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All-Speed Methods and Long-Duration Time Integration for Incorporation into the 7-Equation Two-Phase Model

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Abstract

The numerical simulation of multiphase flows in Light Water (Nuclear) Reactors, LWRs, for normal, accident, and off-normal operation, and for operational optimization must cover a huge disparity of transient time durations, from milliseconds to years. In addition, our recent work has shown that the application of classical Riemann approaches, which pervade modern computational fluid dynamics (CFD), suffer numerical accuracy degradation, especially for compressible liquid flows. In this setting, all-speed or Mach uniform methods are needed which can be accurately and *efficiently* integrated over a very large range of time scales. Thus we need a multi-*time*-scale integration approach to compliment our previously documented multi-*spatial*-scale approach to multiphase flow modeling [1]. This report briefly summarizes our investigations in these areas.

Background

There are key issues in Pressurized Water (nuclear) Reactor, PWR, safety and optimization that rely on in-depth understanding of basic two-phase flow phenomena with heat and mass transfer. The bulk of these can be placed within the context two bubble-dynamic phenomena: boiling (heterogeneous), flashing (homogeneous boiling) and bubble collapse. Other problematic phenomena, such as crud deposition, appear to be intimately connected with the boiling process.

Because of the diversity of physical phenomena occurring in boiling, flashing, and bubble collapse, and of the consequent length- and time-scales in LWR systems, it is imperative that the models have the following features:

- Both vapor and liquid phases (and non-condensable phases, if present) must be treated as compressible,
- Models must be mathematically and numerically well-posed, and

- The methodologies evolved to implement the models must be multi-scale.

In a previous report [1] focus was placed specifically on the compressible, well-posed, and multi-*spatial*-scale requirements of advanced simulation methods for these LWR coolant systems. There it was advocated that because of the expense of developing multiple special-purpose codes and the need to couple information from the multiple length- and time-scales, efforts within CASL should be focused toward development of multi-scale approaches to solve the multiphase flow problems relevant to LWR design and safety analysis. Efforts were recommended aimed at developing well-designed unified physical/mathematical[1] and high-resolution numerical models for compressible, all-speed multiphase flows spanning:

(1) Well-posed general mixture level (true multiphase) models for fast transient situations and safety analysis,

(2) DNS (Direct Numerical Simulation)-like models to resolve interface level phenmena like flashing and boiling flows, and critical heat flux determination (necessarily including conjugate heat transfer), and

(3) Multi-scale methods to resolve both (1) and (2) automatically, depending upon specified mesh resolution, and to couple different flow models (single-phase, multiphase with several velocities and pressures, multiphase with single velocity and pressure, etc.)[2]

Such development would extend the necessary foundations and build the capability to simultaneously solve fluid dynamic interface problems as well as multiphase mixtures arising from boiling, flashing or cavitation of superheated liquid, and bubble collapse, etc. in light water reactor systems. It entails development on two main fronts. The first requires the derivation (design) of *theoretical models* for multiphase and interfacial flows whose mathematical description (equation system) is *well-posed* and exhibits *hyperbolicity*, exhibiting correct wave dynamics at all scales. The second requires the design of appropriate *numerical schemes* to give adequate resolution for *all spatial and time scales of interest*. These models are not as well known as conventional single-fluid models and pose significant numerical challenges, e.g. the numerical approximation of non-conservative terms. In addition, these numerical issues can pose theoretical questions such as shock wave existence in a multiphase mixture, cell averages of non-conservative variables, etc.

[1] That is, the effective, nonlinear system of first order partial differential equations.

[2] Specifically, a well-designed 2-pressure, 2-velocity, seven-equation two-phase mixture model (as in 1) can be systematically reduced analytically to produce a 1-pressure, 1-velocity, five-equation model (as for 2) capable of a DNS-like (Direct Numerical Simlation) resolved interface solution. If such a systematic reduction is accomplished numerically on a local spatial level, then a general algorithm (such as 1) can be made to reduce locally where appropriate to the interface resolved model (2), effectively giving an automatic multi-scale treatment (as 3).

Such two-phase flow phenomena occurring inside light water nuclear reactors includes, especially with departure from nucleate boiling (DNB) and film boiling instability (boiling crisis), coolant phase changes and multiple flow regimes which directly influence the coolant interaction with the fuel elements/assemblies and, ultimately, the reactor performance. Because of the inherent coupling, an understanding of these phemonena, along with subcooled boiling and bubble collapse, is also key to gaining an understanding of crud depostion in these systems [2]. The goal of CASL development needs ultimately to provide models giving highly resolved details where necessary, simultaneously with large scale vessel/component simulation by providing a well-posed, multi-scale model that will:

- Resolve interfaces for larger bubbles (direct numerical simulation, DNS-like) with single velocity, single pressure treatment (interface capturing), and

- Average (or homogenize) the two-phase flow field for small bubbles with two velocities, two pressures.

Of course the resulting algorithms are to be implemented on modern parallel computing machines for solving *large-scale problems* for the design and analysis of advanced technology systems such as nuclear energy.

The primary, enabling feature of the INL (Idaho National Laboratory) multi-scale methodology for multiphase flows involves the way in which we deal with multiphase mixtures. Our multi-scale approach is essentially to ***solve the same equations everywhere with the same numerical method*** [3]**:**

- In pure fluid,

- In multi-velocity mixtures

- In artificial smearing zones at material interfaces or in mixture cells,

- In phase transition fronts and in shocks.

There are several advantages with this approach:

- *Coding simplicity* and *robustness* as a *unique algorithm* is used;

- *Conservation principles* are guaranteed *for the mixture*. Conventional algorithms are able to preserve mass conservation only when dealing with interfaces;

- *Interface conditions are perfectly matched* even for the coupling of complex media (capillary fluids, transition fronts) even in the presence of shocks;

- This approach is the ***only one able to deal with dynamic appearance of interfaces*** (spontaneous flashing (cavitation) and boiling);

- These methods allow the *coupling of multi-velocities, multi-temperature mixtures* to macroscopic interfaces where a single velocity must be present. This capability can be illustrated simply by considering the example of a cloud of bubbles rising up in a liquid to the surface, where a free boundary (interface) is present. Two velocities must be considered for the bubbles rising, while a single velocity must be present just after their crossing through the interface. It is also desirable to resolve large bubbles in which a liquid with small bubbles lies outside our large bubble and/or vapor with small droplets lies inside the bubble. This is the ***only method able to deal with such situations***.

Because of the broad spectrum of phenomena occurring in light water nuclear reactor coolant flows (boiling, flashing, and bubble collapse, choking, blowdown, condensation, wave propagation, large density variation convection, etc.) it is imperative that models accurately describe compressible multiphase flow with multiple velocities. The high-pressure and/or high-velocity conditions involved in these flows require that compressible effects be considered for all phases. Conventional models[3] of two-phase mixtures having two velocities present are represented with a system of six partial differential equations: two mass, two momentum, and two energy equations. With the assumption of pressure equilibrium, these models have a single pressure common to both phases. These models are not hyperbolic and are ill-posed. This means that initial data and boundary conditions do not fully determine the solution at the next instant in time. Wave propagation may have no physical sense with such systems because the square of the sound speed may become negative.

This problem was remedied with the addition of seventh equation, a differential expression (equation) of the pressure nonequilibrium condition, e.g. [4-9], describing the time evolution of the volume fraction[4], and which replaced the pressure equilibrium assumption in the mixture. These terms control the rate at which pressure equilibrium is reached after wave propagation (also as phase velocities equilibrate). Such models have 7- or 8-equations for two-phase flow. (Note: Traditional 6-equation, two-phase models assume both phase have a single pressure, are not hyperbolic, are ill-posed, and give wrong wave dynamics solutions!). With this addition, the model became correctly (well-) posed and unconditionally hyperbolic.

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[3] The complexity of multiphase, multi-component, and/or multi-material flow dictates that they need to be examined in an averaged sense. Traditionally, one would begin with known (or at least postulated) microscopic flow relations that hold on the "small" scale. These include continuum level conservation of mass, balance of species mass and momentum, conservation of energy, and a statement of the second law of thermodynamics often in the form of an entropy inequality (such as the Clausius-Duhem inequality). The averaged or macroscopic multiphase conservation equations and entropy inequalities are then constructed from the microscopic equations through suitable averaging procedures, as shown in the Appendix. At this stage a stronger form of the second law may also be postulated for the mixture of phases or materials. To render the evolutionary material flow balance system unique, constitutive equations and phase or material interaction relations are introduced from experimental observation, or by postulation, or from microlevel numerical simulation) through strict enforcement of the constraints or restrictions resulting from the averaged entropy inequalities. These averaged equations form the governing equation system for the dynamic evolution of these mixture flows.

[4] Specifically, the volume fraction evolution equation is driven, at least in part, by a pressure relaxation effect.

This seven-equation two-phase flow model can be given in slightly different form [10] as

$$\frac{\partial \alpha_1}{\partial t} + u_I \frac{\partial \alpha_1}{\partial x} = \mu\left(p_1 - p_2\right) + \frac{\Gamma_1}{\rho_I}$$
$$\frac{\partial\left(\alpha_1\rho_1\right)}{\partial t} + \frac{\partial\left(\alpha_1\rho_1 u_1\right)}{\partial x} = \Gamma_1$$
$$\frac{\partial\left(\alpha_1\rho_1 u_1\right)}{\partial t} + \frac{\partial\left(\alpha_1\rho_1 u_1^2 + \alpha_1 p_1\right)}{\partial x} = p_I \frac{\partial \alpha_1}{\partial x} - \lambda\left(u_1 - u_2\right) + \Gamma_1 u_I$$
$$\frac{\partial\left(\alpha_1\rho_1 E_1\right)}{\partial t} + \frac{\partial\left[\alpha_1\left(\rho_1 E_1 + p_1\right)u_1\right]}{\partial x} = p_I u_I \frac{\partial \alpha_1}{\partial x} - \mu p_I'\left(p_1 - p_2\right) - \lambda u_I'\left(u_1 - u_2\right) + \Gamma_1 E_I$$

for one phase, coupled to the other phase similarly as

$$\frac{\partial \alpha_2}{\partial t} + u_I \frac{\partial \alpha_2}{\partial x} = \mu\left(p_2 - p_1\right) + \frac{\Gamma_2}{\rho_I}$$
$$\frac{\partial\left(\alpha_2\rho_2\right)}{\partial t} + \frac{\partial\left(\alpha_2\rho_2 u_2\right)}{\partial x} = \Gamma_2$$
$$\frac{\partial\left(\alpha_2\rho_2 u_2\right)}{\partial t} + \frac{\partial\left(\alpha_2\rho_2 u_2^2 + \alpha_2 p_2\right)}{\partial x} = p_I \frac{\partial \alpha_2}{\partial x} - \lambda\left(u_2 - u_1\right) + \Gamma_2 u_I$$
$$\frac{\partial\left(\alpha_2\rho_2 E_2\right)}{\partial t} + \frac{\partial\left[\alpha_2\left(\rho_2 E_2 + p_2\right)u_2\right]}{\partial x} = p_I u_I \frac{\partial \alpha_2}{\partial x} - \mu p_I'\left(p_2 - p_1\right) - \lambda u_I'\left(u_2 - u_1\right) + \Gamma_2 E_I$$

where, for two phases, the second volume fraction equation can be eliminated through the saturation condition $\alpha_1 + \alpha_2 = 1$. We point out that we have here neglected pressure differences that can be sustained due to relative velocity between the phases, e.g. [11], or due to surface tension effects. We refer to these sustained (or steady-state or static) pressure differences as *structural* or *configuration pressures* because they are due to the structure or configuration of the phases. These additional effects can be sustained at steady state – thus for very rapid volume fraction evolution these residual force balances can become an algebraic closure relation. Such pressure differences can be easily accommodated, as appropriate, with modification of the volume fraction evolution equation and the interface pressure expressions in the momentum and energy equations. We neglect these terms here for clarity of presentation and retain only the fastest thermodynamical nonequilibrium terms. For two phases, it holds that $\Gamma_1 + \Gamma_2 = 0$. In addition to equations of state for each phase closure relations for this system require the determination of:

- The interface velocity u_I and pressure p_I representing the velocity and pressure, respectively, that are exerted at the boundary of a cloud of bubbles or droplets,

- The average interface velocity u_I' and pressure p_I' that are exerted in the bulk of a two-phase control volume,
- The relaxation parameters λ and μ that control the rate at which velocities and pressures, respectively, relax to ***mechanical equilibrium***.

This two-phase mixture model has little diffusion. The model can be difficult to solve numerically, in particular with modern algorithms based on the Riemann problem solution (see [1] and the references therein). Notice also that for use with DNS-like interface resolving calculations:

- This model involves two pressures and two velocities,
- At an interface the jump condition corresponds to continuous normal velocities and continuous pressures,
- In order to fulfill this condition we can relax the two pressures and velocities to unique equilibrium values.

These issues can be resolved by using specific relaxation solvers, with locally infinite relaxation parameters, to solve interface problems and multiphase mixtures with two velocities.

With this 7-equation model, reduced models are obtained naturally, characterized by instantaneous equilibrium, or relaxation, (globally or locally) between pressures, velocities, temperatures, and Gibbs energies. This makes it ideal for coupling to simpler codes, "legacy" codes, or continuous reduction to simpler models when appropriate for faster execution speeds. Note this 7-equation model will also form the basis of the new INL, MOOSE-based, RELAP-7 LWR safety analysis code.

All-speed, and Long Time Duration Methods for Two-phase Flows

The success of this multi-scale, multiphase method relies on:

- Use of an unconditionally hyperbolic model for two-phase compressible mixtures,
- Accurate discetization of the nonconservative terms and equations, and
- Use of robust relaxation procedures to restore pressure and velocity interface conditions based on large relaxation parameters.

Consequently, a good all-speed flow integration method is needed for two-phase flows. Recalling from the thermodynamic properties of two-phase mixtures that effective sound speeds in two-phase mixtures can be as low as a few feet per second, effective Mach numbers ranging from nearly 0 to greater than 10 can easily result.

The huge disparity of transient time durations, from milliseconds to years, produces a time stiffness that creates serious numerical difficulties due to the different time scales. For example the short duration, fast transients such as produced by flashing, bubble collapse, and wave dynamics require numerical time steps based on the fastest signal speeds of the system. On the other hand long duration, slow transients require much longer time steps (even several orders of magnitude) to be efficient. This usually implies that some level of implicit time integration be employed to achieve the larger time steps in a stable manner. In addition to this time stiffness, low speed compressible flows can exhibit a coupling which produces a type of "*spatial stiffness*" wherein *an excessive number of spatial mesh points are required to obtain an accurate solution*. This occurs because the numerical flux function must mimic the asymptotic behavior of the continuous equations for $Mach \to 0$. Classical Riemann and approximate Riemann approaches, which form the bulk of modern computational fluid dynamics (CFD) for compressible flows, do not have this property and therefore suffer from this low Mach number problem, especially for compressible liquid.

These ideas can be illustrated with a much simpler benchmark problem that specifies only a single-phase, compressible flow. We consider the benchmark problem, constructed originally for two-phase flow in [12], of transient compressible flow in a converging-diverging nozzle. The flow can be started with nearly arbitrary initial conditions, after which the flow undergoes a rapid transient wave solution, until a steady state is reached.

The converging-diverging nozzle has a cross-sectional area which is specified as a cosine function of position along the axis of the nozzle, x

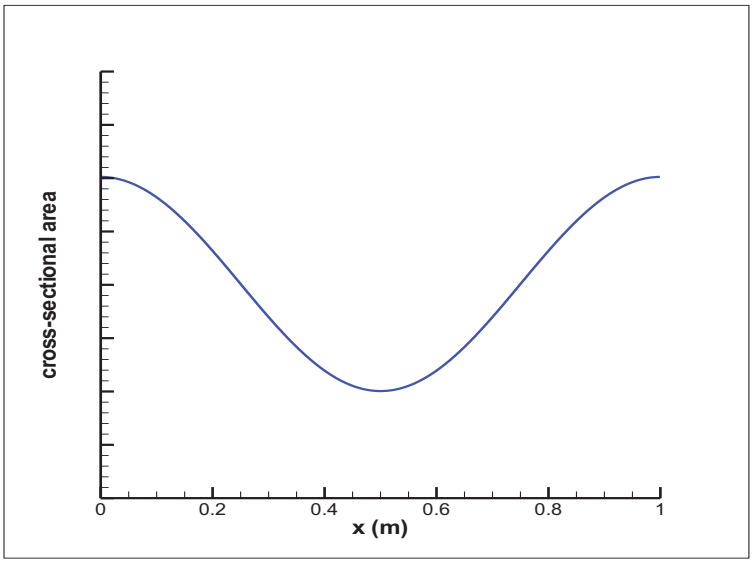
$$A(x) = A_0\left[1 + \frac{\cos(2\pi x)}{2}\right]$$

where $0 \le x \le 1.0$ is in meters and A has units of A_0 (m^2, cm^2, in^2, etc.). The normalized cross-sectional area is shown in the figure below. The inlet and outlet areas are equal. The inlet conditions (left boundary) were specified as stagnation conditions of

$$P_0 = 1\ MPa$$
$$T_0 = 453\ K.$$

The static pressure outlet condition was specified for subsonic flow (right boundary) as

$$p_b = 0.5\ MPa.$$



Normalized nozzle cross-sectional area distribution (cosine function)

It is assumed that the thermodynamic properties for compressible water (or its vapor) are given by the stiffened gas equation of state (SGEOS)

$$e(p,\rho) = \frac{p + \gamma p_\infty}{(\gamma - 1)\rho} + q$$

$$\rho(p,T) = \frac{p + p_\infty}{(\gamma - 1)c_v T}$$

$$h(T) = \gamma c_v T + q$$

$$g(p,T) = (\gamma c_v - q')T - c_v T \ln \frac{T^\gamma}{(p + p_\infty)^{(\gamma - 1)}} + q$$

with parameters given in the following table:

Table 1. Stiffened gas equation of state parameters for water and its vapor [LeMetayer, etal., 2004]

Water	γ_k	$q_k \left(J \cdot kg^{-1}\right)$	$q'_k \left(J \cdot kg^{-1} \cdot K^{-1}\right)$	$p_{\infty k} \left(Pa\right)$	$c_{vk} \left(J \cdot kg^{-1} \cdot K^{-1}\right)$
Liquid	2.35	$-1167 \cdot 10^3$	0	10^9	1816
Vapor	1.43	$2030 \cdot 10^3$	$-23 \cdot 10^3$	0	1040

Phase change is not allowed here (single phase), so local pressures may become negative which is permissible with the SGEOS, at least as long as temperature and density remain positive. Notice that for $p = p_\infty$ the fluid is *nearly incompressible* or *weakly compressible* whereas when p is of the same order as p_∞ the fluid is compressible in the traditional sense. Also note that there are key applications where nearly incompressible is <u>not</u> the same as incompressible.

From this we create two slow transient problems with solutions periodic in time, which are dictated by boundary conditions.

<u>Problem 1</u>

The inlet conditions (left boundary) are specified as stagnation conditions of

$$P_0 = 1\ MPa$$

$$T_0 = 453\ K.$$

A static pressure outlet condition is specified for subsonic flow (right boundary) as a slowly varying function of time

$$p_b = 0.5 + 0.1\sin\left(\frac{\pi t}{10}\right) MPa,$$

where time t is specified in units of seconds. This specified static outlet pressure (back pressure) is periodic over 20 seconds to simulate a longer term transient. Initial conditions must be specified but, due to the scale of this problem, they will have negligible influence on the longer term transient. All flow variables of the "nearly" steady solution will vary slowly as the static outlet pressure is slowly varied. □

<u>Problem 2</u>

An interesting variant of Problem 1 above is specified by maintaining the static outlet pressure (right) at

$$p_b = 0.5\ MPa$$

and specifying that the inlet stagnation conditions (right) vary periodically as

$$p_0 = 1.0 + 0.25\sin\left(\frac{\pi t}{43200}\right) \quad MPa$$

$$T_0 = \hat{K}\left[1.0 + 0.25\sin\left(\frac{\pi t}{43200}\right) + p_\infty\right]^{\frac{\gamma-1}{\gamma}} \quad K$$

where

$$\hat{K} = \frac{453}{\left(1 + p_\infty\right)^{\frac{\gamma-1}{\gamma}}}$$

With these slowly varying stagnation inlet parameters (period = 2 x 43200 = 86400 seconds = 1 day), the pressure distribution of the "nearly" steady solution will not vary at all (in this long term), however the other variables will indeed change slowly. □

To gain better insight to these problems our research has focused in the following areas: (1) low Mach number preconditioning, (2) low Mach number Riemann solvers, (3) IMEX semi-implicit methods, and (4) Point implicit methods. Each of these will be summarized in the sequel.

Low Mach Number Preconditioning

We examined a particular type of Low Mach number preconditioning [13] for each phase in conjunction with our 1-D variable area DEM two-phase method [12]. As stated above, the conventional Godunov method converges to the exact low Mach number solution only if a very fine (excessively so) mesh is used. Such meshes are impractical for more than one space dimension. For transonic to high Mach number flows, conservative formulations of the equations are used and Riemann problem based solution methods work well. However, difficulty arises with conservative formulations when the Mach number tends to zero when the incompressible limit is approached. It appears that the corresponding Riemann solvers give insufficient acoustic dissipation to finite volume methods and fail to provide an accurate approximation of the incompressible equations. Recall that Riemann solvers are based on linearizations, designed to slowly dissipate acoustic waves. The idea behind low Mach number preconditioning is to manage the numerical dissipation in order to improve the numerical convergence at low Mach number. Turkel [14] proposed to enforce pressure time invariance up to Mach number squared fluctuations with the help of a penalization method. This penalization idea can be used to modify the Riemann problem solution while retaining the conservative formulation along with the real equation of state.

We first note that in the low Mach number limit, the solutions of Euler equations are in the form

$$f = f_0(x,t) + f'(x,\tau)$$

where f is any variable of the flow, f_0 the dominant order, and f' its fluctuations. The dominant order of the solution, with a "long" time which is denoted t, is related to the material transport, while the fluctuations, related to acoustics, evolve with the fast time, denoted τ. The relationship between these two times can be written as

$$\tau = M^2 t$$

where M represents a reference Mach number, which can be chosen, for example, as the average Mach number, maximum Mach number, or local Mach number, etc. Briefly, using these transformations, for each phase (single-phase) the 1-D Euler equations (primitive formulation) is transformed to

$$\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + \rho\frac{\partial u}{\partial x} = 0$$
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + \frac{1}{\rho}\frac{\partial p}{\partial x} = 0$$
$$\frac{\partial p}{\partial t} + M^2 u\frac{\partial p}{\partial x} + M^2\rho c^2\frac{\partial u}{\partial x} = 0$$

where the last equation comes from the pressure form of the internal energy equation. This system is hyperbolic with wave speeds $u, u+\tilde{c}_+, and\ u-\tilde{c}_-$ where

$$\tilde{c}_- = \frac{\left(1-M^2\right)u + \sqrt{\left(M^2-1\right)^2 u^2 + 4M^2c^2}}{2}$$
$$\tilde{c}_+ = \frac{\left(M^2-1\right)u + \sqrt{\left(M^2-1\right)^2 u^2 + 4M^2c^2}}{2}$$

These wave speeds are then used in the HLLC solver of the DEM method of [12]. Thus only the Riemann problem for the Euler system (or DEM system) is modified. The fluxes are computed with the HLLC solver and the Godunov method is used with the conservative formulation of the Euler equations (DEM equations) and the unmodified equation of state. This method guarantees conservation and correct jumps across waves – it only acts on the numerical dissipation. The Mach number M above is chosen as a reference, either as a global or local maximum, but notice that by taking its value as 1.0 the unmodified equations result, so the method is also able to compute fast flows. When applied to low Mach compressible liquid flows, this method gives excellent agreement with exact solutions, even when coarse meshes are employed.

There is a drawback, however, with this low Mach number preconditioning approach. The stability restriction for the scheme is more restrictive than the conventional CFL criterion for compressible flows. The time step must abide

$$\Delta t \le M \frac{\Delta x}{\max\left(|u|+c\right)}$$

Because the lower the velocity of the flow, the lower M must be for convergence, the corresponding Godunov scheme with low Mach preconditioning is thus accurate but still expensive due to the time step restrictions. It is thus necessary to derive an implicit scheme. At this juncture, we temporarily put this method aside for later reconsideration with appropriate implicit time integration.

Low Mach Number Riemann Solver

The Godunov method for finite volumes is well developed for the simulation of steady and unsteady compressible flows of moderate and high Mach number flows as well as for the investigation of wave propagation phenomena (including sharp and accurate shock capturing in unsteady flows). When applied to conservative equation systems, the numerical methods are also conservative by construction and they enable efficient time dependent simulations. Godunov type methods, however, can fail in the limit of low Mach number flows. They require modification to overcome this problem wherein the accuracy and the convergence of the Godunov approximation significantly decreases if the Mach number is in the weakly compressible regime, roughly $M \le 0.1$. This slow convergence (the requirement of excessively many spatial cells, or "spatial stiffness", mentioned previously) occurs because of the large difference between the acoustic wave speed $|u|+c$ and the convective speed u. If we define the stiffness or condition number C as the ratio of the largest eigenvalue of the system to the smallest one,

$$C = \frac{|u|+c}{|u|} = 1 + \frac{1}{M},$$

and the maximum time step is limited by the fastest wave speed $|u|+c$, a larger condition number ($M \to 0$) reduces the convergence rate of the numerical scheme. The decrease of accuracy occurs because of the incorrect estimation of the numerical dissipation in the low Mach number limit; especially for compressible liquids where, due to their high acoustic impedance, the decrease of accuracy is even more intensified. This failure can be observed by looking for example at the cell face values of velocity and pressure (used to create the cell edge fluxes in finite volume methods). Assuming that the state variables are smooth, any method based on compatibility relations (method of characteristics) or on Rankine-Hugoniot relations will lead to interface condition comparable to

$$u^* = \frac{(\rho c)_L u_L + (\rho c)_R u_R + (p_L - p_R)}{(\rho c)_L + (\rho c)_R}$$

$$p^* = \frac{(\rho c)_L p_R + (\rho c)_R p_L + (\rho c)_L (\rho c)_R (u_L - u_R)}{(\rho c)_L + (\rho c)_R}$$

Examination of the second equation shows that p^* is dependent upon the velocity difference across the cell face with a very large coefficient, the average acoustic impedance, $\approx \overline{\rho c}$, which is close to a constant value if the Mach number remains small within the flow field. This term also adds to the numerical dissipation in the numerical scheme. In accelerating liquid flow-fields it can easily occur that p^* is not bounded by p_L and p_R unless the mesh is very fine, making it difficult to calculate the numerical "pressure flux" for a smooth water flow. Because Godunov approaches treat all variations as discrete jumps, the calculated interface pressure p^* is extremely sensitive to small variations in the velocity field.

This low Mach number problem is therefore related directly to the numerical approximation of the interface pressure p^*. These Riemann approximations have been investigated [15], and it was found that the numerical error they introduce grows inversely proportional to the Mach number M as long as the number of cells N is kept constant. Thus in order to use these equations it would require a factor of $N:\ M^{-1}$ mesh points (in each direction for multi-dimensional flow), which is usually not practical. To overcome this low Mach number problem for cavitating liquid flow, a simple modified numerical flux was developed [15] for compressible liquid flow using an asymptotically consistent pressure flux definition

$$p^* = \frac{p_L + p_R}{2}.$$

The corresponding cell edge velocity remains the same as above. This simple modification was demonstrated in the 1-D variable area DEM two-phase code [12] to yield very good convergence; equivalent convergence was reached with about two orders of magnitude fewer mesh cells. Notice that this pressure flux definition does not contain the coupling of pressure and velocity that causes the low Mach number problem. Even though this definition doesn't contain the coupling of the Riemann problem above and is less dissipative than the standard approximate Riemann approaches, the numerical stability was well preserved in the simulations. Evidently, the definition of u^* above includes sufficient coupling of pressure and velocity.

IMEX Semi-implicit Method

For simplicity sake, rather than considering the compressible two-phase flow equations with their additional complexities, let us instead consider the 1-D Euler equations for a compressible single-phase flow

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0$$
$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial \left(\rho u^2 + p\right)}{\partial x} = 0$$
$$\frac{\partial E}{\partial t} + \frac{\partial \left[u(E+p)\right]}{\partial x} = 0$$

where $E = \rho e + \frac{1}{2}\rho u^2$ is the total energy and e is the internal energy. Augment this system with the stiffened gas equation of state given previously to represent either a gaseous phase or a compressible liquid phase. A popular method, with many variations, puts the pressure in the momentum equation and the velocity or density x velocity product in the mass conservation equation at the new-time level to create a semi-implicit discetization. The momentum and mass equations are them manipulated to eliminate the new-time momentum variables, leaving a Poisson equation in pressure. This Poisson equation is then solved for new-time pressure, and by back substitution the other variables are found at the new time level. This method is usually called the *segregated approach*.

For our two-phase flow model with two pressures, one for each phase, and with more complicated coupling, such an approach which would, as a minimum, produce two coupled Poisson equations along with another coupling through the volume fraction equation, this approach may not be optimal. To avoid this complication and to eliminate the probable occurrence of a splitting error with this segregated method, an alternative approach, the IMEX semi-implicit method, is described.

Consider the simple flux vector splitting of the 1-D Euler equation system above

$$\frac{\partial U}{\partial t}+\frac{\partial F}{\partial x}=\frac{\partial U}{\partial t}+\frac{\partial F}{\partial U}\frac{\partial U}{\partial x}$$

$$=\frac{\partial U}{\partial t}+Q\begin{bmatrix} u & 0 & 0 \\ 0 & u+c & 0 \\ 0 & 0 & u-c \end{bmatrix}Q^{-1}\frac{\partial U}{\partial x}$$

$$=\frac{\partial U}{\partial t}+Q\begin{bmatrix} u & 0 & 0 \\ 0 & u & 0 \\ 0 & 0 & u \end{bmatrix}Q^{-1}\frac{\partial U}{\partial x}+Q\begin{bmatrix} 0 & 0 & 0 \\ 0 & c & 0 \\ 0 & 0 & -c \end{bmatrix}Q^{-1}\frac{\partial U}{\partial x}$$

$$=\frac{\partial U}{\partial t}+\frac{\partial C}{\partial x}+\frac{\partial P}{\partial x}\quad =0$$

where

$$U=\left(\rho,\rho u,E\right)^T \quad F=\left(\rho u,\rho u^2,\left(E+p\right)u\ \right)^T$$
$$C=u\left(\rho,\rho u,E\right)^T \quad P=\left(0,p,pu\right)^T$$
$$c^2=\left(\frac{\partial p}{\partial \rho}\right)_s \ \textit{isentropic sound speed}$$
$$F=C+P$$

Obviously, the eigenvalues of the Jacobian of C and P are (u,u,u) and $(0,c,-c)$. The information of the convective terms propagates uniformly in the same direction as the velocity u. The information of the pressure terms goes with the convective terms at the speed u and propagates in all directions at the speed c. Intuitively, to remove the acoustic stability limit, at a minimum we should consider an algorithm in which C is evaluated explicitly in time and P is evaluated implicitly in time. Notice that this splitting also tells us that the acoustic information propagations occur due to the coupling of the momentum and energy equations rather than the momentum and mass equations as used for most segregated approaches. This same observation was noted long ago [16] and a similar path has been recently followed [17, 18]. Therefore to follow this line of reasoning, we can envision a predictor-corrector type splitting as follows:

Explicit step

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}=0$$
$$\frac{\partial(\rho u)}{\partial t}+\frac{\partial(\rho u^2)}{\partial x}=0$$
$$\frac{\partial E}{\partial t}+\frac{\partial(uE)}{\partial x}=0$$

Implicit step

$$\frac{\partial \rho}{\partial t}=0$$
$$\frac{\partial(\rho u)}{\partial t}+\frac{\partial(p)}{\partial x}=0\,.$$
$$\frac{\partial E}{\partial t}+\frac{\partial(up)}{\partial x}=0$$

We now recast the implicit step (for an ideal gas) to

$$\frac{\partial \rho}{\partial t}=0$$
$$\frac{\partial u}{\partial t}=-\frac{1}{\rho}\frac{\partial p}{\partial x} \qquad .$$
$$\frac{\partial p}{\partial t}=-(\gamma-1)p\frac{\partial u}{\partial x}$$

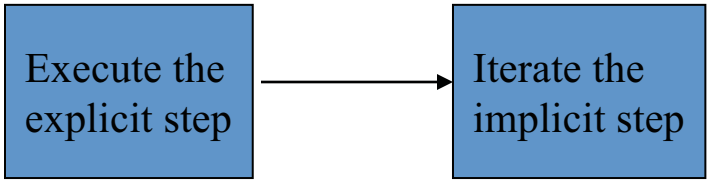
The classical fractional step method to solve these two steps would entail first the solution of the explicit step

$$\rho^{n+1}=\rho^n-\Delta t(\rho u)^n$$
$$(\rho u)^*=(\rho u)^n-\Delta t(\rho u^2)^n$$
$$E^*=E^n-\Delta t(uE)^n$$

to produce the solution vector $\left(\rho^{(n+1)}, u^*, p^*\right)^T$. Notice that $\rho^{(n+1)}=\rho^*$. Next the implicit step is solved

$$u^{(n+1)}=u^*-\Delta t\frac{1}{\rho^{(n+1)}}\left(\frac{\partial p}{\partial x}\right)^{(n+1)}$$
$$p^{(n+1)}=p^*-\Delta t(\gamma-1)p^{(n+1)}\left(\frac{\partial u}{\partial x}\right)^{(n+1)}$$

providing the complete solutions set $\left(\rho^{(n+1)}, u^{(n+1)}, p^{(n+1)}\right)^T$, as shown schematically here.



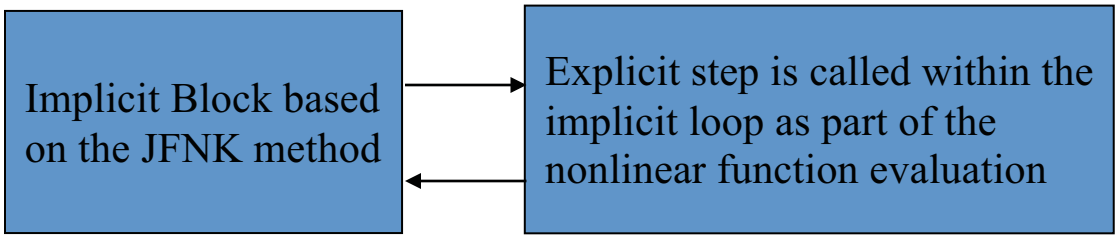
The equations of this implicit step can either be combined to form a Poisson equation or solved as a system interactively. There are some issues associated with this classical approach:

- The explicit and implicit steps are executed independent of each other
- There is no, or limited, influence between the explicit and implicit solutions.

These are the main source of time errors. But there are some additional issues that can become more important, especially when these equations are solved in a multi-physics setting:

- Second order time discretizations do not produce second order time convergent results (time order reduces to one)
- Nonlinearities do not converge completely when coupling different physics.

We therefore recommend the solution of these equations with a self-consistent IMEX approach. With this approach the implicit block is solved based on the JFNK method, and the explicit step is called within this implicit loop as part of the nonlinear function evaluation [19], shown schematically here.



Our tests with compressible flows, gas and liquid, demonstrate there is a significant advantage that is gained with this new approach. There is continuous interaction between the explicit and implicit steps. This means, for each nonlinear iteration, that updated implicit information is immediately felt by the explicit step and the more accurate explicit

solutions are directly used to form the next set of nonlinear residuals. In this way, all the nonlinearities in the system are consistently converged. This leads to an implicitly balanced algorithm that preserves the second order time accuracy of the numerical scheme (no order reductions).

This IMEX semi-implicit approach will allow additional terms (such as interactive sources) to be included along with multiple pressure equations in a more straightforward and accurate manner than segregated approach for the 7-equation two-phase model.

Lastly, there are efficiency gains that can be practically realized with this new approach. During a transient, full IMEX can be employed with the increased stability of dictated by the Courant condition based on material velocity (as opposed to the ordinary Courant condition based on signal speed). This is excellent for rapid and moderately fast transients. However, at steady state one can perform only the implicit step with a very large time step, so for very slow transients, another alternative must be sought. In order to efficiently time integrate these equations with very large time steps for slow transients, we turn now to the final approach we examined, a point implicit method.

Point Implicit Method

We are particularly interested in solving the flow dynamics of nuclear reactors possessing time-scales that are usually many orders of faster/slower than the other dynamics. For example, a fuel behavior simulation may span multiple years of physical time, but it may be necessary to simultaneously couple its behavior to the coolant flow behavior that undergoes very slow, but never-the-less meaningful, transient variations over this time frame. But the flow equations are compressible and hyperbolic, so their natural time frame is much shorter, and most numerical methods for flow solutions are designed for either this faster time frame or for steady-state (no transient). Generally, light water nuclear reactor systems have a need, both operationally and during accidents, to be able treat slow transients with very long duration. This is in addition to the already stringent requirement to treat the very fast transients that could occur during accidents or off-normal operation. For computational efficiency (expediency) for treatment of slow transients one would like to be able to integrate with very large time steps, commensurate with the slow rate of change exhibited by the system. This usually means that implicit time integration methods must be used. However, fully implicit time integration of the 7-equation model, especially in 3-D with highly resolved details may be computationally prohibitive. To treat slow transient and steady state problems, we therefore introduce a point implicit time integration technique that exhibits very large stability (large time steps), but very much-reduced computational requirement (computational efficiency).

This point implicit method does not require implicit iteration, it rather time advances the solutions in the similar spirit of explicit methods except it involves a few additional function evaluation steps.

For simplicity consider the following scalar equation

$$U_t + F\left(U\right)_x = 0 .$$

For numerical solution of this equation, consider the time discretization

$$U_i^{n+1} = U_i^n + \Delta t\, G\left(U_{i-1}^n, U_i^{n+1}, U_{i+1}^n\right)$$

where G is the spatial discretization of $F\left(U\right)_x$. Notice that this equation is implicit in time for only U_i^{n+1}. Define $\Delta U_i = U_i^{n+1} - U_i^n$ and consider the following Taylor series

$$G\left(U_{i-1}^n, U_i^{n+1}, U_{i+1}^n\right) = G\left(U_{i-1}^n, U_i^n, U_{i+1}^n\right) + \frac{\partial G\left(U_{i-1}^n, U_i^n, U_{i+1}^n\right)}{\partial U_i}\Delta U_i .$$

Substitution of these expressions into the time discretized equation above gives

$$\left(\frac{1}{\Delta t} - \frac{\partial G}{\partial U_i}\right)\Delta U_i = G\left(U_{i-1}^n, U_i^n, U_{i+1}^n\right)$$

or

$$\Delta U_i = \frac{\Delta t\, G\left(U_{i-1}^n, U_i^n, U_{i+1}^n\right)}{\left(1 - \Delta t \frac{\partial G}{\partial U_i}\right)}$$

$$U_i^{n+1} = U_i^n + \Delta U_i$$

To treat an equation system with second order time discretization with this approach, see [20] for details.

This point implicit method shares the characteristics of the robust implementation of explicit methods and the stability properties of the unconditionally stable implicit methods. It is specifically designed for slow transient flow problems in that we would like to perform time integrations with very large time steps. We have found that the method can be time inaccurate for fast transient problems, particularly with larger time steps. Therefore, an appropriate solution strategy for a problem that evolves from fast to slow transient would be to integrate the fast transient with an explicit or semi-implicit technique and then switch to this point implicit method as soon as the time variations slow down sufficiently. Note, our time integration algorithm can naturally transition very easily, on demand as flow conditions dictate, from explicit to point implicit.

As another instance, in a typical reactor thermal-hydraulic model problem, the heat conduction parts can vary on a significantly faster time scale in comparison to the flow portion. As a result of the stable nature of numerical solution techniques for heat conduction one can time integrate the heat conducting part with very large time steps. In turn, one may have to perform the time integration for significantly longer times for these kinds of couplings. In this scenario, our point implicit method can stably and effectively time integrate the slowly changing flow portion with whatever the time step sizes imposed by other physics.

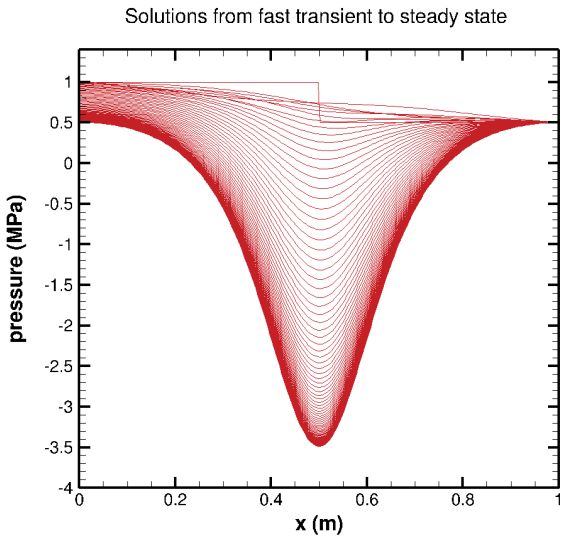
As we pointed out previously, even when considering only two-phase flow scenarios, transitions from single- to two-phase and vice versa exhibits a large disparity of physical time scales due to the corresponding large disparity of fluid and acoustic velocities and the significant smoothing effects of the relaxation processes that can occur in the 7-equation model.

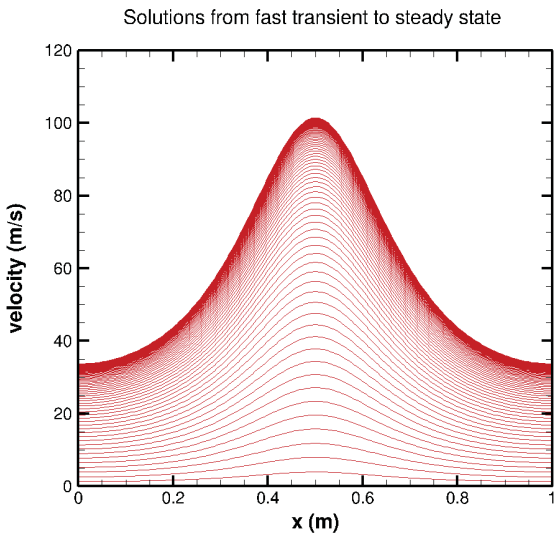
Finally, the numerical implementation of this method is very robust since one can always call this method inside any solver technology as part of the function evaluation routines.

Let us demonstrate, from [20], the point implicit method by application to the first nozzle problem given above. The governing compressible flow Euler equations are slightly modified to

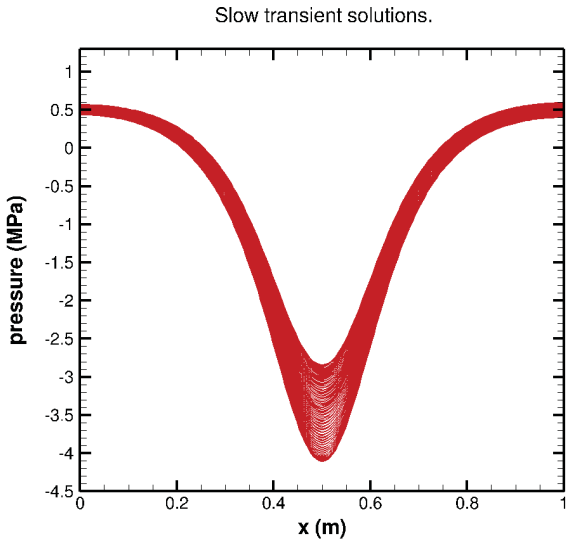
$$\frac{\partial \rho A}{\partial t} + \frac{\partial \rho u A}{\partial x} = 0$$
$$\frac{\partial \rho u A}{\partial t} + \frac{\partial A(\rho u^2 + p)}{\partial x} = p\frac{\partial A}{\partial x}$$
$$\frac{\partial \rho E A}{\partial t} + \frac{\partial u A(\rho E + p)}{\partial x} = 0$$

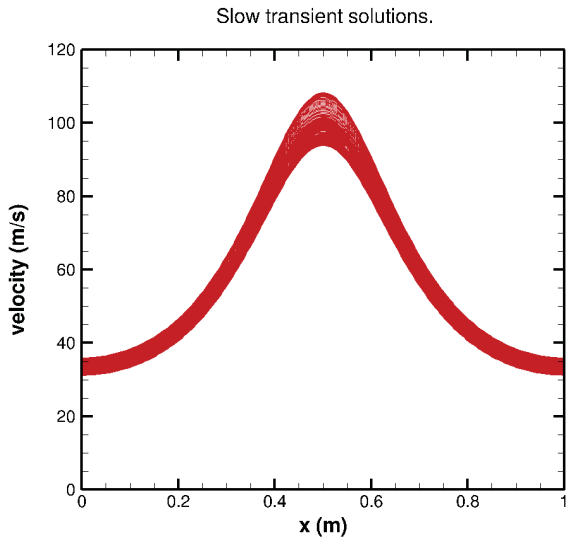
where $A = A(x)$ is the local cross-sectional area. We use the following initial conditions; $p = 1\ MPa$ if $x < 0.5$ else $p = 0.5\ MPa$. The problem is solved in $[0,1]$ interval with 200 grid points. With these settings, a transient flow is initiated. Consider first the flow of *compressible liquid* with SGEOS data give in Table 1. Steady state flow occurs at approximately $t = 0.56\ s$. The solution history of the pressure and flow variables are shown in succession until steady state is reached in the following two figures.





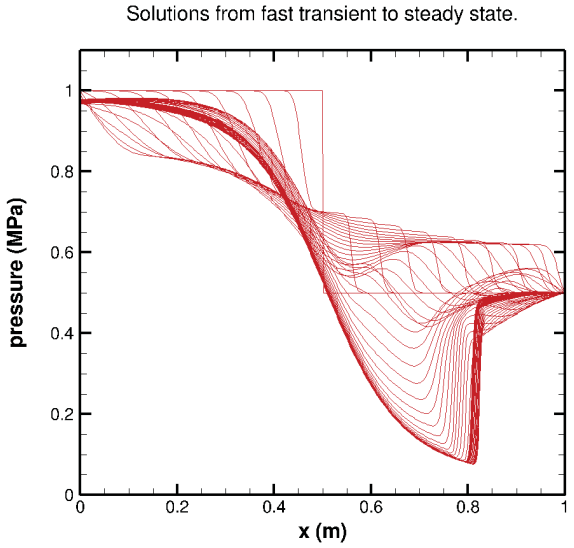
The next two figures show the time succession of pressure and velocity from the slow transient solution that we initiated with the oscillating outlet boundary condition. The red dark regions represent slow transient solution snapshots densely overlain on top of each other. Final time for the slow transient run is $t = 40$. The point implicit time steps used for these simulations are 100 times those required for the explicit acoustic Courant stability condition.

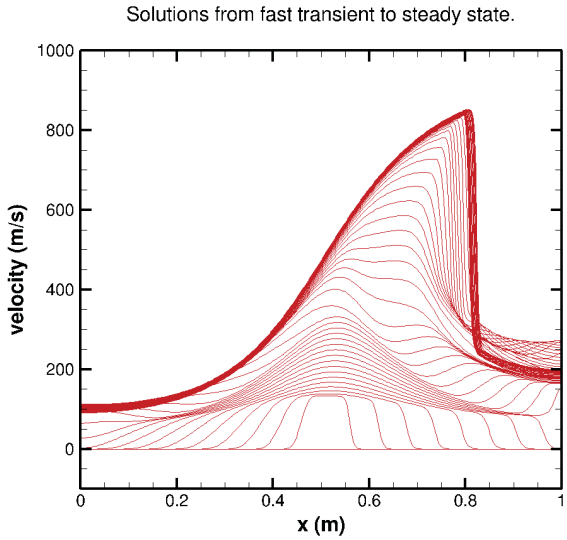




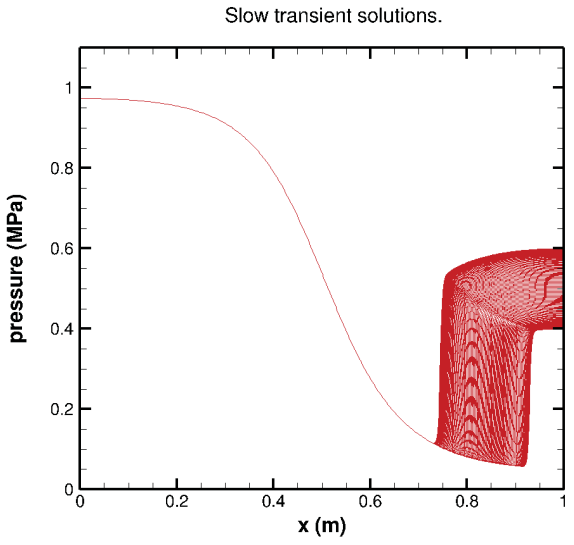
Now consider the exact same nozzle, initial and boundary conditions, but with *compressible gas* as given with SGEOS parameters from Table 1, which corresponds to an ideal gas. With these initial settings, the ensuing transient reaches steady state at approximately $t = 0.21\,s$.

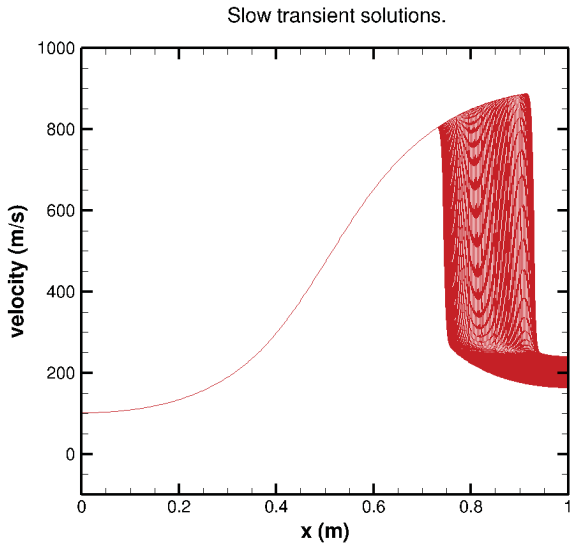
The following two figures show the history of the pressure and velocity until the steady state is reached.





The final two figures show the time succession of pressure and velocity from the slow transient solution that we initiated with the oscillating outlet boundary condition. Again the red dark regions represent slow transient solution snapshots densely overlain on top of each other. Final time for the slow transient run is $t = 20$ (not run for as long because the solution is oscillatory, and this represents a full period). The point implicit time steps used for these simulations are again 100 times those required for the explicit acoustic Courant stability condition.





Conclusions

Four different methods were examined to address the need for all-speed, multi-time scale integration of the two-phase flow equations. Because of budgetary limitations, the latter two, IMEX semi-implicit and point implicit have not yet been applied with two-phase flows, but only single-phase compressible gas and compressible liquid. All four show capability for application within varying physical contexts. Obviously, though not attempted yet, there may also be merit in combining some features of these approaches, e.g. the preconditioned low Mach method (which need some level of implicitness for efficiency) with the point implicit method. These and other variants will be examined in the future. Our immediate next step will be to implement the point implicit method with the 1-D variable area DEM two-phase model, which is restricted currently for stability reasons to an inefficient explicit time stepping regimen.

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