A boundary value “reservoir problem” and boundary conditions for multi-moment multifluid simulations of sheaths

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Multifluid simulations of plasma sheaths are increasingly used to model a wide variety of problems in plasma physics ranging from global magnetospheric flows around celestial bodies to plasma-wall interactions in thrusters and fusion devices. For multifluid problems, accurate boundary conditions to model an absorbing wall that resolves a classical sheath remains an open research area. This work justifies the use of vacuum boundary conditions for absorbing walls to show comparable accuracy between a multifluid sheath and lower moments of a continuum-kinetic sheath.

Multifluid and continuum-kinetic simulations of plasma sheaths often use absorbing walls as boundary conditions in the absence of material emission and other plasma-wall effects. In non-neutral two-fluid modeling of sheath dynamics, in which ions and electrons are treated as independent interpenetrating fluids, boundary conditions need to be specified to appropriately treat subsonic and supersonic quantities. Electrons travel across the sheath edge at bulk speeds lower than their thermal velocity at the boundary whereas ions travel at speeds larger than the Bohm speed. Commonly used models for multifluid sheaths specify a flux at the wall for the subsonic electrons based on the classical Bohm velocity, but this description does not resolve the sheath profile accurately as the Bohm velocity is achieved at the sheath entrance and not at the wall. Also, the exact form of the flux to be specified remains somewhat ad-hoc. Hence, appropriate sheath boundary conditions for multifluid descriptions remain an open research area.

This work proposes using Riemann solvers at the plasma-material wall, with the wall treated as a vacuum. A Riemann solver automatically provides the needed flux for all fluid quantities at the wall, obviating the need to explicitly specify the fluxes. Multifluid simulations of classical sheaths using these Riemann solver boundary conditions are compared to fully kinetic simulations to show that the agreement of the lower moments is excellent. Of course, kinetic physics (or higher-moment models that include pressure-tensor and higher moments) is essential to accurately model the sheath to account for anisotropic temperature, range of collisionalities between a presheath and a sheath, critical role of heat flux and kinetic effects in the presence of magnetic fields. Yet, multi-moment multifluid models remain a computationally tractable reduced model.

Firstly, a generic boundary value problem (BVP) is introduced, denoted as the “reservoir problem”, for a system of hyperbolic equations. Also presented is the solution to this problem in terms of another well-known problem for hyperbolic equations, that is, the Riemann problem. Unlike the reservoir problem, the Riemann problem is an initial value problem (IVP) but its solution can be used to construct a solution to the reservoir problem. The connection to sheath boundary conditions is that the boundary where plasma touches the material surface is a special case of the reservoir problem in which the “reservoir” is a vacuum. However, setting other values for the wall reservoir can allow modeling of other physical processes at the wall, for example, evaporation and condensation in neutral fluid simulations. In this work, “reservoir” is synonymous to setting a ghost cell boundary condition and allowing a self-consistent solution to the Riemann problem at the boundary.

Consider a system of 1D hyperbolic conservation laws written as

$$\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} = 0,$$

where $Q(x,t)$ are the conserved quantities and $F(Q)$ are the fluxes. The reservoir problem can be stated as finding the steady-state solution $Q^\ast$ to this problem with the boundary conditions

$$Q(x < 0, t) = Q_L$$

$$Q(x > 1, t) = Q_R$$

in the domain $x \in [0, 1]$. Note that this system is assumed to be hyperbolic, i.e. the flux Jacobian $A \equiv \frac{\partial F}{\partial Q}$ is diagonalizable and has real eigenvalues.

Consider the simplest case of linear advection,

$$\frac{\partial q}{\partial t} + \lambda \frac{\partial q}{\partial x} = 0.$$  (4)

For this simple case, the solution to the reservoir problem is trivial: if $\lambda > 0$ then $q^\ast = q_L$ and if $\lambda < 0$ then $q^\ast = q_R$. For linear hyperbolic systems, for example, Maxwell equations

$$\frac{\partial}{\partial t} \left[ \frac{E_y}{B_z} \right] + \frac{\partial}{\partial x} \left[ \frac{B_z}{E_y} \right] = 0$$  (5)

(speed of light is set to unity) one can use a diagonalization procedure: add and subtract the two equations to get the un-
Coupled system
\[
\frac{\partial}{\partial t} (E_y + B_z) + \frac{\partial}{\partial x} (E_x + B_z) = 0 \quad (6)
\]
\[
\frac{\partial}{\partial t} (E_y - B_z) - \frac{\partial}{\partial x} (E_x - B_z) = 0. \quad (7)
\]

Hence, one must have \( E_y^* + B_z^* = E_{L,y} + B_{L,z} \) and \( E_y^* - B_z^* = E_{R,y} - B_{R,z} \), and the solution to the reservoir problem is
\[
E_y^* = \frac{1}{2} (E_{R,y} + E_{L,y} - B_{R,z} + B_{L,z}) \quad (8)
\]
\[
B_z^* = \frac{1}{2} (B_{R,z} + B_{L,z} - E_{R,y} + E_{L,y}). \quad (9)
\]

Note that in general there will be (potentially large) finite jumps at the walls.

For nonlinear hyperbolic equations the situation is more complicated. The jump between the reservoir values and the unknown solution \( Q^* \) will lead to a flux and for steady state the flux must be the same at the left and right walls. The solution to the Riemann problem can determine this flux. Consider an interface with left and right values \( Q^- \) and \( Q^+ \) at \( t = 0 \). Then, the Riemann problem is to determine the interface value \( Q \) for \( t > 0 \). Once this is known, then the flux at the interface can be computed as \( F(Q^-) \). Let's denote this flux from the solution to the Riemann problem at the interface as \( F(Q^-, Q^+) \). In terms of this flux one can determine the solution to the reservoir problem as that value which gives
\[
F(Q_L, Q^*) = F(Q^+, Q_R). \quad (10)
\]

In general, this is a nonlinear system of equations that must be solved numerically to determine \( Q^* \). In fact, for complicated systems like Euler equations or ideal MHD equations the Riemann solver itself does not have an explicit analytical solution in terms of elementary functions and must be solved partly numerically. An additional iterative scheme is needed that calls the Riemann solver in a loop till a converged \( Q^* \) is found satisfying this condition.

As an example of a nonlinear system, consider the Euler equations for ideal, inviscid fluids. An exact Riemann solver in the inner loop of a root finding algorithm is used to compute the solution to the reservoir problem. For example, for reservoirs with prescribed mass density, velocity, and pressure corresponding to the notation in Eqs. 2 and 3, \((\rho_L, u_L, p_L) = (1,0,1)\) and \((\rho_R, u_R, p_R) = (0.125,0.01,0.1)\) and gas-adiaic constant, \( \gamma = 3 \), the solution for the intermediate state is \((\rho^*, u^*, P^*) = (0.65,0.61,0.27)\).

Note that for some nonlinear systems the solution \( Q^* \) need not be uniform. As a simple example consider the Burgers’ equation that has a quadratic nonlinear flux. For specific choices of left/right reservoirs \((Q_R = -Q_L)\) a single discontinuity will form in the domain. However, in this specific case a small perturbation to one of the reservoirs will remove the discontinuity.

In a time-dependent sheath problem one only needs the flux, say at the right wall. \( F(Q, Q_R) \), given \( Q \), the solution just to the left of the wall. Typically \( Q_R = 0 \). Often, when an exact Riemann solver is not available an approximate solver can be used to give reasonable estimates of the flux at the wall. The exact Riemann solver may only be needed to compute the wall fluxes and a faster and more tractable approximate solver can be used to update the fluxes at interior cell edges. For example, for the two-fluid model, with the two fluids being ions and electrons coupled with Maxwell’s equations, the exact Riemann solver involving both fluid species and fields is not available and an approximate Riemann solver must be used. For comparison, when applied on the previously described reservoir problem, the approximate Riemann solver used here gives the intermediate state of \((\rho^*, u^*, P^*) = (0.70,0.54,0.25)\).

In order to justify the appropriate multi-moment boundary conditions for reservoir and sheath problems, a kinetic investigation is performed in three stages. For the first stage, non-vacuum reservoirs are set as boundaries on both sides of the computational domain to obtain the intermediate values for a single neutral species. Next, the right reservoir is set to vacuum to ensure that the sonic outflow is recovered accurately. Lastly, the vacuum boundary condition is applied to two species kinetic and multi-moment plasma. The plasma sheath that self-consistently forms is compared between the kinetic and two-fluid simulations.

Here, the reservoir problem is demonstrated using the kinetic Vlasov-BGK (Bhatnagar-Gross-Krook) equations,
\[
\frac{\partial f}{\partial t} + v \cdot \nabla_x f + \frac{q}{m} (E + v \times B) \cdot \nabla_v f = v (f_M - f), \quad (11)
\]
where \( f \) is the particle distribution function, \( q \) and \( m \) are charge and mass, respectively, \( v \) is collision frequency, and \( f_M \) is a Maxwellian particle distribution function which is constructed from the first three moments of \( f \). Note that the part with the Lorentz force matters only for the multi-moment plasma case and not for the single species neutral cases. The equation is implemented in the GKEYLL plasma simulation framework\(^{13}\) using the discontinuous Galerkin (DG) method\(^{15,20}\). The particle distribution is discretized in each cell with a polynomial approximation and a penalty flux is used to reconstruct an intermediate state at cell interfaces\(^{20}\).

Unlike the hyperbolic case of Euler equations discussed in the previous section, the Vlasov-BGK equation contains the effects of finite collisionality and kinetic effects, including heat-flux and higher moments of the distribution function. For example, for finite collisionality a boundary layer forms at the reservoir boundaries (about a mean-free-path in thickness), but such a boundary-layer is absent in the Euler case.

Figure 1 presents the kinetic solutions for the choice of reservoirs with Maxwellian distribution,
\[
f(v) = \frac{n}{\sqrt{2\pi}\nu_{th}^2} \exp\left( -\frac{(v - u)^2}{2\nu_{th}^2} \right), \quad (12)
\]
with \((n_L, u_L, \nu_L) = (1,0,1)\) and \((n_R, u_R, \nu_R) = (0.125,0,0.1)\), where \( \nu = \nu_{th}^2 \), and collisionalities with Knudsen numbers \( (Kn) \) of 0.01, 0.1, and \( \infty \). The density, velocity, temperature, and the heat-flux are presented (in the fluid frame) in
A boundary layer forms at the walls due to particles coming to and from the reservoir with different velocity distributions while undergoing collisional relaxation into a Maxwellian distribution over a finite mean-free-path. Note that this is different from the traditional viscous boundary layer which forms due to no-slip boundaries tangential to the wall in the Navier-Stokes equations. As expected, for lower collisionality the heat-flux near the wall is significant due to the non-Maxwellian shape of the distribution.

The density of the kinetic solution can be understood by looking at the $Kn = \infty$ case. For this case, the intermediate density is the sum of two half-Maxwellians such that the half-Maxwellian with the positive velocity is based on the conditions from the left reservoir while the half-Maxwellian with the negative velocity is based on conditions from the right reservoir. The density obtained using these two half-Maxwellians is exactly the intermediate density value $(n = 0.5625)$ obtained from the kinetic solutions.

Figure 2 presents an expanded scale of the kinetic solutions of Fig. 1 around the left and right reservoir boundaries. The size of the boundary layer depends on the collisionality and is denoted using the shaded regions. The shaded regions have different colors corresponding to the colors of the two collisional cases, and the size of the region represents a single mean-free-path.

The kinetic distribution functions for each of the different collisionalities are presented in Fig. 3 along with a lineout of the distribution from the middle of the domain. As expected, the collisionless case (top panel) represents the half-Maxwellian distributions of each of the left and right reservoirs. The collisionality causes thermalization of the two Maxwellians producing the same zeroth moment (density) at the center of the domain. Note the expansion of the particles due to emission and absorption near the boundaries for the collisional cases. These boundary layers correspond to non-Maxwellian behavior and thermalization, which also is reflected in the non-zero heat-flux at the walls.

Now consider the case where the distribution function in the right reservoir is set to zero (equivalent to having a vacuum reservoir). Simulations are performed by varying the left reservoir conditions while maintaining the right reservoir as a vacuum. Figure 4 presents kinetic results when the left reservoir density is held fixed while varying the pressure in the top panel and a constant pressure left reservoir with varying density is presented in the bottom panel. Note that after reaching a steady-state, the bulk velocity in the middle of domain exactly matches the sound speed for both the cases.

For the collisional case of $Kn = 0.01$, Fig. 5 shows that the intermediate Mach number outside of the boundary layer is exactly 1. The fluid accelerates from zero to a sonic Mach across the left boundary layer, remains sonic across most of the intermediate region, and accelerates to a supersonic Mach number across the right boundary layer. This occurs as the density drops across the boundary layer into the vacuum, hence the velocity must increase to maintain constant flux across the domain. This produces a supersonic outflow at the right boundary illustrating that such a vacuum boundary condition effectively captures an absorbing wall at the right edge of the computational domain.

Finally, this absorbing wall boundary condition is used to simulate a plasma sheath. Each species of ions and electrons are evolved using Eq. 11 and coupled with Maxwell’s equations. A classical sheath is initialized using approximate sheath conditions presented in Ref. [12,122]. The electron
ion populations are initialized with $T_e/T_i = 1.0$. A two-fluid model is also used with the two fluids being ions and electrons coupled with Maxwell’s equations.\cite{11,12,13} Analogous to kinetic simulations where the particle distribution function coming from the wall is set to zero, a fluid vacuum boundary condition of $(n = 10^{-13}, p = 10^{-11})$ can be specified for each species. Maintaining a vacuum density and pressure at the wall produces a self-consistent solution to the Riemann problem given the upstream conditions within the plasma. The solution is then allowed to evolve to a kinetic and two-fluid classical sheath, respectively.

Comparisons of density, electric field, and bulk velocity profiles are presented in Fig. 6 at a time of $t_{0pe} = 200$ comparing the continuum-kinetic and two-fluid results. The density (top), electric field (middle), and velocity (bottom) profiles agree remarkably well between the two models. Note that these are snapshots in time and data have not been averaged. As this simulation was run without collisions, electron momentum fluctuates due to Langmuir waves.\cite{23} These fluctuations can be alleviated by averaging over the plasma frequency to provide electron and ion fluxes that are equal to each other at the wall with value of $0.49 n_0 u_B$. Relying on the Riemann solver at the absorbing boundary to self-consistently produce a plasma sheath, the fluid simulation with the vacuum boundary condition closely reproduces the kinetic solution.

Panel (a) also shows the deviation from quasineutrality by tracking the absolute difference between the electron and ion number densities normalized to the initial uniform density, as denoted by the violet line. Note that as the electric field increases into the presheath towards the sheath, so does the difference in the number densities, which is proportional to the charge density. Due to the smoothness of the density profiles, there is no sharp transition between the quasinetal presheath and charged sheath. An important point in the sheath theory is the location where the ion bulk speed crosses the classical Bohm velocity, $u_B = \sqrt{(T_e + \gamma T_i)/m_i}$. This is marked with vertical gray lines (solid for kinetic and dashed for fluid results). At this point the deviation from quasineutrality is 2.3% for the kinetic code and 2.9% for the fluid code.

This work has shown that the Riemann problem, either approximate or exact, provides a self-consistent boundary condition where the flux is completely determined by prescribed vacuum regions in the boundary. This eliminates the need for
FIG. 6. Comparison of electron and ion number densities (a), electric field (b), and ion bulk velocity (c) between kinetic (solid lines) and fluid (dashed lines) simulations in the region near an ideally absorbing wall. Vertical gray lines mark the crossing of the Bohm velocity. Violet lines in the panel (a) mark the difference between electron and ion densities. Initially the temperatures of the electrons and ions are set to $T_e/T_i = 1$. Solution is shown at $t \tau_{pe} = 200$ and it is not averaged. Figure from Ph.D. dissertation [22]; used with permission.

*ad hoc* implementation of fluxes that have been noted in previously used multifluid simulations of sheaths.

To allow readers to reproduce our results and also use GKEYLL for their applications, the code and input files used here are available online. Full installation instructions are provided on the GKEYLL website [19]. The input files used here are under version control and can be obtained from the repository at https://github.com/ammarhakim/gkeyll-paper-inp

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