. A separate binary switch button **Smoothing of Initial Waveform** allows explicit control over smoothing for discontinuous initial waveforms (Fig. 1).

- **IC algorithm** section

Only the binary switch button **Smoothing of Initial Waveform** is available in the **Numerical scheme** panel since this section is specially created for the IC scheme investigation (Fig. 2a).

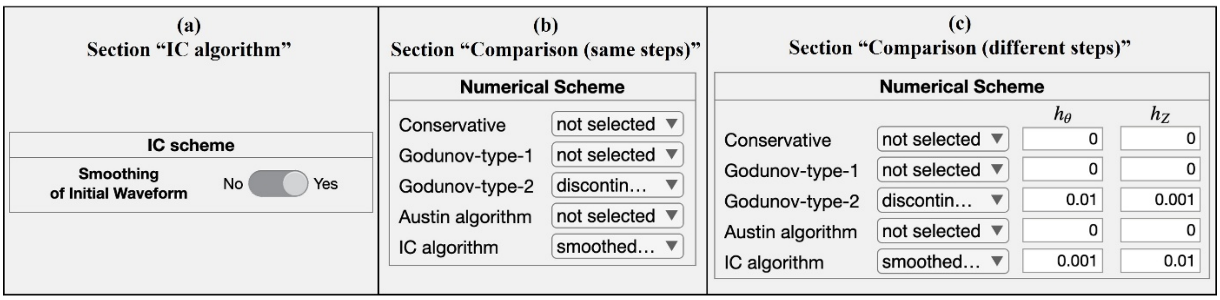

*Figure 2. **Numerical Scheme** panels in different sections: a – section **IC Algorithm**, b – section **Comparison (same steps)**, c – section **Comparison (different steps).***

- Both **Comparison** sections

Algorithm selection is implemented via individual drop-down menus for each scheme. Each menu offers three states: *not selected*, *discontinuous initial waveform*, or *smoothed initial waveform*. This design allows the simultaneous comparison of up to five schemes, each with its own initial-condition treatment, while a single smoothing switch is omitted in favor of the per-scheme menu selection (Fig. 2b,c).

Physical parameters panel

This panel allows the user to define the key physical properties of the simulation:

- **Thermoviscous absorption coefficient** (A): the dimensionless parameter controlling the ratio of nonlinear to thermoviscous effects. Values $A \ll 1$ correspond to strong nonlinear effects, whereas $A > 1$ correspond to weak nonlinearity. Setting $A = 0$ corresponds to a lossless media described by the Riemann equation. Note that A is firmly defined a zero-value for IC algorithm (see Section 5.4 for details).
- **Propagation distance** ($Z_{\max}$): the maximum normalized distance for wave propagation.
- **Time window** (T): the extent of the retarded time axis (θ) used for computation and display (editing is available only for a shock followed by an exponential tail).

Grid parameters panel

This panel controls the discretization of the numerical grid:

- **Time step** (h_θ): the dimensionless step size along the retarded time axis θ (inactive in **Comparison (different steps)** section).
- **Coordinate step** (h_Z): the dimensionless step size along the propagation direction Z (inactive in **Comparison (different steps)** section).
- **Points per shock** (N_{ppsh}): a parameter used to smoothly approximate initially discontinuous waveforms (i.e., N wave, a shock followed by an exponential tail) when required, particularly for the IC scheme or for simulations with $A = 0$. The details of the smoothing methods and points per shock definition are given in Section 4.3.

Visualization panel (axes)

The GUI features different graphical axes for displaying results:

- **UIAxes** (main): the primary axes used in most sections to display pressure P versus retarded time θ (Fig. **Ошибка! Источник ссылки не найден.**a).
- **UIAxes2** (physical coordinates for **IC algorithm** section): used only in the **IC algorithm** section to display the waveform in physical coordinates, which can become multivalued after reaching the shock formation distance (on the left in Fig. **Ошибка! Источник ссылки не найден.**b).
- **UIAxes3** (intrinsic coordinates for **IC algorithm** section): used alongside **UIAxes2** in the **IC algorithm** section to display the same waveform transformed into intrinsic coordinates (waveform angle ψ versus arc length s), where it remains single-valued (on the right in Fig. **Ошибка! Источник ссылки не найден.**b).

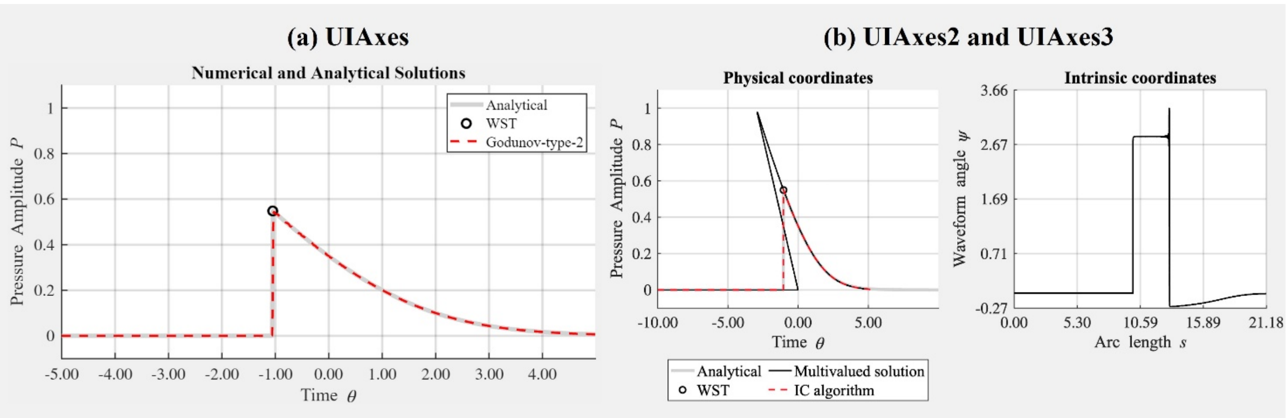

Figure 3. Visualization axes for different sections.

Main action buttons

A dedicated series of control buttons provides the primary simulation and visualization commands. These buttons allow the user to initialize, compute, and manage the graphical output.

- **Initial Waveform:** plots the selected initial condition.
- **Waveform at Z_{max}:** computes and displays the waveform at the user-specified maximum propagation distance Z_{max}.
- **Waveform Evolution:** animates the wave propagation from the zero point up to Z_{max}, allowing observation of distortion and shock formation in real-time.
- **Clear All:** clears all plots from the graphical axes.
- **Stop Animation:** pauses/resumes the waveform evolution animation.

3.3. Operating sections description

The GUI is built around four distinct operating sections, accessed via the MENU. This modular design separates different use cases, reducing interface clutter and guiding the user.

Section **Algorithms**

The main purpose of this section is to investigate the performance, accuracy, and grid steps requirements of a single selected numerical scheme in detail. During the operation, the user selects one of the five numerical schemes, defines all physical and grid parameters and chooses whether to smooth the initial waveform. The section provides scheme-specific stability and accuracy recommendations for the grid steps. Several recommendations on the choice of the steps h_Z and h_θ and the number of points per shock are given in the green fields. They were chosen for each numerical scheme to ensure a compromise between sufficient accuracy compared to the analytical solution and a short run time. General recommendations are marked in blue under the **Grid Parameters** panel. These recommendations are related to stability and accuracy criteria for the numerical schemes under consideration. The user can visualize the initial condition, the final waveform at Z_{max}, or animate the entire propagation.

The calculation time of each chosen numerical algorithm is shown on the screen after execution.

Section **IC Algorithm**

The section provides a specialized environment for the Intrinsic Coordinates scheme, which operates with lossless propagation ($A = 0$) condition as is accounts for thermoviscous absorption by the equal area rule after transforming the solution from intrinsic back to physical coordinates. Thus, the absorption coefficient A is by default set to zero. Upon running a simulation, two synchronized plots are generated: one shows the potentially multivalued solution in physical coordinates (P vs θ), and the other shows the equivalent single-valued waveform in intrinsic coordinates (ψ vs s). This visually demonstrates the core principle of the IC method.

Section **Comparison (same steps)**

The main feature of this section is to compare the output and computational efficiency of multiple numerical schemes under identical discretization conditions. The user selects which schemes to include (up to five) from drop-down menus, each with the option to use a discontinuous or smoothed initial waveform. A single set of grid parameters (h_θ, h_Z) is applied to all selected schemes. The results are overlaid on the main axes for visual comparison, either at Z_{max} or during an evolution animation.

Note that even when the investigated propagation regime is absorptive, the selected IC scheme in this section still operates with $A = 0$.

Section **Comparison (different steps)**

Unlike the previous one, this section provides the performance comparison where each scheme uses its own optimal grid parameters, reflecting its inherent numerical properties. Similarly to **Comparison (same grid steps)**, the user selects schemes for comparison. However, individual input fields for h_θ and h_Z are provided for each selected algorithm. This allows the user to configure each scheme according to its stability criteria or to achieve a target accuracy, facilitating a comparison of computational efficiency when each method is tuned to its best performance. The **Waveform Evolution** button is disabled in this section.

Note that even when the investigated propagation regime is absorptive, the selected IC scheme in this section still operates with $A = 0$.

4. Theoretical background

4.1. The Burgers equation

To simulate the propagation of plane, high-amplitude acoustic waves in absorptive media accounting for the competing effects of nonlinear steepening and thermoviscous absorption, the Burgers equation serves as the fundamental theoretical model implemented in the **B-Sim** software:

$$\frac{\partial p}{\partial z} = \frac{\beta}{c_0^3 \rho_0} p \frac{\partial p}{\partial \tau} + \frac{\delta}{2c_0^3} \frac{\partial^2 p}{\partial \tau^2}, \tag{1}$$

where p is the acoustic pressure, z is the propagation coordinate, $\tau = t - z/c_0$ is the retarded time, c_0 is the sound speed, ρ_0 is the density of a medium, β and δ are the nonlinearity and thermoviscous absorption coefficients in the media, respectively.

For the convenience of numerical modeling, the following dimensionless variables are introduced:

$$P = p / p_0, \ \theta = \omega_0 \tau, \ Z = z / l_{\text{sh}}. \tag{2}$$

Here, p_0 and ω_0 are the maximum pressure and the characteristic frequency of the initial harmonic or pulsed waveform, respectively; $l_{\text{sh}} = \rho_0 c_0^3/(\beta\omega_0 p_0)$ is the characteristic nonlinear length, e.g. the shock formation distance in case of the initially harmonic wave.

Thus, the Burgers equation (1) in dimensionless variables (2) takes the form:

$$\frac{\partial P}{\partial Z} = P \frac{\partial P}{\partial \theta} + A \frac{\partial^2 P}{\partial \theta^2}, \tag{3}$$

where the combined effects of nonlinearity and thermoviscous absorption depend on the single dimensionless parameter $A = \delta\rho_0\omega_0/(2\beta p_0)$, which is equal to the ratio of the nonlinear length l_{sh} to the absorption length $l_{\text{abs}} = 2c_0^3/(\delta\omega_0^2)$. Note that the regime $A \ll 1$ corresponds to strong nonlinear effects, whereas $A > 1$ corresponds to weak nonlinearity.

4.2. Types of predefined initial waveforms

The **B-Sim** software implements five canonical initial pressure waveforms to investigate nonlinear propagation and shock formation under various physical conditions. The waveforms are divided into two categories: symmetric shocks and moving shocks, based on the dynamics of the resulting shock which can form during wave propagation or exist initially. The nature of the shock is determined by the amplitude distribution in the predefined initial waveform.

1) *Waveforms with symmetric shocks*

Symmetric shocks maintain a fixed shock position in retarded time during propagation. This occurs when the absolute values of the positive and negative pressure peaks adjacent to the forming discontinuity are equal. Such a balance ensures that the nonlinear steepening from one side of the shock is matched by that from the opposite side, maintaining the shock at a fixed retarded time. These waveforms originate from initial conditions, where peak positive and peak negative pressures of equal magnitude steepen towards the same zero-crossing. Two initial waveforms evolving into symmetric shocks are implemented into the software: a periodic sine wave and a single cycle of a sine wave turning into S wave. These waveforms are presented in Figure 4.

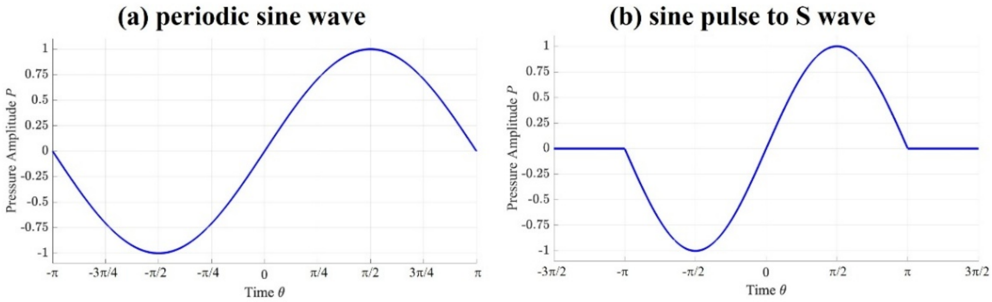

Figure 4. Initial waveforms with symmetric shocks formed during their propagation.

- **Periodic sine wave:** $P(\theta) = \sin(\theta)$

This is the fundamental harmonic initial condition, primary to studying nonlinear distortion in continuous wave regimes relevant to high intensity focused ultrasound (HIFU) and finite amplitude sound beams. During propagation the positive half-cycle and the negative half-cycle of equal magnitude steepen towards their common zero-crossing. This leads to the formation of a stationary shock at each period, ultimately creating the sawtooth waveform (S wave) in a lossless medium. Its selection allows for the investigation of periodic shock formation and harmonics generation.

The GUI displays one period of the initial sine waveform in the range $\theta \in [-\pi; \pi]$. It is important to note that the temporal axis for the ***IC algorithm*** is zero-padded to the right, in contrast to all other numerical algorithms implemented in the software, in which the temporal axis boundaries remain fixed at $\pm\pi$. This extension ensures the correctness of waveform calculations and display up to distances of $Z_{\max} = 10$ (refer to Section 5.4 for a detailed explanation).

- **Sine pulse to S wave:** $P(\theta) = \begin{cases} \sin(\theta), & |\theta| \le \pi \\ 0, & |\theta| > \pi \end{cases}$

This waveform models a single cycle of a sine wave, representing finite-duration acoustic pulses such as those from transient excitations. The dynamics of this initial profile illustrates the nonlinear evolution of a finite-duration pulse into an S shaped wave.

The time window length for this initial condition is predefined in the software, and the temporal axis is set as $\theta \in [-1.5\pi; 1.5\pi]$ for all implemented numerical algorithms except for the IC one. For the ***IC algorithm***, this window is extended to the right to ensure a correct simulation of the pulse's evolution up to distances of $Z_{\max} = 10$, accounting for its progressive shift to the left (see Section 5.4 for details).

2) Waveforms with moving shocks

Moving shocks transfer in retarded time as the wave propagates. This occurs when the amplitude distribution in the shock is imbalanced, breaking the symmetry that maintains it in place. These waveforms originate from initial conditions in which the maximum and minimum pressure values of the region adjacent to the shock are of unequal magnitude or in which peaks of equal amplitude steepen away from each other, leading to shock motion. Three representative waveforms were chosen for analysis in the software.

- **Shock followed by an exponential tail:** $P(\theta) = \begin{cases} \exp(-\theta), & \theta > 0 \\ 0, & \theta < 0 \end{cases}$

This waveform is a primary model for the disturbance produced by explosions, both underwater and in the atmosphere, such as blast waves, etc. and are characterized by a sharp pressure rise followed by an exponential decay. The initial waveform contains only a positive-pressure phase (Fig. 5a). The high-amplitude region immediately behind the initial discontinuity does not have a symmetrical negative peak to balance the shock. This causes the discontinuity to move forward in retarded time with a decreasing amplitude as propagation distance increases.

The duration T of the computational time window for this initial waveform is set by the user via the *Time window T* field in the **Physical Parameters** panel, allowing flexible adaptation to the simulation requirements.

- **N wave:** $P(\theta)=\begin{cases}-\theta, & |\theta| \le 1\\ 0, & |\theta|>1\end{cases}$

It is a canonical nonlinear acoustic waveform that illustrates disturbances produced by supersonic projectiles, sonic booms (far from the aircraft), bursting spherical balloons and electric sparks in air. This waveform consists of a leading shock, a tail shock and an intervening region of linear pressure variation. The shock at the positive-pressure front and the shock at the negative-pressure front (Fig. 5b) propagate at different speeds due to their opposite amplitudes. This imbalance causes both shocks to move apart from each other as the N wave broadens during propagation, demonstrating shock motion and amplitude decay.

The time window length for four implemented numerical algorithms is set to the interval $\theta \in [-4; 4]$, providing the position of the moving shock within the temporal interval for distances up to $Z_{\max} = 10$. This window is extended to the right for the ***IC algorithm*** for the same reasons as for a sine wave evolving into S wave (see Section 5.4 for details).

- **Sine pulse to N wave:** $P(\theta)=\begin{cases}-\sin(\theta), & |\theta| \le \pi\\ 0, & |\theta|>\pi\end{cases}$

This single cycle of a negative sine wave (Fig. 5c) represents a finite-duration, initially smooth acoustic pulse. Unlike the sine evolving into S wave pulse, here the positive half-cycle does not move towards an equal-magnitude negative section. Upon propagation, the positive phase outruns the negative one. This imbalance leads to the formation of two moving shocks at the waveform's extremities and its subsequent evolution into a broadening N wave. It connects the study of idealized discontinuous pulses to that of smooth initial conditions, illustrating how an inherent imbalance in the waveform's shape governs the subsequent motion of the shocks.

The time window length is also predefined in the software for such an initial condition: $\theta \in [-2.5\pi; 2.5\pi]$ providing the position of the moving shock within the temporal interval for distances up to $Z_{\max} = 10$. This window is also extended to the right for the ***IC scheme*** as mentioned above (see Section 5.4 for details).

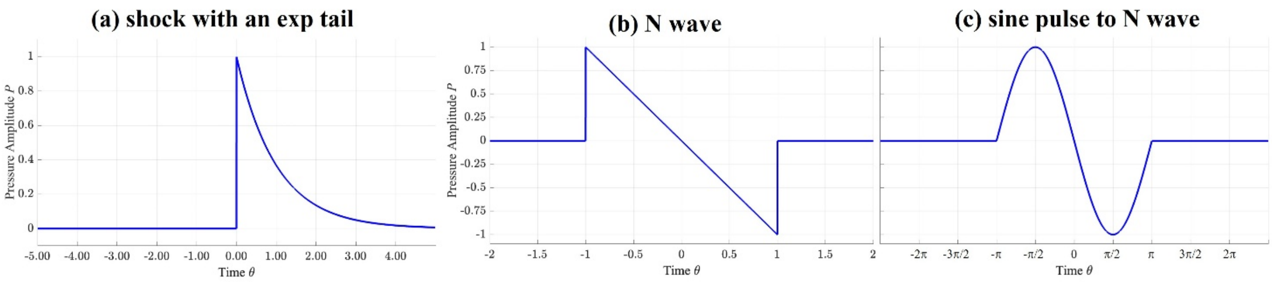

Figure 5. Initial waveforms with moving shocks.

4.3. Initial waveform smoothing

The **B-Sim** software includes an option to apply smoothing to initially discontinuous waveforms: *a shock followed by an exponential tail* and *N wave*. This feature is implemented for two primary reasons. First, in case of zero thermoviscous absorption (A = 0), the ***IC algorithm*** is fundamentally designed for smoothed waveforms and cannot process discontinuous ones. Smoothing provides a finite-thickness shock in the initial waveform which the ***IC algorithm*** can correctly transform and propagate in the intrinsic coordinates. Moreover, smoothing of initially discontinuous waveforms provides more accurate results for the ***Godunov-type algorithm*** in order to increase time and spatial steps, thereby speeding up the calculations. Second, when simulating propagation with non-zero thermoviscous absorption ($A > 0$), it is physically consistent to define the initial waveform as a quasi-stationary solution of the Burgers equation itself. A true discontinuity cannot persist in an absorbing media; dissipation immediately acts to spread the shock over a finite width. Therefore, for $A > 0$, initializing the simulation with a smoothed profile that already represents a balance between nonlinear steepening and thermoviscous absorption provides a more accurate and numerically stable initial condition.

If $A > 0$, the smoothing waveforms are derived from the quasi-stationary solution of the Burgers equation (1), (3). This solution describes a shock of a constant amplitude $\Delta P = P_2 - P_1$, where $P(\theta \to -\infty) = P_1$, $P(\theta \to +\infty) = P_2$, and a constant propagation speed. To obtain it, we introduce a coordinate system $\theta_1 = \theta - Z/v$, moving with the shock speed v. Substituting $P = P(\theta_1)$ into the Burgers equation (3) leads to a following differential equation:

$$v\frac{dP}{d\theta_1} + \frac{1}{2}\frac{dP^2}{d\theta_1} + A\frac{d^2P}{d\theta_1^2} = 0. \tag{4}$$

Double integration over θ_1 gives the solution in a form of a hyperbolic tangent profile, which represents a shock of finite width determined by the thermoviscous absorption coefficient A:

$$P = \frac{P_1 + P_2}{2} + \frac{P_2 - P_1}{2}\tanh\left[\frac{P_2 - P_1}{4A}\left(\theta - \theta_0 + \frac{P_1 + P_2}{2}Z\right)\right], \tag{5}$$

where θ_0 is the initial time of shock arrival at a distance $Z = 0$. Thus, the initial condition for a constant amplitude moving shock takes the form:

$$P = \frac{P_1 + P_2}{2} + \frac{P_2 - P_1}{2}\tanh\left[\frac{P_2 - P_1}{4A}\left(\theta - \theta_0\right)\right]. \tag{6}$$

For the specific two initial waveforms (*a shock followed by an exponential tail* and *N wave*) in **B-Sim**, this general solution (6) is adapted.

For *a shock followed by an exponential tail* the quasi-stationary profile is used as a local approximation at the discontinuity with $P_1 = 0$, $P_2 = 1$and $\theta_0 = 0$, and the smoothed initial condition is constructed as:

$$P = \frac{1}{2}\left(1 + \tanh\left(\frac{1}{4A}\theta\right)\right)\cdot \mathrm{e}^{-\theta}. \tag{7}$$

The *N wave* contains two discontinuities of opposite polarity: $P_1^{\text{left}} = 0$ and $P_2^{\text{left}} = 1$ at $\theta_0^{\text{left}} = -1$ for the left shock and $P_1^{\text{right}} = -1$ and $P_2^{\text{right}} = 0$ at $\theta_0^{\text{right}} = 1$ for the right shock. Each is treated as an independent shock transition. Applying the quasi-stationary solution symmetrically at both shocks yields the smoothed profile:

$$P = \frac{1}{2}\left(\tanh\left(\frac{1}{4A}(\theta - 1)\right) - \tanh\left(\frac{1}{4A}(\theta + 1)\right)\right) \cdot \theta. \tag{8}$$

The width of the smoothed shock front $\Delta\theta$ is an important parameter for smoothing the initial waveform. In the software, $\Delta\theta$ is defined as the interval in θ over which the pressure rises from 10% to 90% of its maximum absolute value (P_{max}) across the shock. For a hyperbolic tangent waveform, this width is directly proportional to the thermoviscous absorption parameter A (Fig. 6):

$$\Delta\theta \approx 10A. \tag{9}$$

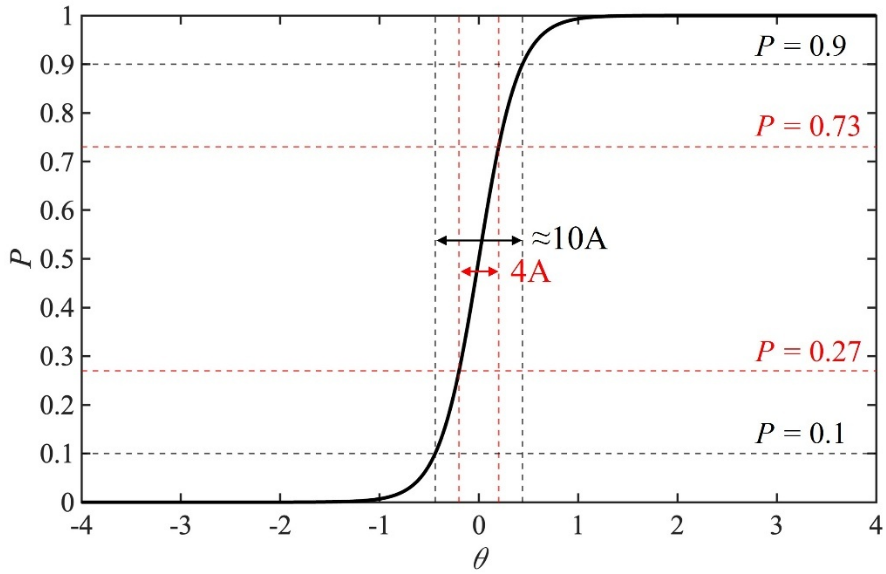

Figure 6. The smoothed shock width definition.

This relationship provides the correspondence between the physical absorption and the numerical shock width.

Thus, the smoothing logic in the **B-Sim** software distinguishes between two propagation regimes:

1. When $A > 0$, the physical thermoviscous absorption coefficient A directly defines the shock width. In this case, the initial waveform is smoothed according to the (7) for *a shock followed by an exponential tail* and (8) for *N wave*, respectively, using the value of A which is set by the user. The field **Points per shock N_{ppsh}** is inactive in this regime.
2. For case $A = 0$ there is no physical absorption to set a shock width. Here, the user defines the desired shock resolution by specifying the number of time grid points N_{ppsh} in the **Points per shock N_{ppsh}** field that should span the $\Delta\theta$ width of the initial smoothed profile. Then an effective numerical absorption coefficient A_{eff} is calculated to produce this width on the given temporal grid from the following relation:

$$\Delta\theta = 10A_{eff} = N_{ppsh} \cdot h_\theta. \tag{10}$$

This A_{eff} is then used in the smoothing functions (7)–(8) to generate the initial waveform. This mechanism allows precise control over the initial shock thickness for algorithms like the ***IC scheme***, ensuring it is resolvable on the computational grid while maintaining the formal condition $A = 0$ for the propagation itself.

4.4. Benchmark analytical solutions

4.4.1. Zero thermoviscous absorption case

To validate the numerical results and provide benchmark solutions, the **B-Sim** software incorporates analytical models for all five implemented types of initial waveforms. Analytical solutions are presented for the case of zero thermoviscous absorption ($A = 0$) and derived from the weak shock theory (WST) and the equal-area rule applied to the lossless Burgers (Riemann) equation. These benchmark solutions allow for a direct assessment of the accuracy and convergence of the implemented time-domain numerical algorithms.

WST for discontinuous initial waveforms

WST provides an analytical framework for predicting the evolution of waveforms containing shocks. The theory is based on the assumptions that the shocks are weak, that energy dissipation is concentrated almost entirely at the shock fronts, and that the shock thickness is negligible compared to the overall duration of the wave. Under these conditions, the continuous regions of the waveform between shocks can be described by the lossless (Riemann) solution, while the shock amplitudes and positions are governed by simple differential equations derived from conservation laws. In **B-Sim**, WST solutions are used as benchmarks for two initially discontinuous waveforms: the *shock followed by an exponential tail* and the *N wave*. For both waveforms, the solution describes the evolution of the shock amplitude P_{sh} and its temporal position θ_{sh}.

Applying WST to the initial *shock with exponential decay* yields the following relationships:

$$P_{sh}(Z) = \frac{\sqrt{1+2Z}-1}{Z},\ \theta_{sh}(Z) = -\ln(P_{sh}) - Z \cdot P_{sh}. \quad (11)$$

The approximate analytical solution for the waveform shape in the software is constructed as follows:

$$P(Z,\theta) = \begin{cases} \dfrac{1+\ln\left[(2y+1)/\left(1+\ln(y+1)\right)\right]}{y+(2y+1)/\left(1+\ln(y+1)\right)} \cdot \mathrm{e}^{-\theta}, & \theta > \theta_{sh}(Z) \\ 0, & \theta < \theta_{sh}(Z) \end{cases}, \quad (12)$$

where $y = Z \cdot \mathrm{e}^{-\theta}$.

For *N wave* initial condition, the WST solution describes the location of the head shock and the decay of its amplitude as follows:

$$P_{sh}(Z) = \frac{1}{\sqrt{1+Z}},\ \theta_{sh}(Z) = -\sqrt{1+Z}. \quad (13)$$

The location of the tail shock is found using the asymmetricity of the initial waveform and the waveform shape is constructed using its property to maintain a linear shape during a distortion governed by a Riemann equation.

These WST solutions are implemented in the software and are displayed alongside the numerical results for comparison, providing a quantitative measure of accuracy in regimes with zero thermoviscous absorption.

Equal area rule for smoothed initial waveforms

For initially smooth waveforms such as a *periodic sine wave*, a *sin pulse evolution into S wave*, and a *sin pulse evolution into N wave*, an analytical solution in the lossless case ($A = 0$) is obtained using the equal area rule applied to the multivalued solution of the simple wave (Riemann) equation. Unlike the discontinuous initial waveforms, these signals do not have a pre-existing shock whose evolution is governed by WST. Instead, the shock forms during propagation as the waveform steepens and becomes multivalued. The equal area rule is a geometrical method that determines the correct shock position within the multivalued region, ensuring conservation of the waveform's area and providing a single-valued physical solution. Figure 7 presents the idea of the equal area rule implementation in the software for constructing analytical solutions to both symmetric and moving shocks.

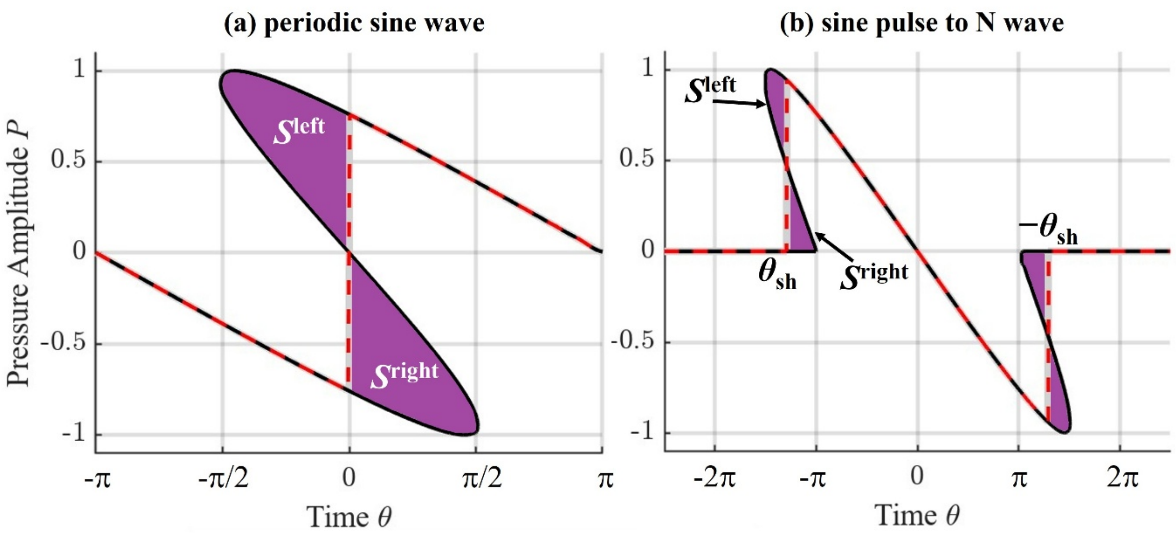

Figure 7. Equal area rule implementation principle for constructing analytical solutions to the waveforms with symmetric (a) and moving (b) shocks.

The implementation of the equal area rule is based on the method of characteristics that uses the implicit solution $P(Z, \theta) = P(0, \theta_{shift} = \theta - P \cdot Z)$. This solution becomes multivalued at $Z > 1$. To recover a single-valued waveform with a shock, the equal area rule is applied: the shock is placed at the retarded time θ_{sh} such that the two areas between the multivalued curve and the vertical line at θ_{sh} are equal. This condition conserves the integral of pressure and yields the correct weak shock solution.

In the **B-Sim** implementation, the general computational algorithm is as follows:

1. For a given propagation distance Z, the waveform is computed along characteristics: the time axis shifts as θ_{shift}, that typically produces a multivalued array θ_{shift}.
2. The algorithm identifies the region where the shifted time θ_{shift} is not a single-valued function of θ. This is done by searching for local extrema in the θ_{shift} array.
3. An iterative search is performed within the boundaries of the multivalued region to find the shock position θ_{sh}. For each trial θ_{sh}, the areas S^{left} on the left and S^{right} on the right are calculated by integrating the upper and lower branches of the multivalued curve relative to the trial vertical line. The iteration continues until the difference between the areas is closest to or equals zero.
4. Once θ_{sh} is found, the multivalued data is replaced by a single-valued waveform. The part of the curve for $\theta_{shift} < \theta_{sh}$ is retained up to the point intersecting θ_{sh}, and the part for $\theta_{shift} > \theta_{sh}$ is retained after the intersection. The shock itself is represented as a mathematical discontinuity between these two segments.

Specific implementation details vary slightly for the different initial conditions to handle their unique symmetry or asymmetry:

- For the examples of a *periodic sine wave* and a *sin pulse evolution into S wave*, the shock forms at the zero-crossing due to symmetry. The algorithm often exploits this symmetry to simplify the area calculation and waveform reconstruction.
- For a *sin pulse evolution into N wave*, the iterative equal rule implementation is performed only for a head shock and the solution to the tail shock is reconstructed using the symmetricity.

The resulting single-valued analytical solutions from these functions are used as benchmark references when comparing numerical results in the $A = 0$ regime, providing a rigorous test for the accuracy of tested numerical schemes.

4.4.2. Non-zero thermoviscous absorption case

When thermoviscous absorption is present in the medium ($A > 0$) benchmark solutions are obtained numerically using a high-resolution ***Conservative scheme*** with very fine discretization. Specifically, the reference solution is computed with 100 grid points per shock width that ensures the numerical dissipation and dispersion errors are negligible compared to the physical thermoviscous absorption. This finely resolved ***Conservative scheme*** solution serves as the benchmark for assessing the accuracy and convergence of the other implemented time-domain algorithms in thermoviscous media. For a detailed description of the ***Conservative scheme***, its discretization parameters and special features, the reader is referred to Section 5.1.

5. Numerical schemes

Time-domain numerical modeling has proven to be the most effective approach for simulating strongly nonlinear sound fields with shocks. In contrast to frequency-domain methods, whose computational cost depends quadratically on the number of harmonics, time-domain algorithms scale linearly with the number of time grid points, making them preferable when thousands of harmonics are required to accurately represent steep shock fronts. The **B-Sim** software implements four time-domain marching schemes widely used in nonlinear acoustics. These include conventional finite-difference ***Conservative scheme***, a shock-capturing ***Godunov-type method***, an algorithm based on the exact implicit solution of the lossless Burgers equation (***Austin algorithm***), and a scheme that operates in intrinsic coordinates (***IC algorithm***), operating with zero thermoviscous absorption. Each scheme has distinct features, stability characteristics and computational efficiencies, making it suitable for different physical regimes, such as propagation with or without thermoviscous absorption and for waveforms with symmetric or moving shocks. This chapter provides a detailed description of each numerical scheme, its discretization, key implementation aspects, and practical recommendations for its use within the software.

5.1. Conservative Scheme

The ***Conservative scheme*** is a conventional explicit finite-difference method based on the conservation-law form of the Burgers equation. When thermoviscous absorption is neglected ($A = 0$), the dimensionless Burgers equation (3) reduces to the Riemann equation:

$$\frac{\partial P}{\partial Z} = P\frac{\partial P}{\partial \theta}. \tag{14}$$

This equation can be written in divergence form as:

$$\frac{\partial P}{\partial Z} = \frac{1}{2}\frac{\partial P^2}{\partial \theta}, \tag{15}$$

which expresses the momentum conservation along the propagation direction Z. The ***Conservative scheme*** directly discretizes this conservation law.

For simulations with thermoviscous absorption ($A > 0$), the dissipative term is added explicitly, leading to the following discretized equation for the pressure value $P(Z + h_Z, \theta) \equiv P_j^{n+1}$ at each subsequent spatial step $n + 1$:

$$P_j^{n+1} = P_j^n + \frac{h_Z}{4h_\theta}\left(\left(P_{j+1}^n\right)^2 - \left(P_{j-1}^n\right)^2\right) + \frac{h_Z}{h_\theta^2}A\left(P_{j+1}^n - 2P_j^n - P_{j-1}^n\right), \tag{16}$$

where h_Z and h_θ are spatial and temporal steps, respectively. The second term on the right-hand side approximates the nonlinear flux using a second-order centered template. The third term is the standard three-point finite-difference approximation of the absorption operator.

This scheme is explicit, provides second-order accuracy in time, and is widely used as a reference in nonlinear acoustics. However, it is subject to numerical instabilities in the presence of steep shocks. In the non-absorptive propagation regime ($A = 0$) this method is generally unstable even if the grid steps h_Z and h_θ satisfy stability constraints derived from the Courant–Friedrichs–Lewy condition for the nonlinear term. Adding thermoviscous absorption to the equation helps to make it stable provided that the diffusion stability condition for the thermoviscous term is satisfied:

$$h_Z < \frac{h_\theta^2}{2A}. \tag{17}$$

This restriction is further implemented in recommendations in the **B-Sim**.

The ***Conservative scheme*** possesses distinct features that influence its optimal application:

1. It is robust for moderate nonlinearities and its conservational law form ensures convergence to the correct weak solutions.
2. Without additional thermoviscous absorption the scheme diverges at discontinuities in the waveform (when $Z > 1$), and Gibb's oscillations occur when thermoviscous absorption coefficient A is very small.
3. The scheme requires fine temporal discretization (100 points per shock) for a non-zero absorption and small spatial steps due to stability restrictions, leading to many propagation steps and increased runtime for long distances.

Despite limitations, the ***Conservative scheme*** serves as a valuable benchmark in the **B-Sim** due to its conservative nature and simplicity. It is especially useful for validating results in the regimes where shocks are not yet fully developed or where significant absorption keeps the waveform smooth.

5.2. Godunov-type algorithm (1 & 2)

The ***Godunov-type algorithm*** implemented in the **B-Sim** is a high-resolution shock-capturing finite-difference method based on the conservative form of the Burgers equation. Unlike the conventional ***Conservative scheme***, which becomes unstable and oscillatory near discontinuities, the ***Godunov-type scheme*** is specifically designed to handle steep shock fronts accurately while maintaining numerical stability. The scheme achieves high resolution of discontinuities using only 2–3 grid points per shock front for plane waves, making it computationally efficient for strongly nonlinear problems with moving shocks.

The numerical template of the ***Godunov-type scheme*** is as follows:

$$P_j^{n+1} = P_j^n + \frac{h_Z}{h_\theta}\left(H^n_{j+\frac{1}{2}}(Z) - H^n_{j-\frac{1}{2}}(Z)\right) + \frac{h_z A}{h_\theta^2}\left(P_{j+1}^n - 2P_j^n + P_{j-1}^n\right) \tag{18}$$

Here $H^n_{j\pm\frac{1}{2}}$ are the numerical fluxes at the cell interface between nodes j and $j+1$. The fluxes are computed as:

$$H^n_{j\pm\frac{1}{2}}(Z) = \frac{1}{4}\left(\left(P^+_{j\pm\frac{1}{2}}\right)^2 + \left(P^-_{j\pm\frac{1}{2}}\right)^2\right) + \frac{a^n_{j\pm\frac{1}{2}}(Z)}{2}\left(P^+_{j\pm\frac{1}{2}} - P^-_{j\pm\frac{1}{2}}\right), \tag{19}$$

where $a^n_{j\pm\frac{1}{2}}(Z) = \max\left|P^+_{j\pm\frac{1}{2}}, P^-_{j\pm\frac{1}{2}}\right|$ are the local wave speeds at the center of the numerical cell. $P^+_{j+\frac{1}{2}}$ and $P^-_{j+\frac{1}{2}}$ are reconstructed pressure values on the right and left sides of the grid node (n, j), obtained from a piecewise-linear reconstruction within each cell:

$$P^{+}_{j+\frac{1}{2}} = P^{n}_{j+1}(Z) - \frac{h_\theta}{2}\left(\frac{\partial P}{\partial \theta}\right)^{n}_{j+1}, \quad P^{-}_{j+\frac{1}{2}} = P^{n}_{j}(Z) + \frac{h_\theta}{2}\left(\frac{\partial P}{\partial \theta}\right)^{n}_{j},$$
$$P^{+}_{j-\frac{1}{2}} = P^{n}_{j}(Z) - \frac{h_\theta}{2}\left(\frac{\partial P}{\partial \theta}\right)^{n}_{j}, \quad P^{-}_{j-\frac{1}{2}} = P^{n}_{j-1}(Z) + \frac{h_\theta}{2}\left(\frac{\partial P}{\partial \theta}\right)^{n}_{j-1}. \tag{20}$$

The temporal derivatives $\left(\frac{\partial P}{\partial \theta}\right)^{n}_{j,j\pm1}$ are calculated using the slope limiter to ensure stability at slopes:

$$\left(\frac{\partial P}{\partial \theta}\right)^{n}_{j} = \min\bmod\left(\frac{b\left(P^{n}_{j} - P^{n}_{j-1}\right)}{h_\theta}, \frac{P^{n}_{j+1} - P^{n}_{j-1}}{2h_\theta}, \frac{b\left(P^{n}_{j+1} - P^{n}_{j}\right)}{h_\theta}\right), \tag{21}$$

where the weighting coefficient b is $1 \le b \le 2$. For $b = 1$(***Godunov-type-1*** in the software) the limiter introduces more numerical dissipation, improving stability. For $b = 2$ (***Godunov-type-2*** in the software), the scheme is less dissipative, yielding higher accuracy. The minmod limiter for the temporal derivatives is introduced as:

$$\min\bmod(x_1, x_2, \ldots) = \begin{cases} \min\limits_i\left(|x_i|\right), & x_i > 0 \ \forall i \\ \max\limits_i\left(|x_i|\right), & x_i < 0 \ \forall i \\ 0, & \text{otherwise} \end{cases}. \tag{22}$$

Because the scheme is explicit, the grid steps h_Z and h_θ must satisfy stability constraints derived from the Courant–Friedrichs–Lewy condition for the nonlinear term:

$$h_Z < \frac{h_\theta}{2\max|P|}, \tag{23}$$

and the diffusion stability condition for the viscous term:

$$h_Z < \frac{h_\theta^2}{2A}. \tag{24}$$

In simulations with both nonlinearity and absorption ($A > 0$) the more restrictive of the two conditions (23) or (24) must be satisfied. In practice, for reliable simulations of shock-forming waves, the following combined recommendation is used in the **B-Sim**:

$$h_Z < \min\left(\frac{h_\theta}{2\max|P|}, \frac{h_\theta^2}{2A}\right). \tag{25}$$

Because the ***Godunov-type scheme*** includes built-in numerical dissipation through the flux limiter, it is generally more robust than the conventional ***Conservative scheme*** and can remain stable even when the CFL condition is approached.

The ***Godunov-type scheme*** has several features for nonlinear acoustic simulations:

1. The scheme captures steep shocks within 2–3 grid points, making it suitable for modeling moving shocks in, e.g., an *N wave*, a *shock followed by an exponential tail*, and *one cycle of a sine wave evolving into N wave*.

2. Despite its more complex flux computation, the scheme can use larger numerical grid steps compared to the conventional ***Conservative scheme***, thus gaining in performance.
3. Though the scheme remains stable in non-absorptive cases even for non-smoothed discontinuous initial waveforms, implementation of initial waveform smoothening improves its accuracy.

In the **B-Sim**, the ***Godunov-type scheme*** is particularly recommended for simulations with moving shocks when thermoviscous absorption is small or equal to zero. Its ability to handle discontinuities with minimal grid points per shock makes it a preferred choice for efficient modeling of strongly nonlinear propagation regimes.

5.3. Austin algorithm

The ***Austin algorithm*** is a time-domain marching scheme based on the exact implicit solution of the lossless Burgers (Riemann) equation combined with a Crank-Nicolson treatment of thermoviscous absorption. The algorithm exploits the analytical solution to handle nonlinear distortion exactly, thereby avoiding numerical diffusion and dispersion errors associated with finite-difference approximations of the nonlinear term. Absorption is incorporated using an implicit scheme that ensures unconditional stability for the linear dissipative part.

The algorithm employs operator splitting technique to separate the effects of nonlinearity and thermoviscous absorption within each propagation step h_Z. The solution at $Z + h_Z$ is obtained in two stages: solution to an absorption term and to nonlinear term.

Thermoviscous absorption is treated by solving the linear diffusion equation:

$$\frac{\partial P}{\partial Z} = A\frac{\partial^2 P}{\partial \theta^2} \tag{26}$$

using the Crank-Nicolson scheme, which is second-order accurate and unconditionally stable. The discrete equation for each numerical grid point is:

$$\frac{P_j^{n+1} - P_j^n}{h_Z} = \frac{A}{2}\left(\frac{P_{j+1}^{n+1} - 2P_j^{n+1} + P_{j-1}^{n+1}}{h_\theta^2} + \frac{P_{j+1}^{n} - 2P_j^{n} + P_{j-1}^{n}}{h_\theta^2}\right). \tag{27}$$

This leads to a tridiagonal linear system which is then solved using the Thomas algorithm with Dirichlet boundary conditions at the edges of the time window.

The nonlinear term in the Burgers equation has the implicit solution: $P(Z, \theta) = P(0, \theta - P\cdot Z)$. This represents a time-grid transformation where each point of the waveform is shifted by an amount proportional to its local pressure. In discrete form, for the j-th time sample at propagation step $n + 1$:

$$\theta_j^{n+1} = \theta_j^n - P_j^n \cdot h_Z. \tag{28}$$

After applying this shift, the waveform is resampled onto the original uniform time grid θ using piecewise-cubic Hermite interpolation (PCHIP). This interpolation preserves monotonicity and avoids overshoots near shocks.

The overall scheme has a second order of accuracy in both time and space. To prevent the formation of multivalued solutions for nonlinear term, the spatial step must satisfy the following condition:

$$h_Z < \frac{h_\theta}{\max\left|P_j^n - P_{j-1}^n\right|}, \tag{29}$$

which ensures that no two characteristic lines cross within one spatial step.

The Crank–Nicolson scheme is unconditionally stable for the linear diffusion equation. There is no step-size restriction from the absorption term, allowing bigger h_Z when A is large.

The ***Austin algorithm*** has some specific peculiarities that influence its recommended usage in the **B-Sim**:

1. The algorithm requires that the time-shifted waveform remains single-valued within each propagation step. This imposes the practical constraint (29). When the waveform becomes very steep it requires smaller h_Z to avoid multivalued interpolants and maintain accuracy.
2. For waveforms with moving shocks (e.g., an *N wave*, a *shock followed by an exponential tail*, and *one cycle of a sine wave evolving into N wave*) in lossless media, the algorithm does not correctly reproduce the shock velocity given by the Rankine-Hugoniot relation; that is, the shock remains stationary. Consequently, the algorithm is not recommended for moving shock waveforms when $A = 0$.
3. When thermoviscous absorption is present, the algorithm requires a sufficiently time resolution (around 50 points per shock) of the waveform for moving shocks. If the shock is under-resolved, the propagation speed of the shock is distorted. Thus, for asymmetric shocks with $A > 0$ careful choice of the temporal grid spacing relative to the shock width is essential.
4. For waveforms that evolve into symmetric shocks (e.g., a *periodic sine wave*), the algorithm achieves high accuracy with large spatial steps regardless of absorption presence, making it the most computationally efficient scheme in the **B-Sim** for such cases.

5.4. IC (Intrinsic Coordinates) algorithm

The ***IC (Intrinsic Coordinates) algorithm*** was originally developed for modeling nonlinear wave propagation in media with relaxation and geometrical spreading (spherical or cylindrical waves). In the **B-Sim**, the method is implemented for the simpler case of plane waves while retaining its core mathematical framework. It is a specialized time-domain method designed for solving the Burgers equation, operating with ($A = 0$) and accounting for thermoviscous absorption via equal area rule. The main feature of this approach is a coordinate transformation that converts the potentially multivalued solution in physical coordinates (θ, P) into a single-valued representation in intrinsic coordinates (ψ, s). This transformation eliminates the numerical difficulties associated with shock formation and allows the use of larger adaptive spatial steps without the need for explicit shock-capturing or artificial viscosity.

The conversion to intrinsic coordinates is performed via the following relations:

$$\psi = \tan^{-1}\frac{\partial P}{\partial \theta},\quad s = \int_{\theta_0}^{\theta} \sqrt{1 + \left(\partial P / \partial \theta\right)^2}\, d\theta, \tag{30}$$

where ψ is the angle of the tangent to the waveform slope and s is the arc length along the waveform, a monotonic parameter that uniquely labels each point on the profile. In these coordinates, the lossless Burgers equation turns to:

$$\frac{\partial \psi}{\partial Z} = \sin^2\psi + \frac{\partial \psi}{\partial s}\int_0^s \sin\psi \cos\psi\, ds. \tag{31}$$

This equation describes how the tangent angle changes with propagation distance. Crucially, it remains single-valued even when the physical waveform becomes multivalued after shock formation. In the **B-Sim** software equation (31) is integrated in Z using a Runge-Kutta algorithm based on the fourth-order-accurate method of Dormand and Prince. The spatial step h_Z is adjusted dynamically based on local curvature, allowing larger steps where the waveform changes slowly.

After solving Eq. (31) for $\psi(s, Z)$, the physical waveform is recovered by integrating:

$$P(\theta,Z) = P(\theta_0,Z) + \int_0^s \sin\psi ds, \quad \theta = \int_0^s \cos\psi ds + \theta_0, \tag{32}$$

where θ_0 is the starting time of the signal.

If the result in physical coordinates is multivalued, a shock is inserted using the equal-area rule (described in Section 4.4) to obtain a weak solution that conserves the waveform's integral. This step is applied after the inverse transformation and is identical to the analytical equal-area procedure used for benchmark solutions.

Since the equation in intrinsic coordinates is smooth for most waveforms, the algorithm is inherently stable without a Courant-type restriction. The adaptive Runge–Kutta routine automatically controls the local error, typically allowing much larger spatial steps than explicit finite-difference schemes. The only stability-related requirement is that the initial waveform be sufficiently smooth to compute ψ accurately.

The ***IC algorithm*** has several distinctive characteristics that determine its optimal use in the **B-Sim**:

1. The method operates with $A = 0$ and uses the equal area rule to account for absorption. In the **B-Sim**, the absorption coefficient is automatically set to zero when this scheme is selected.
2. Because the coordinate transformation (30) involves derivatives, initially discontinuous profiles must be smoothed (see Section 4.3). The smoothing width is defined by the **Points per shock N_{ppsh}** parameter, which determines how many grid points span the initial shock transition.
3. For accurate reconstruction of the physical solution after shock formation the time window must be extended beyond the original signal duration to accommodate the spreading of multivalued regions. In the **B-Sim**, the default time window is automatically enlarged for the ***IC scheme*** when simulating to $Z_{max} \leq 10$ for all the signals except for *a shock followed by an exponential tail*, where time window T is a custom value set by the user.
4. The use of an adaptive Runge–Kutta solver allows the spatial step h_Z to vary according to the local rate of change of ψ. This results in efficient computation, with larger steps in regions of gentle waveform variation and finer steps near developing shocks, making the ***IC algorithm*** the fastest among the implemented schemes for waveforms with moving shocks at moderate propagation distances. At very long distances the need to extend the time window reduces this advantage.

The ***IC algorithm*** represents an elegant and computationally efficient approach to nonlinear lossless wave propagation, particularly valuable for educational demonstration of coordinate transformation principles and for efficient simulations of pulsed signals with moving discontinuities.

6. Critical user inputs: guidelines and recommendations

The accuracy, stability, and computational efficiency of simulations in the **B-Sim** depend critically on several user-defined parameters. This section provides practical guidelines for selecting appropriate values based on the physical problem, the chosen numerical scheme, and the desired trade-off between precision and runtime. Following these recommendations will help users obtain reliable results while avoiding common pitfalls such as numerical instability, excessive diffusion, or unnecessarily long computation times.

6.1. Absorption coefficient (A)

The dimensionless absorption coefficient A is a fundamental parameter in the Burgers equation which quantifies the relative strength of thermoviscous dissipation compared to nonlinear distortion. The value of A directly influences the wave propagation regime, shock structure, and the appropriate choice of numerical scheme.

Two primary propagation regimes are distinguished based on the A value:

1. Nonlinear regime with $A < 0.1$: in this regime nonlinear steepening dominates over dissipation. Shocks form rapidly, resulting in sharp, narrow fronts. Waveforms can become multivalued in the lossless limit ($A = 0$). This regime is typical for high-amplitude sound waves in water, soft tissue, or air over moderate distances, where cumulative nonlinear effects are significant.
2. Quasi-linear regime with $A > 0.1$: here dissipative effects are comparable to or stronger than nonlinearity. Shock formation is suppressed and shocks are substantially broadened by viscosity. This regime occurs for low-amplitude signals or in highly viscous/relaxing media, or when propagation distances are shorter relative to the shock-formation distance.

Note that the threshold $A \approx 0.1$ is a practical guideline, the transition between regimes is gradual.

The value of A dictates which numerical schemes are applicable and how they should be configured:

- ***IC algorithm*** accounts for absorption via equal area rule and thus does not provide a precise description of smooth solutions. Therefore, it should be used for $A \ll 1$ or $A = 0$. Selecting the ***IC scheme*** automatically sets $A = 0$ for this algorithm.
- ***Austin algorithm*** is effective mostly for $A > 0$. For $A = 0$ it provides correct results only for *waveforms with symmetrical shocks*. For *moving shocks* at $A > 0$ the algorithm requires high temporal resolution to accurately resolve the shock front. It was estimated that around 40–50 point per shock are required for a correct behavior. If A is extremely small (e.g., $A < 0.001$) the shock width becomes very narrow, necessitating an impractically fine grid. Therefore, it is not recommended to use $A < 0.001$ with ***the Austin algorithm*** for *moving shocks*.
- ***Conservative scheme*** requires $A > 0$ for stability in shock-forming regimes. In the lossless limit ($A = 0$) the scheme becomes unstable after shock formation ($Z > 1$). A small but finite A provides necessary damping for stable simulations. This scheme, however needs fine temporal resolution with around 100 point per shock to accurately describe the waveform. This imposes a severe restriction on grid steps, drastically increasing computational cost. Therefore, using $A < 0.001$ with the ***conservative scheme*** is not recommended for typical simulations.

- *Godunov-type schemes* are robust for all A, performing well in both nonlinear and quasi-linear regimes. In contrast to the ***Austin algorithm*** and ***conservative scheme***, the ***Godunov-type algorithm*** requires not more than 10 points per shock for an accurate shock description. Still, to avoid impractical runtimes, it is recommended to use $A \geq 0.001$ with ***Godunov-type schemes***.

Note that both explicit schemes (***Conservative*** and ***Godunov-type***) must satisfy the diffusion stability condition (17), (24).

In the **B-Sim** interface, the absorption coefficient is entered in the **Physical Parameters** panel. To maintain reasonable computation times, it is advisable to keep $A \geq 0.001$ for explicit schemes (***conservative*** and ***Godunov-type***) and for the ***Austin algorithm*** when simulating *moving shocks*.

6.2. Initial waveform smoothing recommendations

The treatment of initially discontinuous waveforms (a *shock followed by an exponential tail* and *N wave*) plays a critical role in the accuracy and stability of numerical simulations in the **B-Sim**. The software provides an option to smooth these discontinuities before propagation, and the choice of smoothing parameters depends on the thermoviscous absorption coefficient A and the selected numerical scheme.

As follows from Section 4.3, smoothing of initially discontinuous waveforms (*N-wave* and a *shock followed by an exponential tail*) is recommended for all propagation regimes to ensure physically consistent and numerically robust simulations. The smoothed waveforms are constructed using the quasi-stationary hyperbolic tangent shock solution of the Burgers equation. The shock width $\Delta\theta$ is defined as the interval over which the pressure rises from 10% to 90% of its maximum absolute value. For a tanh profile: $\Delta\theta = 10A$.

The software distinguishes two smoothing regimes:

1. $A = 0$: no physical absorption is present. The user defines the desired shock resolution by specifying the number of time grid points per shock N_{ppsh} in the corresponding field **Points per shock N_{ppsh}**. The software then calculates an effective thermoviscous absorption coefficient A_{eff} to produce that width on the given temporal grid. In this regime only ***Godunov-type*** and ***IC scheme*** produce correct results for *initially discontinuous shocks*. Below are the recommendations for smoothing for these algorithms.

   - ***IC algorithm***
     To achieve maximum agreement with analytical weak shock theory solutions (errors in shock rise time and amplitude are below 1%), the following recommendations were established. For propagation distances $Z_{\max} < 5$ it is recommended to use 10 points per shock and for $Z_{\max} > 5$ the recommended number is 20 points per shock. These values ensure that the initially smoothed profile is sufficiently resolved to accurately capture shock motion and deformation over the simulated distance. However, the user may freely adjust this number depending on the chosen time step h_θ to avoid making the initial profile too wide relative to the waveform's characteristic scale, which could artificially delay shock formation or alter the waveform's early evolution.

   - ***Godunov-type algorithms***
     Because these schemes are designed to capture shocks using only 2–3 grid points per discontinuity, there is no benefit in using more than 3–4 points per shock in the initial smoothing. The exact shape of the smoothed initial profile does not significantly affect

the final result unless this number is too big, as the shock-capturing mechanism quickly adjusts to the correct solution. Using more points only increases the initial computational cost without improving accuracy.

2. $A > 0$: the physical thermoviscous coefficient A directly determines the shock width. The initial waveform is smoothed using this value, and the **Points per shock N_{ppsh}** field becomes inactive. For all the algorithms except for the ***IC scheme***, smoothing is recommended because it corresponds to the physical reality of a viscous shock front. In this case, the smoothing parameters are automatically determined by the **B-Sim** based on the physical absorption coefficient A, as described in Section 4.3. The user does not need to specify **Points per shock N_{ppsh}**, the software constructs a tanh profile whose width is consistent with the stationary shock solution for the given A.

Thus, the key points for users are organized in the following table:

Propagation regime	Algorithm	Smoothing option	Points per shock N_{ppsh}	Comments
$A = 0$	IC	Mandatory	10 ($Z_{max} < 5$) 20 ($Z_{max} > 5$)	Accuracy loss may occur with too different N_{ppsh} values
	Godunov-type	Recommended	2–4	Accuracy loss beyond 10 points per shock
$A > 0$	Conservative Godunov-type Austin	Recommended	N/A	Smoothing width is calculated automatically according to A value

By adhering to these recommendations, users can ensure that their simulations start from a physically and numerically appropriate initial condition, leading to reliable results and efficient computation.

6.3. Grid steps choice

The choice of the temporal step h_θ and the spatial step h_Z are critical for achieving accurate, stable, and computationally efficient simulations in the **B-Sim**. The software provides built-in recommendations for these parameters described in the **Algorithms** section, displayed in the green fields on the right to the **Grid Parameters** panel and in the field **General recommendation**, where recommended relations between h_Z and h_θ are given. These recommendations are derived from a combination of stability criteria according to Eqs. (17), (25), (29) (to prevent numerical divergence) and accuracy considerations (to ensure the solution converges to within 1% of the asymptotic fine grid result). The recommended values and their relationships depend on both the numerical scheme and the propagation regime ($A = 0$ or $A > 0$).

The recommendations on the relation between h_Z and h_θ are based on the following principles:

1. Stability conditions:

For explicit schemes (***Conservative*** and ***Godunov-type***) the steps must satisfy the parabolic stability condition for the viscous term when $A > 0$ (17), (24). The ***Godunov-type algorithm*** must also satisfy the Courant-Friedrichs-Lewy (CFL) condition for the nonlinear term when $A = 0$ (23). In the B-Sim the resulting stability restrictions are: $h_Z < \dfrac{h_\theta^2}{2A}$ (17) for ***Conservative scheme*** and $h_Z < \min\left(\dfrac{h_\theta}{2\max|P|}, \dfrac{h_\theta^2}{2A}\right)$ (25) for ***Godunov-type algorithm***. For the ***Austin algorithm*** the primary constraint is the uniqueness condition to prevent multivalued interpolants: $h_Z < \dfrac{h_\theta}{\max\left|P_j^n - P_{j-1}^n\right|}$ (29).

The ***IC algorithm*** is inherently stable; its step h_Z is adaptive and controlled by the ODE solver's error tolerance.

2. Accuracy criterion:

For each scheme and regime, the recommended steps relationships were determined by performing convergence tests. The chosen steps are the largest for which further refinement changes key solution metrics (e.g., shock amplitude and temporal position) by less than 1%. Next, the recommendations on h_θ, depending on the propagation regime (A = 0 or A > 0), were chosen to provide the proper accuracy (less than 1% change in results with altered h_θ) with the chosen steps relationship.

The table below summarizes the default recommendations implemented in the **B-Sim**. In the interface, specific numerical values are pre-filled based on these formulas.

Algorithm	Propagation regime	Recommended h_θ	Recommended h_Z	Comments
Conservative	$A = 0$	0.01	$h_Z < 0.5h_\theta$	Only for *initially smooth waveforms* before shock formation
	$A > 0$	$0.1A$	$h_Z < \dfrac{h_\theta^2}{2A}$	Recommendations for stability and accuracy criteriums satisfaction
Godunov-type 1 & 2	$A = 0$	0.01	$h_Z = 0.1h_\theta$	More restrictive recommendation for accuracy criterium satisfaction
	$A > 0$	$\min(2.5A, 0.1)$	$h_Z < \min\left(0.1h_\theta, \dfrac{h_\theta^2}{2A}\right)$	h_θ recommendation to avoid too large time steps at large A
Austin	$A = 0$	0.01	$h_Z = 0.9h_\theta$	Grid steps primarily limited by accuracy for *symmetric shocks*
	$A > 0$	$0.25A$	$h_Z = 0.1h_\theta$	Grid steps primarily limited by accuracy for *moving shocks*
IC	$A = 0$	0.001	$h_Z = 0.01$ (adaptive)	The internal ODE solver uses adaptive step, the entered h_Z determines the maximum value. A finer h_θ for accurate *moving shocks* results

Adhering to the suggested steps and their relationships ensures a balance between accuracy and computational speed. Using significantly larger steps may lead to instability or large errors, while much finer steps will increase run time without appreciably improving the result. By understanding and applying these guidelines, users can reliably set up their simulations to produce accurate results without unnecessary computational expense.

7. Summary table of algorithms usage

Here, as a conclusion, a brief summary table is provided on the applicability, key features and limitations of using a particular numerical algorithm, depending on the propagation mode (lossless or absorptive) determined by the coefficient A.

<table>
<tr><th>Algorithm</th><th>Propagation regime</th><th>Applicability</th><th>Key features</th><th>Limitations</th></tr>
<tr><td rowspan="2">Conservative</td><td>$A = 0$</td><td>Limited</td><td>Simple implementation
Fast</td><td>Unstable after shock formation ($Z > 1$)
Not suitable for practical simulation</td></tr>
<tr><td>$A > 0$</td><td>Applicable</td><td>Simple implementation
A benchmark solution</td><td>Requires high temporal resolution
Stability limits restrict h_Z</td></tr>
<tr><td rowspan="2">Godunov-type 1 & 2</td><td>$A = 0$</td><td>Applicable</td><td>Stable and correct
Fastest at long distances</td><td>Stability limits restrict h_Z
Initial waveform smoothing is recommended</td></tr>
<tr><td>$A > 0$</td><td>Applicable</td><td>Only 2–3 points per shock needed
Fastest for moving shocks</td><td>Stability limits restrict h_Z
Initial waveform smoothing is recommended</td></tr>
<tr><td rowspan="2">Austin</td><td>$A = 0$</td><td>Limited</td><td>Exact nonlinearity treatment
Fastest for symmetric shocks</td><td>Inaccurate shock speed for moving shocks
Uniqueness condition restrict h_Z</td></tr>
<tr><td>$A > 0$</td><td>Applicable</td><td>Fastest for symmetric shocks
Unconditionally stable</td><td>Needs fine resolution for moving shocks</td></tr>
<tr><td rowspan="2">IC</td><td>$A = 0$</td><td>Applicable</td><td>Adaptive spatial step
Fastest for moving shocks at short distances</td><td>Initial waveform smoothing is required
Requires prolongated waveforms at long distances</td></tr>
<tr><td>$A > 0$</td><td>Inapplicable</td><td>-</td><td>-</td></tr>
</table>