Knudsen number dependence of single-mode Rayleigh-Taylor fluid instabilities

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We present a study of single-mode Rayleigh-Taylor instabilities (smRTI) with a modified Direct Simulation Monte Carlo (mDSMC) code. The mDSMC code is aimed to capture the dynamics of matter at all Knudsen numbers within one approach. Our method combines the traditional Monte Carlo technique to efficiently propagate particles and the Point-of-Closest-Approach method for high spatial resolution. To validate our results for the smRTI at early times we compare the growth rate to an analytic prediction from linear theory. We find good agreement and observe the development of secondary instabilities at later times, similar to hydrodynamic simulations and experiments. In addition to the continuum limit we also perform simulations using different particle mean-free-paths. As expected, an increase of the latter favors particle diffusion and the development of a diffusion layer. Furthermore, large particle mean-free-paths reduce the occurrence of secondary instabilities and have an impact on the growth rate of the smRTI. Finally, to facilitate the comparison of our approach in the continuum regime with hydrodynamic simulations we introduce and test an algorithm that minimized particle diffusion from one fluid into the other.

Keywords: Kinetic simulation; Monte Carlo; fluid instabilities; fluid dynamics; Rayleigh-Taylor

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I. INTRODUCTION

Dynamical simulations that are based on interacting particles are increasingly applied in different physical fields. Unlike conventional hydrodynamics which operates in the continuum limit, they are able to simulate matter at all Knudsen numbers $K = l/L$ whereas $l$ is the mean-free-path of the particles the system is comprised of and $L$ is a characteristic length scale. Examples of research areas that apply particle methods include computational aerodynamics and space-flight studies \cite{1,2}, material science \cite{3,5}, nuclear collisions \cite{6,12}, and plasma physics \cite{13,15}. In astrophysics, particle methods have a long history in radiation transport \cite{16-22} and cosmological N-body simulations \cite{22}. Modern usage also include simulations of flow in accretion disks \cite{24}, nuclear matter in neutron star crusts and white dwarfs \cite{25,27}, and neutrino transport in core-collapse supernova (CCSN) \cite{28,29}. Particle methods are also receiving a large interest from studies of inertia confinement fusion (ICF) capsule implosion performed at the National Ignition Facility (NIF) \cite{13,15,30,33}. Advantages of particle methods include their flexibility with regard to optical depths, the facility to include complex geometries and distributions of matter, and the correct representation of the Boltzmann transport of many particles in three dimensions (3D). A current drawback in comparison to hydrodynamic simulations is the large number of particles that is required to accurately represent a given physical problem and reduce statistical noise. For example, large optical depths require many particle interactions and the corresponding simulations become increasingly slow. However, as computational power increases, the relatively straightforward parallelization and scalability of particle codes, also on graphics processing units \cite{34,36}, could outweigh the computational costs. Depending on the physical problem, different particle-based simulation techniques are used, for example Molecular Dynamics \cite{37,38}, Direct Simulation Monte Carlo \cite{39,41}, Particle-in-Cell \cite{42,43}, and Dissipative Particle Dynamics \cite{44,46}. While all approaches have been primarily developed to describe non-equilibrium matter, they are able retrieve macroscopic variables like density, fluid velocity, pressure, and temperature. Furthermore, they can model the evolution of hydrodynamic phenomena such as shock waves \cite{47,53} and fluid instabilities \cite{54,58}. Both are important components in plasma and astrophysics, and are discussed to play a crucial role during the compression of ICF capsules \cite{59,60} and the evolution of CCSNe \cite{61}.

A core-collapse supernova is the explosion of a massive star at the end of its life when the gravitational pressure of its iron core cannot be balanced anymore by the thermal pressure and the Fermi degeneracy pressure of the electrons \cite{62,63}. As a consequence, the core collapses within less than a second and nuclei which make up the core are compressed to homogeneous matter of neutrons and protons. The collapse is reversed as infalling matter re-bounces at the center of the core due to the repulsive nuclear force between neutrons and protons that sets in at around nuclear matter saturation density $n \sim 2.4 \times 10^{14}$ g/cm$^3$. This bounce creates an outgoing shock wave. However, the latter does not directly lead to the explosion of the star but, as has been
shown in 1D simulations, stalls due to energy loss at a distance of several 100 km from the center. Although different shock revival mechanisms are discussed, the consensus of modern 3D simulations seems to be that neutrino heating combined with fluid instabilities is the likely cause for the explosions. Details of the interplay between neutrino heating and 3D fluid instabilities are still debated vigorously; however, in order to understand the supernova dynamics a correct 3D simulation including detailed neutrino transport seems to be inevitable.

Inertial confinement fusion is one of the two major ways to achieve fusion in the laboratory (the other one being the magnetic confinement fusion). NIF has been extensively exploring this possibility by compression and heating of fusion fuel (deuterium and tritium) in form of a spherical pellet via intense laser beams and Hohlraum X-ray radiation. A recent breakthrough has been achieved when the energy generated through fusion reactions exceeded the amount of deposited energy. However, current difficulties to achieve a self-sustaining burn or ignition seem to lie in the formation of Rayleigh-Taylor instabilities (RTIs) during the compression of the fuel capsule. Small perturbations on the surface of the pellets serve as seeds for the instabilities. As the latter grow, they lead to a turbulent mixing of hot and cold fuel which decreases the efficiency of the laser compression. In addition, non-equilibrium effects have also been discussed to impact the ICF dynamics.

Our goal is to develop a large-scale kinetic transport code that can handle particles in a computationally efficient way, and thereby simulate matter in non-equilibrium and in the hydrodynamic regime. With that, we want to study astrophysical phenomena such as CCSNe. Furthermore, this approach could be applied in the simulation of ICF capsule dynamics. Our modified DSMC code (mDSMC) has already been successfully tested on shock wave phenomena applying test-particles in non-equilibrium and in the continuum regime. In this work we present our first detailed study of fluid instabilities. Hereby, we focus on the single-mode Rayleigh-Taylor instability (smRTI). Our motivation is the possible important role of RTIs in ICF and CCSN dynamics. The advantage of the smRTI is that at early stages, it can be compared to an analytic solution from linear theory. Furthermore, smRTIs are often used by hydrodynamic codes as validation tests. With that, we can also refer to the latter and experiments for comparison. Fluid instability simulations including RTIs have been performed by various particle codes in the past (see e.g. references therein). However, with the current work, we present a detailed and comprehensive analysis of the smRTI for a range of particle mean-free-paths and different particle numbers. Furthermore we introduce and test an approach to suppress particle diffusion that can facilitate the comparison with hydrodynamic codes.

In the following we will give a short introduction of RTIs in section II followed by an overview of our mDSMC code in section III. We will then proceed to the setup of our simulations and discuss the obtained results for varying particle mean-free-paths in sections IV and V. We will introduce a method to suppress particle diffusion in section VI and present results of the corresponding calculations. The paper closes with a summary and outlook in section VII.

II. RAYLEIGH-TAYLOR INSTABILITIES

Rayleigh-Taylor instabilities form at the interface of two fluids with different densities when the less dense fluid is pushing against the one with higher density. A typical example for such a situation is a heavy fluid resting on top of a lighter one in the presence of a gravitational acceleration $g$. In such a case, small perturbations at the fluid interface grow and result in the development of RTIs. The latter can be found in many different physical environments - ranging from astrophysical systems, to geophysical phenomena, and plasma physics. Due to their large dynamical impact and the direct connection with turbulent mixing, RTIs receive a wide interest and studies have been performed analytically, experimentally, and numerically (see e.g. references therein). With the growing computational power, RTI phenomena can be studied in greater detail and for increasingly larger systems.

In a realistic environment, fluid instabilities of many different wavenumbers can be present. For validation studies, it is easier to focus on the so-called single-mode RTI which arises from an initial perturbation $\eta(x)$ with a defined wavelength $\lambda$. Its evolution can be divided into several major stages:

1. **During the first stage**, the amplitude of the initial perturbation is $B \lesssim 0.5 \lambda$ and the instability undergoes exponential growth which can be described by linear analysis:

   \begin{align}
   \eta(x,t) &= \frac{1}{2} (e^{\gamma t} + e^{-\gamma t}) \eta_0(x), \\
   \gamma &= \frac{\sqrt{A g k}}{c}, \quad A = \frac{p_2 - p_1}{p_2 + p_1}, \quad k = 2\pi/\lambda.
   \end{align}

   Here, $\gamma$ is the growth rate, $A$ is the Atwood number, and $k$ is the wavenumber. The densities of the high- and low-density fluids are given by $p_2$ and $p_1$, respectively. During the second stage, when the amplitude of the perturbation is $B > \lambda$, non-linear effects start to dominate. Bubbles of low-density fluid rise into the high-density matter, while the latter sinks in spikes downwards. Perturbations with larger wavenumbers are generated and secondary Kelvin-Helmholtz instabilities
(KHI) at the tip of the sinking fingers lead to the transformation of low-density bubbles into mushroom-like structures. As bubbles and spikes start to interact with each other, the dynamics become chaotic leading to turbulent mixing.

Note, that eq.\[1\] describes the behavior of an incompressible and inviscid fluid. Compressibility, viscosity, and surface tension have been studied regarding their effect on the evolution of the RTI in the past\[51,52\]. Hereby, surface tension and viscosity seem to stabilize perturbations. Simulations using fluids with a finite compressibility experience delays in the formation of secondary KHI\[s\] while spikes of the sinking heavy fluid become more blurred. Challenges in numerical studies of RTIs arise in the non-linear regime when a finer computational grid leads to the development of more secondary instabilities. This is partly due to the finer resolution and partly due to a different impact of the grid. Convergence tests are generally performed to ensure that the dynamics of the simulated system does not change with resolution.

III. MODIFIED DSMC APPROACH

In this section, we will give a short overview of our simulation method, whereas a more detailed discussion can be found in\[48\]. The foundation of our approach is a modified DSMC method where the phase-space of the physical problem is represented by \(N\) delta-functions or so-called test-particles:

\[ f(\mathbf{r}, \mathbf{p}, t) = \sum_{i=0}^{N} \delta^3(\mathbf{r} - \mathbf{r}_i(t)) \delta^3(\mathbf{p} - \mathbf{p}_i(t)). \]  

(3)

Here, \( \mathbf{r}_i \) is the position and \( \mathbf{p}_i \) the momentum of the \( i \)-th test-particle. This distribution function is then used as input into the Boltzmann equation\[83\] and results in \(2N\) ordinary differential equations of motion for each test-particle with mass \(m_i\):

\[ \frac{d}{dt} \mathbf{p}_i = \mathbf{F}(\mathbf{r}_i) + \mathbf{C}(\mathbf{p}_i), \]

(4)

\[ \frac{d}{dt} \mathbf{r}_i = \frac{\mathbf{p}_i}{m_i}, \quad i = 1, \ldots, N. \]  

(5)

Particles interact with each other via one-body mean-field forces \(\mathbf{F}(\mathbf{r}_i)\), such as gravity and nuclear forces. In addition, they undergo two-body interactions which are symbolized by \(\mathbf{C}(\mathbf{p}_i)\). For realistic fluids, the latter must contain the appropriate cross-section \(\sigma\). In the current study, we want to test the continuum behavior of our code. Particle interactions are therefore modeled as simple elastic collisions and the cross-sections are related to a particle effective interaction radius:

\[ \sigma = 4\pi r_{\text{eff}}^2. \]  

(6)

The latter is linked to the particle mean-free-path \(l\) and the particle number density \(n = N/V\) via:

\[ r_{\text{eff}} = \left(4\pi nl\right)^{-1/2}. \]  

(7)

As in our previous works, \(l\) will be used as an input variable. We determine the particle effective radius and apply it in one of the steps of our collision partner search\[45\]. Hereby, we calculate the time at which the effective radii of both particles overlap:

\[ t_{0,1,2} = t_{\text{p}} \pm \sqrt{t_{\text{rel}}^2 + t_{\text{eff}}^2}, \]

(8)

\[ t_{\text{p}} = -\frac{(\mathbf{r}_{\text{rel}} \cdot \mathbf{v}_{\text{rel}})}{|\mathbf{v}_{\text{rel}}|^2}; \]

(9)

\[ t_{\text{rel}} = |\mathbf{r}_{\text{rel}}|/|\mathbf{v}_{\text{rel}}|; \]

(10)

\[ t_{\text{eff}} = (r_{\text{eff},A} + r_{\text{eff},B})/|\mathbf{v}_{\text{rel}}|. \]  

(11)

If either \(t_{01}\) or \(t_{02}\) is a real number, a collision can take place. Otherwise, the particles are too far away from each other. For the actual interaction time we choose the Point-Of-Closest-Approach (PoCA) method which is different from the usual DSMC approach. This is done to prevent causality violations, which are otherwise present in DSMC type of simulations\[12\]. The combination DSMC and PoCA results in a very favorable scaling of the computational time with the number of particles (from DSMC)\[48,84\] and an improved accuracy of e.g. shock wave and instability localization (from PoCA). The collision time is taken as \(t_{\text{p}}\) in eq.\[6\] and is the time when the distance of closest approach is reached. Outgoing velocity vectors are determined randomly in the center-of-mass (cm) frame of the colliding pair with:

\[ \phi = 2\pi \kappa, \quad \kappa \in [0,0,1.0], \]  

(12)

\[ v_{x,\text{out,cm}} = v_{\text{in,cm}} \cos(\phi), \]

(13)

\[ v_{y,\text{out,cm}} = v_{\text{in,cm}} \sin(\phi), \]  

(14)

\[ v_{\text{in,cm}} = \sqrt{v_{x,\text{in,cm}}^2 + v_{y,\text{in,cm}}^2}. \]  

(15)

We only deviate from this approach when we use guided collisions in our diffusion suppression study (see section VI). However, more complex interactions have to be implemented in future CCSNe simulations, as has already been done in previous works\[55,57\]. Our code can perform simulations in 2D and 3D whereas the particle degrees of freedom and thereby the equation of state of matter they represent change accordingly. The collision partner search is parallelized using shared memory parallelization via OpenMP. However, a distributed memory version using MPI is under development\[84\].

At the beginning of each time step, particles are sorted into their spatial cells or bins and can only interact with partners within their own cell or bins in their collision neighborhood. To prevent particles from traveling significantly farther than their neighborhood during \(\Delta t\) we limit the latter to a value that is given by cell size \(\Delta x\) and the maximum particle velocity:

\[ \Delta t = \frac{\Delta x}{v_{\text{max}}(t)}. \]  

(16)
At the moment we predominantly use Euler’s method to iterate the equations of motion:

\[ \mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \mathbf{v}_{\text{old},i} \Delta t + \mathbf{v}_{\text{new},i}(\Delta t - t_p) \quad (17) \]
\[ \mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \mathbf{v}_{\text{old},i} \Delta t. \quad (18) \]

Equation (17) is used when a collision takes place and eq. (18) when the particle do not interact during \( \Delta t \).

We avoid computationally expensive sorting algorithms by representing each grid bin via a linked list of the particles it contains. This way, spatial particle sorting is not necessary as it is replaced by a simple coordinate check. The scaling of the collision partner search is close to ideal for 2D as well as for 3D setups [48, 84]. Our study of the smRTI uses the same algorithm as is discussed in [48]. Differences include a change in the boundary conditions to adapt the code for the long-time evolution of the RTI (see next section) and the application of guided collisions in one of our studies (see section VII).

IV. SIMULATION SETUP

A. Particle Initialization

The smRTI is initialized as a heavy fluid with density \( \rho_2 \) lying on top of a light one with \( \rho_1 = 0.5 \rho_2 \). The box size is chosen as \( 0 \leq x \leq L_x \) and \( 0 \leq y \leq L_y \). Both fluids are initially at rest with a pressure \( P_0 \) at the fluid interface. The units of all quantities are given by the dimensions of length \( L \), density \( \rho \), and pressure \( P \) [88]. Consequently, the units for velocity are \( \sqrt{P/\rho} \), the units for time \( L/\sqrt{\rho/P} \), and the units for the gravitational acceleration \( \rho g/\bar{L} \). The value of the gravitational acceleration is \( g = -1.0 \), i.e. it is pointing in the negative y-direction. The simulation space is divided into two equally sized volumes \( V_1 = V_2 \) whereas \( V_2 \) contains the high-density fluid while the low-density fluid is in \( V_1 \). Both sub-spaces contain the same number of test-particles \( N_1 = N_2 \). The test-particle masses are determined via:

\[ m_{1,2} = \rho_{1,2} V_{1,2}/N_{1,2}. \quad (19) \]

To keep track of their motion during the simulation, particles in \( V_2 \) are assigned a particle type \( \tau_2 = 2 \) while particles in \( V_1 \) are given \( \tau_1 = 1 \). The pressure is a function of the y-position assuming constant densities \( \rho_1 \) and \( \rho_2 \):

\[ P_{1,2}(y) = P_0 + \rho_{1,2} g (y - 0.5 L_y). \quad (20) \]

with \( P_0 = 2.5 \). We initialize the particle velocities via Maxwell-Boltzmann (MB) distributions. The root-mean-square velocity

\[ \sqrt{\text{rms}}(y_i) = \sqrt{2T(y_i)/m_i} \quad (21) \]

associated with particle \( i \) is determined using the ideal gas equation of state:

\[ T_{1,2}(y_i) = P_{1,2}(y_i)/n_{1,2}. \quad (22) \]

A Monte Carlo algorithm calculates the absolute velocity of \( i \) according to the \( y \)-dependent MB distribution from \( \sqrt{\text{rms}}(y_i) \).

To initialize the smRTI, a small amplitude perturbation \( \eta_0(x) \) is introduced at the interface of both fluids. In principle, this can be a perturbation in the velocity fields or directly in the shape of the interface. In the current work we choose the latter and define the position of the interface as:

\[ \eta_0(x) = 0.5 L_y + B_0 \cos(2 \pi x / \lambda). \quad (23) \]

Here, the initial amplitude of the perturbation is \( B_0 = 0.01 \) and its wavelength is \( \lambda = 0.5 L_x \). As discussed in section II eq. (1) describes its growth rate in the linear regime.

B. Boundary Conditions

Our previous studies applied simple reflective boundary conditions [48]: If during \( \Delta t \) a particle with velocity \( \mathbf{v}_{\text{old}} \) and position \( \mathbf{r}_{\text{old}} \) is found to cross the box boundary at e.g. \( y = b_y = 0 \), its motion and location are updated via:

\[ \mathbf{v}_{\text{new},x} = \mathbf{v}_{\text{old},x}, \quad \mathbf{v}_{\text{new},y} = -\mathbf{v}_{\text{old},y}, \quad (24) \]
\[ x_{\text{new}} = x_{\text{old}}, \quad y_{\text{new}} = -y_{\text{old}}. \quad (25) \]

For the current tests, we modify this simple approach. In addition to the usual particle motion, we have to consider that the gravitational acceleration is present at all times. Therefore, when a particle is moving towards \( b_y = 0 \), it is accelerated downwards. Once it is reflected and moves into the opposite direction, its \( y \)-velocity is decreased due to gravitation. In addition, our RTI tests are running for \( \mathcal{O}(10^5) \) time steps. With these long timescale, the sinusoidal form of the instability paired with the simple reflective boundary conditions could lead to the development of standing waves in the simulation box. As these could potentially impact the evolution of the smRTI, we modify the boundary conditions from simple reflective to random reflective.

To implement the latter together with the gravitational acceleration, we first determine the particle-boundary collision time \( t_b \) from:

\[ b_y = y_{\text{old},y} + t_b + 0.5 g t_b^2 \]
\[ t_b = -v_{\text{old},y} g + \sqrt{(v_{\text{old},y} g)^2 - 2 (y_{\text{old},y} - b_y) g}. \quad (26) \]

whereas \( b_y = L_y \) or \( b_y = 0 \). The incoming \( y \)-velocity at \( b_y \) is then given by:

\[ v_{b,y} = v_{\text{old},y} + g t_b. \quad (28) \]

Together with the unchanged particle motion in the \( x \)-direction, the absolute velocity \( v_b \) at \( b_y \) becomes:

\[ v_b = \sqrt{v_{b,y}^2 + v_{x,old}^2}. \quad (29) \]
To determine the velocity after the reflection on the boundary, the outgoing direction of motion is randomized. For that, we create random numbers $\kappa_x \in [-1.0,1.0]$ and $\kappa_y \in [0.0,1.0]$ or $\kappa_y \in [-1.0,0.0]$, depending on whether the reflection is performed at $b_y = 0$ or $b_y = L_y$, respectively. The random numbers are scaled so that $\kappa_x^2 + \kappa_y^2 = 1$, and the new velocity components and positions calculated as:

\[
\begin{align*}
    v_{\text{new},y} &= v_{\text{old},y} + g \Delta t - t_b, \\
    v_{\text{new},x} &= v_{\text{old},x}, \\
    y_{\text{new},y} &= y_{\text{old},y} + 0.5 g \Delta t - t_b^2, \\
    x_{\text{new},x} &= x_{\text{old}} + v_{\text{old},x} t_b + v_{\text{new},x} \Delta t - t_b.
\end{align*}
\]

\[
\begin{align*}
    \kappa &= \frac{\Delta y}{\Delta x}.
\end{align*}
\]

\[
\begin{align*}
    l &= 4 \text{ growth of large-scale instabilities. Fig.1 shows the evolution, these can serve as seeds for the development and small surface and fluid interface irregularities. If not suppressed, this can serve as seeds for the development and growth of large-scale instabilities. Fig.1 shows the evolution of an initially smooth interface over a time period of } t = 4.0 \text{ using } 4.0 \times 10^7 \text{ test-particles. The initialization of the simulation is as described in section IV, however with the difference that the box dimensions are chosen as } 0.8 \times 0.5 \text{ with } 2560 \times 1600 \text{ calculation bins and } 320 \times 200 \text{ output bins. The mean-free-path is } l = 10^{-4} \Delta x \text{ to ensure hydrodynamic behavior. It can clearly be seen how the seemingly smooth fluid interface starts to develop a diffusion layer with small dips and peaks. This mixing is due to the particle nature of our approach as some particles move from one fluid into the other. The peaks and dips are caused by the previously mentioned irregularities of the fluid interface as a consequence of the finite number of test-particles and their random initial positioning. Since the simulation should be in the continuum limit, we expect the fluid interface to remain a sharp line. The observed particle diffusion might indicate that we are not exactly reproducing this regime. Fig.1 shows how the small perturbations grow over time and result in the formation of RTIs with different wavelengths. We will find similar behavior in our continuum smRTI simulation. To prevent the development of these small-scale structures that can dominate the smRTI evolution, we implement a diffusion suppression algorithm that is discussed in section VI.}
\]

\[
\begin{align*}
    \tau &= 1 \text{ for } t = 25, \text{and} \quad \tau &= 2 \text{ for } t = 75. \text{ The corresponding results for } \tau \text{ are plotted in Fig.3 for (a1) } t = 0.5, \text{ (a2) } t = 1.25, \text{ (a3) } t = 3.5, \text{ and (a4) } t = 7.5. \text{ For } t \leq 1.25 \text{ we add the analytic solution from linear analysis (see eq.(1) and eq.(23)) as a dashed line. Figure 4 gives the contour lines corresponding to } \tau = 1.2 \text{ (red, bottom line), } \tau = 1.5 \text{ (middle, black line), and } \tau = 1.8 \text{ (top, blue line). The small value of } l \text{ should generally lead to the continuum solution and be directly comparable to hydrodynamic simulations [48]. However, as seen in Fig.3 the formation of a diffusion layer for } t \leq 0.5 \text{ is clearly visible. Again, small finite structures are developing at the interface. Still, at } t = 0.5, \text{ the amplitude of the instability is nearly unchanged and is in good agreement with the analytic prediction. The observed small perturbations serve as seeds for fluid instabilities that become clearly visible at } t = 1.25. \text{ Here, in addition to the growth of the smRTI, small bubbles of light fluid are moving upwards. Overall, the analytic prediction is matched by the envelope of the bubble maximum. As the small perturbations grow in size, they develop secondary instabilities themselves (see Fig.3a3). For } t \geq 3.75, \text{ the smRTI has spread to the } x\text{-edges of the simulation space where its evolution is influenced by the interaction with the box walls.}
\]

\[
\begin{align*}
    \text{V. MEAN-FREE-PATH STUDIES}
\end{align*}
\]

\[
\begin{align*}
    \text{B. Simulation in the Continuum Limit}
\end{align*}
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We start our 2D smRTI studies with a test in the continuum limit by setting $l = 10^{-3} \Delta x$. The box dimensions are $0.25 \times 1.6$ with $800 \times 5120$ calculation bins, and $100 \times 640$ output bins. The boundary conditions are random reflective and particles are interacting with each other via simple elastic collisions according to the PoCA algorithm. Fig.2 shows the initial (a) particle type $\tau$, (b) particle number normalized by $N_0 = N/(L_x \times L_y) = 625$, and (c) the pressure as given by eq.(20). All quantities are shown as averages per bin. For better visualization, we mirror the output at $x = 0$. We let the simulation evolve up to a time of $t = 3.75$. The corresponding results for $\tau$ are plotted in Fig.3 for (a1) $t = 0.5$, (a2) $t = 1.25$, (a3) $t = 2.5$, and (a4) $t = 3.75$. For $t \leq 1.25$ we add the analytic solution from linear analysis (see eq.(1) and eq.(23)) as a dashed line. Figure 4 gives the contour lines corresponding to $\tau = 1.2$ (red, bottom line), $\tau = 1.5$ (middle, black line), and $\tau = 1.8$ (top, blue line). The small value of $l$ should generally lead to the continuum solution and be directly comparable to hydrodynamic simulations [48]. However, as seen in Fig.3 the formation of a diffusion layer for $t \leq 0.5$ is clearly visible. Again, small finite structures are developing at the interface. Still, at $t = 0.5$, the amplitude of the instability is nearly unchanged and is in good agreement with the analytic prediction. The observed small perturbations serve as seeds for fluid instabilities that become clearly visible at $t = 1.25$. Here, in addition to the growth of the smRTI, small bubbles of light fluid are moving upwards. Overall, the analytic prediction is matched by the envelope of the bubble maximum. As the small perturbations grow in size, they develop secondary instabilities themselves (see Fig.3a3). For $t \geq 3.75$, the smRTI has spread to the $x$-edges of the simulation space where its evolution is influenced by the interaction with the box walls.}

\[
\begin{align*}
    \text{C. Mean-free-path comparison}
\end{align*}
\]

As previously mentioned, the advantage of particle approaches is that they can describe the dynamics of matter at different values of the Knudsen number, unlike hydrodynamic methods. Figures 3(b) - (g) show the evolution of the smRTI with particle mean-free-paths ranging from (b) $l = 1.5 \Delta x$, (c) $l = 3.0 \Delta x$, (d) $l = 5.0 \Delta x$, (e) $l = 10.0 \Delta x$, (f) $l = 30.0 \Delta x$, and (g) $l = 100.0 \Delta x$. Snapshot times are as in the continuum limit: (1) $t = 0.5$, (2) $t = 1.25$, (3) $t = 2.5$, and (4) $t = 3.75$, and Fig.4 shows again the corresponding contour lines. The large step in the mean-free-path from $l = 10^{-3} \Delta x$ to $l = 1.5 \Delta x$ is motivated by our previous finding that shock wave dynamics do not differ much for $l \lesssim 1.0 \Delta x$. As shown in the same work, an increase in $l > 1.0 \Delta x$ reduces the number of interactions per
FIG. 1: Evolution of fluid instabilities at an unperturbed interface between a high density fluid (top, blue) and a low density fluid (bottom, red) in the presence of a gravitational acceleration. The particle number is $N = 4.0 \times 10^7$ and we plot the average particle type $\tau$ per output bin at times (a) $t = 0$, (b) $t = 0.5$, (c) $t = 1.0$, (d) $t = 2.0$, (e) $t = 3.0$, and (f) $t = 4.0$.

FIG. 2: Initialization of smRTIs with (a) average particle type $\tau$ per bin, (b) average particle number $N_{\text{bin}}$, normalized by $N_0 = 625$, and (c) average pressure $p$ per bin.

It can be seen in Fig. 3(1) and Fig. 4(1) that the thickness of the mixed fluid layer increases with $l$, as particles have more freedom to move from one fluid into the other. At the same time, the small wavelength perturbation that are present for $l = 10^{-3} \Delta x$ are smoothed out. Although the growing width of the diffusion layer prohibits a clear definition of the fluid interface, the position of the latter seems to match well with the analytic prediction for $l \leq 10.0 \Delta x$ up to $t \sim 1.25$. At later times, the simulations start to lag behind, as can be seen in Fig. 3(2). For $l = 30.0 \Delta x$ and $l = 100.0 \Delta x$, a clear separation between the fluids cannot be determined and both seem to simply mix with each other over time. The further impact of the mean-free-path on the evolution of the smRTI with $l \leq 10.0 \Delta x$ can clearly be seen for $t \geq 2.5$. Here, $l$ seems to influence the growth rate in the non-linear regime, as the height of the light fluid bubble clearly decreases with larger $l$.

Despite their different mean-free-paths, smRTIs with $l \leq 5.0 \Delta x$ reach a similar height at the end of the simulation. Fig. 3 shows the amplitude of the smRTI as a function of time $t$ and scaled time $t_s = t(\Delta y/\lambda)^{0.5}$. We define the amplitude $B$ as the average between the highest point with $\tau = 1.8$ and the height of the layer with $\tau = 1.2$ at the same $x$-coordinate. Furthermore, we scale $B$ with the wavelength of the initial perturbation $\lambda$. The continuum simulation with $\lambda = 10^{-3} \Delta$ matches the analytic prediction up to $t \sim 1$ whereas a larger mean-free-path leads to earlier deviations. For $t > 1$, the linear solution continues to increase exponentially while the simulations flatten, their growth rate decreasing with larger $l$. timestep and therefore leads to a slower equilibration. Of course, for our smRTI tests particles are already initialized in equilibrium (see section IV). Nevertheless, we expect that large mean-free-paths will have an effect on the simulations, for example, the resolution and amount of particle diffusion from one fluid into the other. Furthermore, $l$ can also impact matter compressibility and viscosity, and thereby influence the growth rate and overall evolution of the smRTI.
FIG. 3: Time evolution of the average particle type $\tau$ per bin in the smRTI simulation for: (a) $l = 0.001 \Delta x$, (b) $l = 1.5 \Delta x$, (c) $l = 2.0 \Delta x$, (d) $l = 5.0 \Delta x$, (e) $l = 10.0 \Delta x$, (f) $l = 30.0 \Delta x$, and (g) $l = 100.0 \Delta x$. Snapshots are taken at times (1) $t = 0.5$, (2) $t = 1.25$, (3) $t = 2.5$, and (4) $t = 3.75$. The number of test-particles is $N = 4.0 \times 10^7$ with $800 \times 5120$ simulation bins covering a space of $0.25 \times 1.6$. The output is mirrored at $x = 0$. 
FIG. 4: Same as in Fig.3 but as contour plots for $\tau = 1.2$ (red, lower line), $\tau = 1.5$ (black, middle line), and $\tau = 1.8$ (top, blue line).

Fig.4 shows the thickness of the diffusion layer $D$ for $l \leq 30 \Delta$. The width of the layer is the difference in the $y$-coordinate of the highest point with $\tau = 1.8$ and the $y$-coordinate for $\tau = 1.2$ at the same $x$-position. Particle diffusion is always present and increases with $l$. Furthermore, a comparison between Fig.3 and Fig.4 shows that diffusion dominates the evolution of the smRTI at early times. For larger $l$, this behavior persists longer. However, once the mixed fluid layer is established, it stops growing and even shrinks at later times.

For better comparison, we plot different quantities of the smRTI simulations at $t = 3.75$ in Fig.4.
VI. DIFFUSION SUPPRESSION

Both, the formation of the diffusion layer for large $l$ and the occurrence of large wavenumber instabilities for small $l$, originate in the particle nature of our approach. For a better comparison to hydrodynamic studies, we would like to minimize both effects. Therefore, we apply larger mean-free-paths and the typical mushroom shape of the smRTI is only present for $l \lesssim 5 \Delta x$. Fig. 7(1) shows two additional interesting phenomena. First, with larger values of $l$, particle densities at the top of the simulation box seem to decrease over time. This can be seen for $l = 30 \Delta x$ and $l = 100 \Delta x$ and is most likely caused by the absence of scattering. Initially, particle velocities are set up according to MB distributions. Over time, the gravitational acceleration increases components in the negative $y$-direction. The absence of particle interaction makes it impossible for these velocity components to be transferred into motion in other directions and the particles eventually move downwards. Since the absolute particle velocity decrease with height, this effect is most pronounced at the top of the simulation box and explains the observed lower values of $\rho$. The second effect which is present for simulations with smaller $l$ indicates a finite matter compressibility. It is visible for Fig. 7(a1) - (c1). Here, densities at the foot of the smRTI seem to be slightly higher than e.g. the ones at the tip of the light fluid bubble.

To better understand at which point the vorticity and matter compression set in, we compare the densities and velocities of the smRTI at $t = 1.25$ and $t = 2.5$. The results are shown in Fig. 8 whereas subfigures (1) and (2) correspond to $t = 1.25$ and $t = 2.5$, respectively. Figures 8(a)-(c) give $\rho$, $v_x$, and $v_y$. Particle velocities are small at $t \sim 1.25$ and start to increase at later times. Compressibility effects are not visible either for $t = 1.25$ or $t = 2.5$, and therefore seem to appear at later times when mushroom shape of the smRTI is more developed. Here, density variations are most likely caused by the rapid motion of the light fluid bubble that stretches and compresses matter. Although a finite fluid compressibility is realistic for physical fluids, our simulations should be able to reproduce the ideal fluid solution for small $l$. More tests have to be performed with higher test-particle numbers and different particle interactions. It is interesting to note that compressible fluids have been found to lead to a later development of secondary instabilities [78], an effect which is seen in our simulations for large $l$.

Our 2D RTI studies are long-time simulations. With 20 processors and OpenMP parallelization, the $l = 10^{-3} \Delta x$ simulation ran for about $1.2 \times 10^5$ timesteps in ca. 718 hours. Although larger mean-free-paths decrease the computational time due to fewer particle interactions an efficient MPI parallelization should be implemented to enable the usage of many nodes and speed up the calculations.
an algorithm for diffusion suppression which prevents particles of one fluid to diffuse into the other. The details of the algorithm are described in appendix A. Our algorithm uses guided collisions. The interaction neighborhood of a particle $i$ of type $\tau = 1$ is first checked for all particles $j$ with $\tau = 2$. If the latter exist, a normalized repulsive acceleration is calculated between $i$ and $j$ along their relative position vector. After the neighborhood search, all acceleration vectors are summed up and normalized again. When the collision between $i$ and its final interaction partner is performed and the collision partner has $\tau = 2$, the outgoing velocities are set along the repulsive acceleration vector.

With that, particles of one fluid will always obtain a post-collision motion that is pointing away from the other fluid. With our approach we do not explicitly use repulsive particle potentials or a surface tension. However, with the introduction of a defined accelerations we technically apply a force. To minimize its impact on the evolution of the smRTI we limit its application to $t \leq 0.5$.

We simulate the smRTI for $N = 4.0 \times 10^7$ and $N = 1.0 \times 10^7$, both, with $l = 10^{-3} \Delta x$. The results are shown in Fig. 8 whereas we plot $\tau$ and $\rho$ in subfigures (1) and (2), respectively. The density is normalized as in eq. (5) with $N_0 = 666.67$. The different snapshots
The bubble rises continuously, stretching the mushroom shape. No further formation of secondary instabilities is observed. This can be due to the fast rise of the fluid bubble or the small size of the simulation box which, at this point, restricts the evolution of smRTI. As before, we can make out effects of finite compressibility for $t \geq 3.75$ density variations from the bottom of the sinking dense fluid fingers to the top of the simulation box.

A comparison of the results with $N = 4.0 \times 10^7$ and $N = 1.0 \times 10^7$ allows us to get an idea about the particle number dependence. For $N = 1.0 \times 10^7$, we adjust the number of calculation bins to $200 \times 1200$. In Fig. 9 no significant differences can be found for $t = 0.5$. At later times, the lower resolution of the simulation with smaller $N$ as well as the more pronounced statistical noise become apparent. However, both smRTIs reach similar amplitudes and have similar structures, although in the large $N$ simulation the light fluid bubble is slightly higher. The latter can be attributed to a different shape of the smRTI. Another possibility are different finite compressibility effects in connection with the particle number.

The introduction of diffusion suppression is a useful tool for comparison studies with hydrodynamic codes. However, it should be noted that it is not based on physical forces and is therefore not suited for simulations of realistic problems. Eventually, a sufficiently large particle number should ensure that perturbations on the interface between two fluids are not due to a low particle number but are of physical nature. Hydrodynamic simulations face similar challenges as grid size, resolution, and advection scheme can impact the evolution of small-wavelength instabilities. These effects can change the evolution of e.g. astrophysical systems. Therefore, like in hydrodynamic simulations, we have to perform convergence tests to ensure that the dynamics of the physical system will not change significantly with resolution or particle number.

VII. SUMMARY AND OUTLOOK

We present simulations of single-mode Rayleigh Taylor instabilities (smRTIs) with a large-scale modified Direct Simulation Monte Carlo Code. Our approach combines the computational scaling of DSMC methods and the spatial accuracy of the Point-of-Closest-Approach technique. The aim of the current work is to test our kinetic code on its ability to reproduce fluid instabilities. The code has already been validated in the hydrodynamic regime by 2D and 3D shock wave studies and is able to simulate matter up to large Knudsen numbers. For our RTI simulations, we apply $N = 4.0 \cdot 10^7$ test-particles. In the early regime of the smRTI the growth rate can be analytically obtained from linear theory while for late
time behavior the onset of secondary instabilities and eventually turbulent mixing is seen by hydrodynamic codes and experiments. We compare the results of our simulations to the expected behavior of the smRTI in these regimes. Applying different particle mean-free-paths \( l \), we simulate smRTIs in the hydrodynamic regime and for non-equilibrium matter. We find that even for small values of \( l \) the formation of a mixed fluid layer is present. It is caused by particles diffusing from one fluid into the other. Furthermore, for small mean-free-paths, initial irregularities of the fluid interface result in the formation of large wavenumber instabilities which evolve into RTIs themselves. With increasing \( l \), the diffusion layer becomes wider and the small-scale structures are blurred out. For \( l \leq 5 \Delta x \) we find the formation of Kelvin-Helmholtz instabilities at the tips of the sinking heavy fluid. Secondary instabilities lead to the characteristic mushroom shape of the smRTI which is observed in hydrodynamic simulations and experiments. To prevent the formation of small-scale instabilities and minimize the width of the mixing layer, we introduce a diffusion suppression algorithm that uses guided particle collisions. The latter is applied in the beginning of the simulation for \( t \leq 0.5 \) and allows the smRTI to sufficiently grow in amplitude and dominate any possible small-scale perturbations. We find that the analytic prediction for the instability position is very well reproduced until \( t \lesssim 0.5 \). For later times the simulation starts to lag behind, which becomes apparent at e.g. \( t \sim 1.25 \).

Overall, our simulations agree with the analytic prediction from linear theory for early times and have a similar shape and size as we would expect from hydrodynamic simulations. We conclude that our kinetic approach can reproduce the general features of smRTI. Observations that need to be explored in future studies include the formation of a diffusion layer, even for very small particle mean-free-paths which is not seen in ideal hydrodynamics codes.

In the future, we plan to perform convergence tests as well as more general RTI studies. Furthermore, we will complement our fluid instability test suite with the Kelvin-Helmholtz and the Richtmeyer-Meshnikov instabilities. With that, together with the already successfully passed shock wave tests, we will be able to point our attention to the simulation of e.g. astrophysical

FIG. 9: (1) Particle type \( \tau \) and (2) mass density \( \rho \) for the smRTI with diffusion suppression, \( l = 10^{-3} \Delta x \), \( N = 4.0 \times 10^7 \) (for \( x < 0 \)) and \( N = 1.0 \times 10^7 \) (for \( x > 0 \)). The diffusion suppression is released at \( t = 0.5 \). The snapshot times are (a) \( t = 0.5 \), (b) \( t = 1.25 \), (c) \( t = 2.5 \), (d) \( t = 3.75 \), (e) \( t = 4.0 \), (f) \( t = 4.5 \), and (g) \( t = 5.0 \).
systems, like core-collapse supernovae.

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Appendix A: Diffusion suppression via guided collision

Our general approach for detection and performance of particle interactions is described in detail in [8]. Two collision partners, particles $i$ and $j$, are transformed into their center-of-mass (cm) frame where their initial cm-velocities are calculated as:

$$v_{i,cm} = v_i - v_{cm}, \quad v_{j,cm} = v_j - v_{cm}.$$  \hspace{1cm} (A1)

The outgoing cm-velocity vector of particle $i$ is then assigned via:

$$u_{i,cm} = a_i v_{i,cm},$$ \hspace{1cm} (A2)

whereas $u_{i,cm} = v_{i,cm} = |v_{i,cm}|$ and $a_i$ is a normalized direction vector with randomly assigned components. The cm-velocity of particle $j$ is arranged equal and opposite to the one of particle $i$, i.e. $u_{j,cm} = -u_{i,cm}$. Both velocity vectors, $u_{i,cm}$ and $u_{j,cm}$, are then transformed back into the laboratory frame via the inverse of eq.(A1).

When we perform guided collisions, $a_i$ is not determined randomly anymore: For each particle $i$, we iterate through all particles $j$ in the collision neighborhood. If $i$ and $j$ have different types $\tau_i \neq \tau_j$ and their relative distance $r_{rel,ij} = |r_i - r_j| \leq 1.5 \Delta x$, a normalized vector $\alpha_{ij}$ is calculated via:

$$\alpha_{ij} = (r_{rel,ij}) / (r_{rel,ij}).$$  \hspace{1cm} (A3)

If particle $i$ is located in a bin that is next to a border of the simulation space, its collision neighborhood is not complete. In this case we mimic the effects of possible particles beyond the walls by setting up a reflection axis through the center of the collision neighborhood. Mirror particles $jm$ of neighborhood particles $j$ are created if $\tau_j \neq \tau_i$ by mirroring the latter on the axis. For example, if particle $i$ is located at $(L_x - dx) \leq x \leq L_x$ or $0 \leq x \leq dx$, we calculate the corresponding vector $\alpha_{ijm}$ via:

$$\alpha_{ijm,x} = \frac{x_{rel,ijm}}{r_{rel,ijm}}, \quad \alpha_{ijm,y} = \alpha_{ij,y}.$$ \hspace{1cm} (A4)

Hereby:

$$r_{rel,ijm} = (x_{ijm}^2 + y_{ijm}^2)^{0.5},$$ \hspace{1cm} (A5)

$$x_{ijm} = x_i - x_{jm},$$ \hspace{1cm} (A6)

$$x_{jm} = 2L_x - dx - x_j, \quad (L_x - dx) \leq x \leq L_x,$$ \hspace{1cm} (A7)

$$x_{jm} = dx - x_j, \quad 0 \leq x \leq dx,$$ \hspace{1cm} (A8)

whereas $y_{rel,ij}$ and $r_{rel,ij}$ are as above. We then normalize and sum all direction vectors

$$\alpha_i = \sum_j (\alpha_{ij} + \alpha_{ijm}),$$ \hspace{1cm} (A9)

normalize $\alpha_i$ again, and assign it as a property of particle $i$ before proceeding with the usual collision partner search. Once final collision partners, particle 1 and 2, have been determined, we check whether they have different types $\tau_1 \neq \tau_2$, and whether $\alpha_1 \neq 0$, and $\alpha_2 \neq 0$. If this is not the case, we proceed with our usual collision routine by randomly assigning $a_1$ (see above). If the collision happens between particles of different types, we first average:

$$a_1 = (\alpha_1 - \alpha_2)/2, \quad a_2 = -a_1.$$ \hspace{1cm} (A10)

To determine the post-collision velocities in the laboratory frame $u_{1,2}$ from the in-coming velocities $v_{1,2}$ and the accelerations as determined in eq.(A10), we use energy and momentum conservation during the collision:

$$E = m_1v_1^2 + m_2v_2^2 = m_1u_1^2 + m_2u_2^2$$ \hspace{1cm} (A11)

$$p = m_1v_1 + m_2v_2 = m_1u_1 + m_2u_2$$ \hspace{1cm} (A12)

With $a_1$ from eq.(A10) and $u_1 = a_1 u_1$, we rewrite:

$$p = m_1a_1 u_1 + m_2 u_2$$ \hspace{1cm} (A13)

$$\Rightarrow u_2 = (1/m_2) (p - m_1 a_1 u_1).$$ \hspace{1cm} (A14)

From this we arrive at:

$$m_2 u_2^2 = \frac{(p - m_1 a_1 u_1)^2}{m_2} + \frac{(p_y - m_1 a_y u_1)^2}{m_2}$$  \hspace{1cm} (A15)

Now, eq.(A11) can be written as:

$$E = m_1 u_1^2 + \frac{(p_x - m_1 a_x u_1)^2}{m_2} + \frac{(p_y - m_1 a_y u_1)^2}{m_2},$$  \hspace{1cm} (A16)

and therefore:

$$E = u_1^2 \left(\frac{m_1 m_2 + m_2^2}{m_2}\right) - 2 m_1 u_1 (p_x a_x + p_y a_y) \frac{p_x^2 + p_y^2}{m_2}.$$ \hspace{1cm} (A17)
Equation (A17) has the form:

\[
\begin{align*}
  u_1^2 - c u_1 + d &= 0, \\
  d &= \frac{p_x a_x + p_y a_y}{m_1 + m_2},
\end{align*}
\] (A18)

and can be solved as:

\[
  u_1 = -\frac{1}{2} c \pm \sqrt{\frac{1}{4} c^2 - d},
\] (A20)

With given \(a_1\) we can then determine \(u_1\) and \(u_2\).
