Three Dimensional Simulations of Multiphase Flows Using a Lattice Boltzmann Method Suitable for High Density Ratios – 12126

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ABSTRACT

Multiphase flows involving gas and liquid phases can be observed in engineering operations at various Department of Energy sites, such as mixing of slurries using pulsed-air mixers and hydrogen gas generation in liquid waste tanks etc. The dynamics of the gas phase in the liquid domain play an important role in the mixing effectiveness of the pulsed-air mixers or in the level of gas pressure build-up in waste tanks. To understand such effects, computational fluid dynamics methods (CFD) can be utilized by developing a three-dimensional computerized multiphase flow model that can predict accurately the behavior of gas motion inside liquid-filled tanks by solving the governing mathematical equations that represent the physics of the phenomena.

In this paper, such a CFD method, lattice Boltzmann method (LBM), is presented that can model multiphase flows accurately and efficiently. LBM is favored over traditional Navier-Stokes based computational models since interfacial forces are handled more effectively in LBM. The LBM is easier to program, more efficient to solve on parallel computers, and has the ability to capture the interface between different fluid phases intrinsically. The LBM used in this paper can solve for the incompressible and viscous flow field in three dimensions, while at the same time, solve the Cahn-Hillard equation to track the position of the gas-liquid interface specifically when the density and viscosity ratios between the two fluids are high. This feature is of primary importance since the previous LBM models proposed for multiphase flows become unstable when the density ratio is larger than 10. The ability to provide stable and accurate simulations at large density ratios becomes important when the simulation case involves fluids such as air and water with a density ratio around 1000 that are common to many engineering problems.

In order to demonstrate the capability of the 3D LBM method at high density ratios, a static bubble simulation is conducted to solve for the pressure difference between the inside and outside of a gas bubble in a liquid domain. Once the results show that the method is in agreement with the Laplace law, buoyant bubble simulations are conducted. The initial results obtained for bubble shape during the rising process was found to be in agreement with the theoretical expectations.

INTRODUCTION

As a result of atomic weapons production, millions of gallons of radioactive waste was generated and stored in underground tanks at various U.S Department of Energy (DOE) sites. DOE is currently retrieving, transferring, and processing some of these wastes, employing a variety of methods. Various waste retrieval and processing methods are employed during the transfer of the waste. One such method, pulsed-air mixing, involves injection of discrete pulses of compressed air or inert gas at the bottom of the tank to produce large bubbles that rise due to buoyancy and mix the waste in the tank as a result of this rising motion. Pulsed-air mixers are operated by controlling the pulsing frequency and duration, the sequence of injection plates and gas pressure. Low equipment cost, high durability, easy decontamination and low operating costs are some of the advantages of pulsed-air mixers over other waste mixing technologies.

The pulsed-air technology is commercially available and its effectiveness has been demonstrated at Pacific Northwest National Laboratory (PNNL) (Powell & Hymas, 1996), however, understanding the physical nature of the mixing phenomena by injection of air bubbles and the effects of the air release process to the tank environment need to be studied by considering various waste conditions. Such an analysis can be made possible by developing a numerical method that can simulate the process of air bubble generation inside liquid filled tanks including suspending solids. The final computational program would serve as a tool for the site engineers to predict various mixing scenarios and improve operational procedures of pulsed-air mixing efficiently.

In this paper, a numerical method, lattice Boltzmann method (LBM), is presented that can model multiphase flows accurately and efficiently. Special attention was given to two-phase flows with high density ratios since this brings another challenge in terms of instabilities to LBM simulations for multiphase flows with density ratios larger than 10. The instability is considered to be generated as a result of large density gradients in the interfacial region between two phases. The current LBM presented in this paper is able to provide stable and accurate simulations at large density ratios between the fluid and the gas phases.

The outline of the paper is given as the following: first an overview of various multiphase LBM approaches is presented. Second, the governing equations for the lattice Boltzmann method used in this paper are introduced. Later, applications to static and dynamic bubbles are shown. Finally, conclusions are drawn and discussions for future work are presented.

LBM FOR HIGH-DENSITY RATIO MULTIPHASE FLOWS

One common limitation of the multiphase LBM is that its applications were limited to low density ratios between phases. The density ratio obtained by the Swift's free-energy method (Swift, Osborn, & Yeomans, 1995) was less than 10, which was also the limit for the index-function method of (He, Chen, & Zhang, 1999). Attempts to improve Gunstensen's color method (Gunstensen, Rothman, Zaleski, & Zanetti, 1991) to higher density ratios were only successful to achieve density ratios up to 4 (Tolke, Krafczyk, Schulz, & Rank, 2002) and 20 (Reis & Phillips, 2007). (Lishchuk & Halliday, 2008) have claimed to extend the color method to density ratios up to 500, however, they have reported simulations with density ratios less than 10 due to computational expense of the method at larger density ratios. The exact reasons of this low-density-ratio limit in LBM multiphase models have not yet been explained clearly, however, the inherent compressible characteristic of the LBM is considered to be one of the reasons.

(Inamuro, Ogata, Tajima, & Konishi, 2004) proposed a method based on the free energy method to extend its capability to incorporate fluids with large density ratios up to 1000. They used a pressure correction step in order to enforce the continuity equation after the collision and streaming step. The projection step required solving the Poisson's equation for the whole flow field and has reduced the computational efficiency of the method. Problems with assigning a cut-off value for the order parameter, evolved by the Cahn-Hilliard interface evolution equation, and a lack of analytical expression of the surface tension coefficient has been brought forward as deficiencies of the method (Zheng, Shu, & Chew, 2005; Zheng, Shu, & Chew, 2006). In addition, the additional terms that show up in the recovered interface evolution equation caused the method to lack Galilean invariance.

(Lee & Lin, 2005) have used the index function method of (He, Chen, & Zhang, 1999) in order to develop a stable version for multiphase flows with large density ratios up to 1000 and viscosity ratio varying from 40 to 100 (Lee & Lin, 2005). A modified pressure was introduced in order to avoid the large pressure fluctuations across the interface causing the scheme to be unstable at high density ratios in the index function model. The forcing term in the pre-streaming collision step and post-collision step were treated differently in order to improve the stability of the method. The results were verified for a stationary drop using the Laplace's law and their method was observed to have a high degree of isotropy. Using a D3Q19 lattice model, a 3D droplet oscillation case is solved for a density ratio of 1000 and a viscosity ratio of 100. The oscillation periods for droplets with various radius size and thicknesses were verified against analytical results with maximum errors being less than 5%. Droplet splashing on a thin liquid film was also analyzed where the density ratio was 1000, maximum viscosity ratio was 40 and the Weber number was 8000. However, their model was criticized for not recovering the lattice Boltzmann equation for the interface to the Cahn-Hilliard equation (Zheng, Shu, & Chew, 2006).

NUMERICAL METHOD

The lattice Boltzmann method presented in this paper is based on the continuous Boltzmann equation given by

$$ - + \cdot \nabla + \cdot \nabla = . \tag{1}$$

Here f is the single particle density distribution function, ξ is the particle velocity, $\boldsymbol{F}$ is the interfacial force and Ω is the collision term. For single-phase flows the interfacial force term drops out and we obtain

$$ - + \cdot \nabla = . \tag{2}$$

The continuous Boltzmann equation given in Eq. (2) can be discretized in the velocity space by expressing as

$$ - + \cdot \nabla = , \tag{3}$$

where

$$ \equiv \; = \begin{array}{lll} (0,0,0) & , & = 0, \\ (\pm 1,0,0),\ (0,\pm 1,0),\ (0,0,\pm 1) & , & = 1-6, \\ (\pm 1,\pm 1,0),\ (\pm 1,0,\pm 1),\ (0,\pm 1,\pm 1) & , & = 7-18. \end{array} \tag{4}$$

In Eq. (4) α is the discrete particle velocity distribution using the D3Q19 lattice structure for three dimensional domains, e is the particle velocity between lattice points.

Using a collision matrix Λ, the collision term on the right hand side of Eq. (2) is represented by

$$ = - \quad - \quad . \tag{5}$$

The equilibrium distribution function, f_α^{eq}, is written as

$$ = \quad 1 + \frac{}{} + \frac{(\quad)}{} , \tag{6}$$

where w_α is the weight function given by

$$= \begin{array}{ll} 1/3, & = 0, \\ 1/18, & = 1 - 6, \\ 1/36, & = 7 - 18. \end{array} \qquad (7)$$

The evolution equations given above for the particle density distribution function are mapped into the moment space by multiplying the terms in Eq. (2) with the transformation matrix **T**

$$= \begin{array}{c} \langle\ |, \langle\ |, \langle\ \ |, \langle\ \ |, \langle\ \ |, \langle\ \ , \langle\ \ , \langle\ |, \langle\ \ |, \langle 3\ \ \ |, \langle 3\ \ \ \ |, \langle\ \ \ \ |, \langle\ \ \ \ |, \\ \langle\ \ \ , \langle\ \ \ , \langle\ \ |, \langle\ \ |, \langle\ \ \ , \langle\ \ | \end{array} , \qquad (8)$$

where

$$|\ \rangle = |\ \ |\ , \qquad (8a)$$

$$|\ \rangle\ = 19|\ \ | - 30 \qquad (8b)$$

$$|\ \ \rangle\ = (21|\ \ | - 53|\ \ | + 24)/2, \qquad (8c)$$

$$|\ \rangle\ =\ \ _{,}\ , \qquad (8d)$$

$$|\ \ \rangle\ = [5|\ \ | - 9]\ \ _{,}\ , \qquad (8e)$$

$$\rangle\ =\ \ _{,}\ , \qquad (8f)$$

$$\rangle\ = [5|\ \ | - 9]\ \ _{,}\ , \qquad (8g)$$

$$|\ \rangle\ =\ \ _{,}\ , \qquad (8h)$$

$$|\ \ \rangle\ = [5|\ \ | - 9]\ \ _{,}\ , \qquad (8i)$$

$$|\ \ \ \rangle\ = 3\ \ _{,}\ - |\ \ |\ , \qquad (8j)$$

$$|\ \ \ \rangle\ = (3|\ \ | - 5)\ 3\ \ _{,}\ - |\ \ |\ \ , \qquad (8k)$$

$$|\ \ \ \rangle\ =\ \ _{,}\ -\ \ _{,}\ , \qquad (8l)$$

$$|\ \ \ \rangle\ = (3|\ \ | - 5)\ \ _{,}\ -\ \ _{,}\ , \qquad (8m)$$

$$\rangle\ =\ \ _{,}\ \ _{,}\ , \qquad (8n)$$

$$\rangle\ =\ \ _{,}\ \ _{,}\ , \qquad (8o)$$

$$|\ \ \rangle\ =\ \ _{,}\ \ _{,}\ , \qquad (8p)$$

$$|\ \ \rangle\ =\ \ _{,}\ -\ \ _{,}\ \ \ _{,}\ , \qquad (8r)$$

$$\rangle\ =\ \ _{,}\ -\ \ _{,}\ \ \ _{,}\ , \qquad (8s)$$

$$|\ \ \rangle\ =\ \ _{,}\ -\ \ _{,}\ \ \ _{,}\ , \qquad (8t)$$

The resulting evolution equation in moment space takes the form

$$\frac{}{} + \ \cdot \nabla\ \ = -\ \ \ \ -\ \ \ , \qquad (9)$$

where

$$=\ \ , \qquad (10)$$

$$= \quad , \qquad (11)$$

and

$$= \quad . \qquad (12)$$

The equilibrium distribution function is written as

$$(\quad) = \; , \quad ,(\quad) \; , \; , \quad , \; , \quad , \; , \quad ,3 \quad ,3 \quad , \quad , \quad , \quad , \quad , \quad , \quad , \quad , \qquad (13)$$

where the equilibrium distributions of the moments are given by

$$= -11 \quad + 19(\quad + \quad + \quad)/ \; , \qquad (14)$$

$$(\quad) \quad = 3 \quad -—(\quad + \quad + \quad)/ \; , \qquad (15)$$

$$= -- \quad , \qquad (16)$$

$$= -- \quad , \qquad (17)$$

$$= -- \quad , \qquad (18)$$

$$= - \; 2 \quad - \quad + \quad / \; , \qquad (19)$$

$$= -- \quad , \qquad (20)$$

$$= \quad - \quad / \; , \qquad (21)$$

$$= -- \quad , \qquad (22)$$

$$= \quad / \; , \qquad (23)$$

$$= \quad / \; , \qquad (24)$$

$$= (\quad)/ \; , \qquad (25)$$

$$= 0, \qquad (26)$$

$$= 0, \qquad (27)$$

$$= 0. \qquad (28)$$

The collision matrix in the moment space, , is given as

$$= \quad [\; , \; , \; , \; , \; , \; , \; , \; , \; , \; , \; , \; , \; , \; , \; , \; , \; , \; , \;]. \qquad (29)$$

The diagonal elements are inverses of relaxation times for the distribution functions in the moment space, , and they are used to relax to the equilibrium distribution functions in the moment space, . In this work, the diagonal elements are selected as $s_1 = s_4 = s_6 = s_8 = 0$, $s_2 = 1.19$, $s_3 = s_{11} = s_{13} = 1.4$, $s_5 = s_7 = s_9 = 1.2$, and $s_{17} = s_{18} = 1.2$, $s_{19} = s_7 = 1.98$. The parameters s_{10}, s_{12} and $s_{14\text{-}16}$ are related to the relaxation time, τ where $s_{10} = s_{12} = s_{14\text{-}16} = 1/\tau$ and are used to determine the viscosity, $\nu = -$ — and the Reynolds number, $= \; /$.

The macroscopic properties such as fluid density, velocity and pressure are obtained by

$$= \sum \quad , \qquad (30)$$

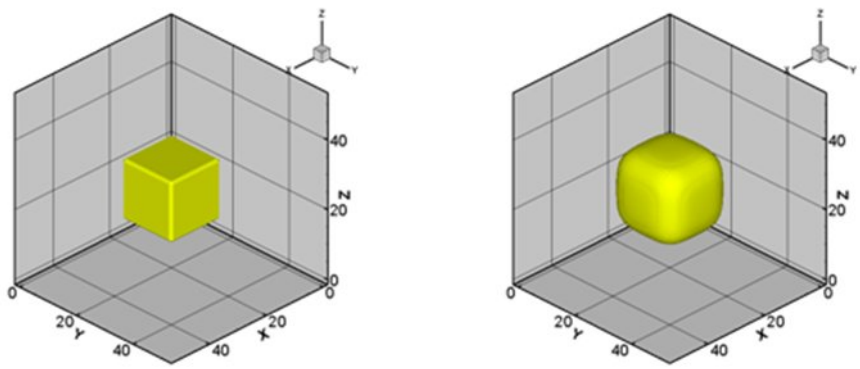
$$= \sum \quad , \qquad (31)$$

$$= \ /3. \quad (32)$$

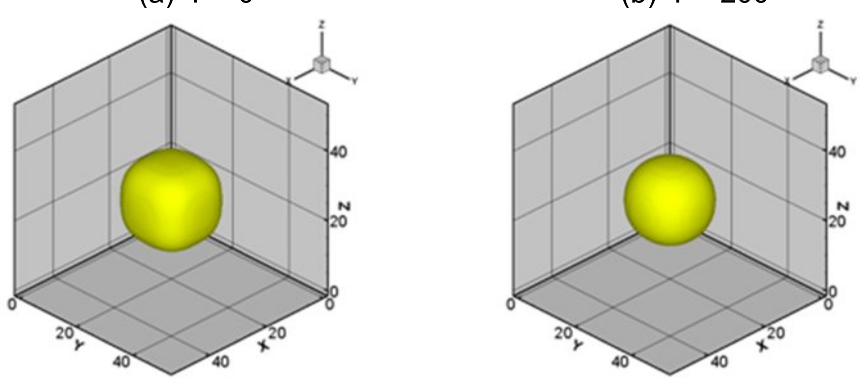
STATIC AND DYNAMIC BUBBLE SIMULATIONS

The multiphase model proposed by Lee and Lin (2005) simulates the Navier-Stokes equations for the hydrodynamics and the Cahn-Hillard equation for tracking the evolution of the interface. This is achieved by solving a set of lattice Boltzmann equations that yields pressure and velocity fields represented by the *f* distribution function and the density field represented by the *g* distribution function. The multiphase mode allows simulating two-phase systems with arbitrary fluid density and viscosity ratios.

In the first numerical test case presented here, a cubical three-dimensional bubble was generated in a fluid domain by assigning an initial density profile. The fluid domain was 51x51x51 lattice units (lu) in size and the bubble radius was 15 lu. The surface tension was imposed as an input parameter. The density ratio was set to 1.11 and the viscosity ratio between the fluids was 1.11. This test case was performed for demonstration of the effect of surface tension on the bubble shape. As seen in Figure 1, the interfacial tension on the bubble tends to minimize the surface area of the bubble and a spherical bubble shape is obtained as time progresses in the simulation.



(a) T = 0 (b) T = 200



(c) T = 500 (d) T = 1000

Fig 1. Evolution of a initially cubical bubble during time into a spherical bubble due to the effect of surface tension (T is given in dimensionless lattice time units).

In order to validate the implementation of the surface tension, the initial condition was changed to a spherical bubble at a fixed radius with imposed surface tension and an initial pressure distribution. The initial conditions were set to have density and viscosity ratios of 100 between the two fluids. The initial pressure field in the fluid domain was uniform; however, as the system converged to an equilibrium state, a pressure difference between the fluid domain and the gas domain was created. The relaxation of the interface between the two fluids was tested against the Laplace's law that expresses the pressure difference between the inside and the outside of a bubble as a function of the surface tension and the radius as given in two-dimensions by, $\Delta \; = \; /$. The difference of pressure between the inside and the outside of the bubble, P_{diff}, was computed at every time step and the relative error against the exact value is calculated as, $= (\; - \Delta \;)/\Delta$. The convergence of was measured at every 10 iterations by $(\;) = (\; (\;) - \; (\; - 1))$ and the simulation was assumed to converge to a steady state result when $= 0.1 \sum \; (\;) < 0.05$.

Fig 2 shows the calculated pressure difference across the fluid interface for various bubble radii. The slope of the linear curve fit to the data provides the obtained surface tension value from the simulations. It was found that an error of 1.5 % - 9.6 % was obtained for the calculated pressure difference as compared to the analytical solution.

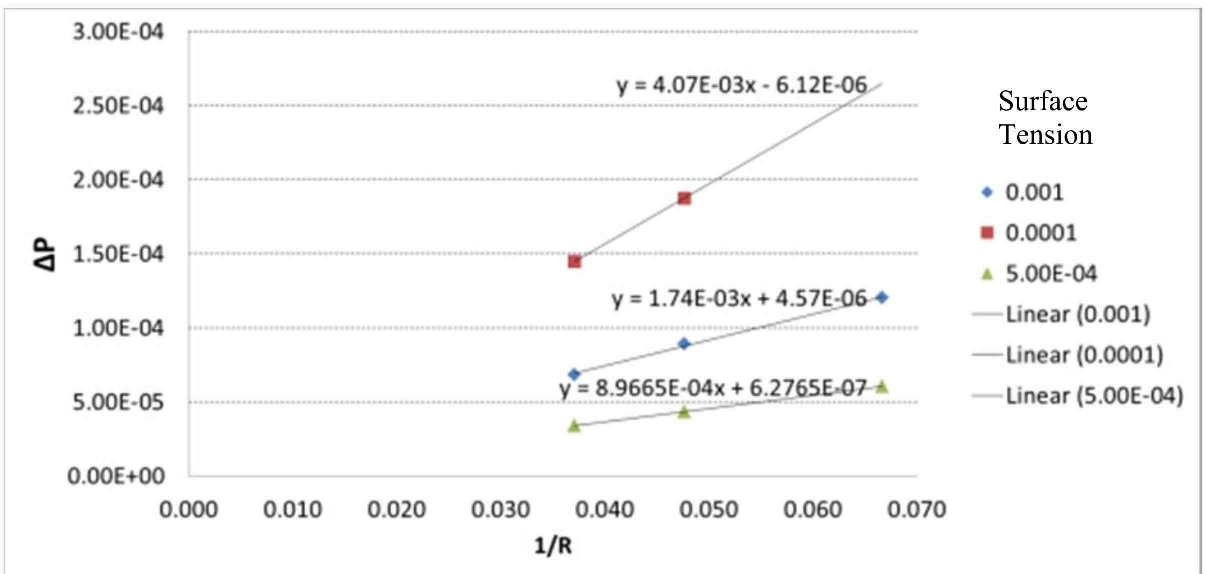
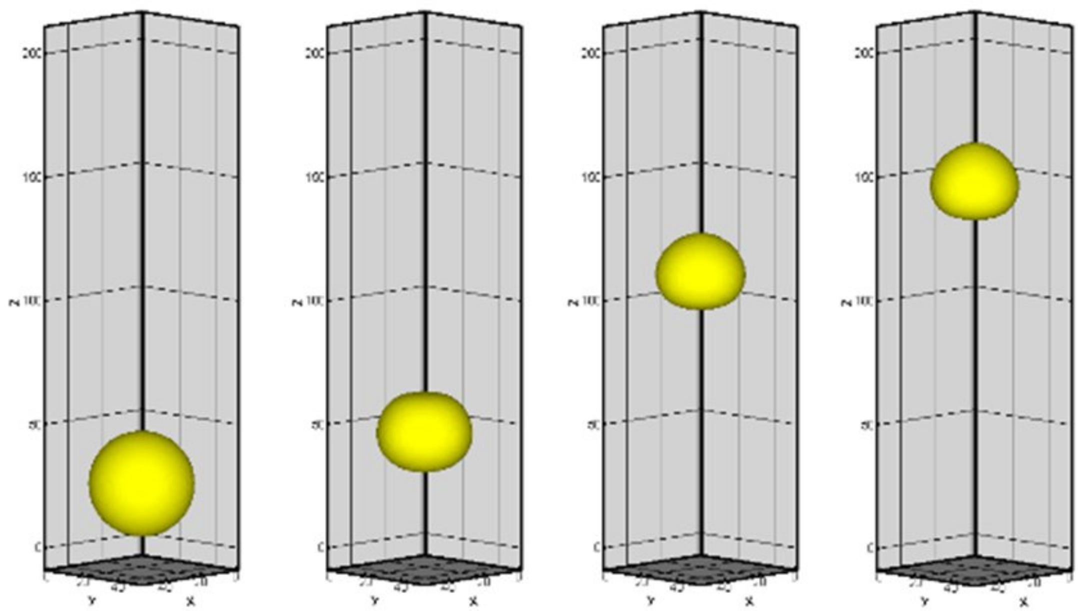


Fig 2. Pressure difference across the bubble as a function of radius for different values of surface tension (given in dimensionless units).

The LBM was verified for static bubble cases where the buoyancy force applied on the bubble was ignored however the effect of the gravity should be considered when using computer simulations to solve the engineering problems related to DOE waste handling operations. Therefore the LBM is expected to be applicable to such cases where the buoyancy force applied on the gas phase should be considered. In order to evaluate whether the LBM used in this study can successfully simulate multiphase flows with external body forces such as gravity applied on one phase of the system, a preliminary test case was simulated for a dynamic bubble moving under the effect of a buoyancy force. The fluid domain was 51x51x201 lattice units (lu) in size and the bubble radius was 20 lu. The surface tension was imposed as an input parameter (σ=0.0001). The density ratio was set to 4 and the viscosity ratio between the fluids was 4. Periodic boundary conditions were applied at all sides of the computational domain. The gravitational force was applied by modifying the macroscopic velocity and evolution equations with the additional buoyancy force term, – Δ . Fig 3 shows the shape evolution of the spherical bubble during the rising process. As expected the shape of the bubble changes due to the surrounding fluid as it rises in the vertical direction and an ellipsoidal bubble shape is obtained. Although this analysis needs to be verified against benchmark solutions, the preliminary results obtained using LBM for buoyant 3D bubbles are encouraging and suggest that the proposed multiphase LBM presented in this paper can be useful for multiphase systems with moving discrete phases.



T = 0 T = 10000 T = 20000 T = 22500

Fig 3. 3D Multiple Relaxation Time LBM simulation for the evolution of a rising bubble (T= dimensionless lattice time units).

CONCLUSIONS AND FUTURE WORK

In this paper, the implementation of an Multiple Relaxation Time LBM based on the Lee and Lin multiphase model was presented for static and dynamic bubbles in three dimensional domains. Validation cases against analytical solutions for static bubble have been presented and the capability of the method to simulate dynamic interface tracking for a buoyant bubble rising problem has been shown. The numerical method based on a multiphase LBM established with this research effort were able to provide promising preliminary results. However, further analysis of the accuracy of the method needs to be performed and the validation of the dynamic bubble simulations with appropriate wall boundary conditions to simulate flows in closed domains will follow as future work.

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