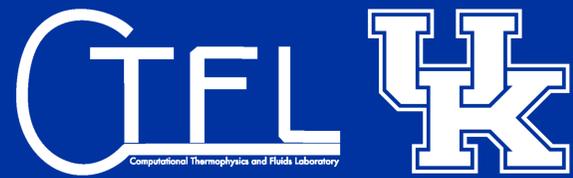# A framework to capture phase-change of atmospheric ice particles in hypersonic flows

Carlos E. Americo (ceam223@uky.edu), Ethan H. Huff, and Savio J. Poovathingal (saviopoovathingal@uky.edu)

Department of Mechanical and Aerospace Engineering, University of Kentucky, Lexington, KY, 40506, USA.
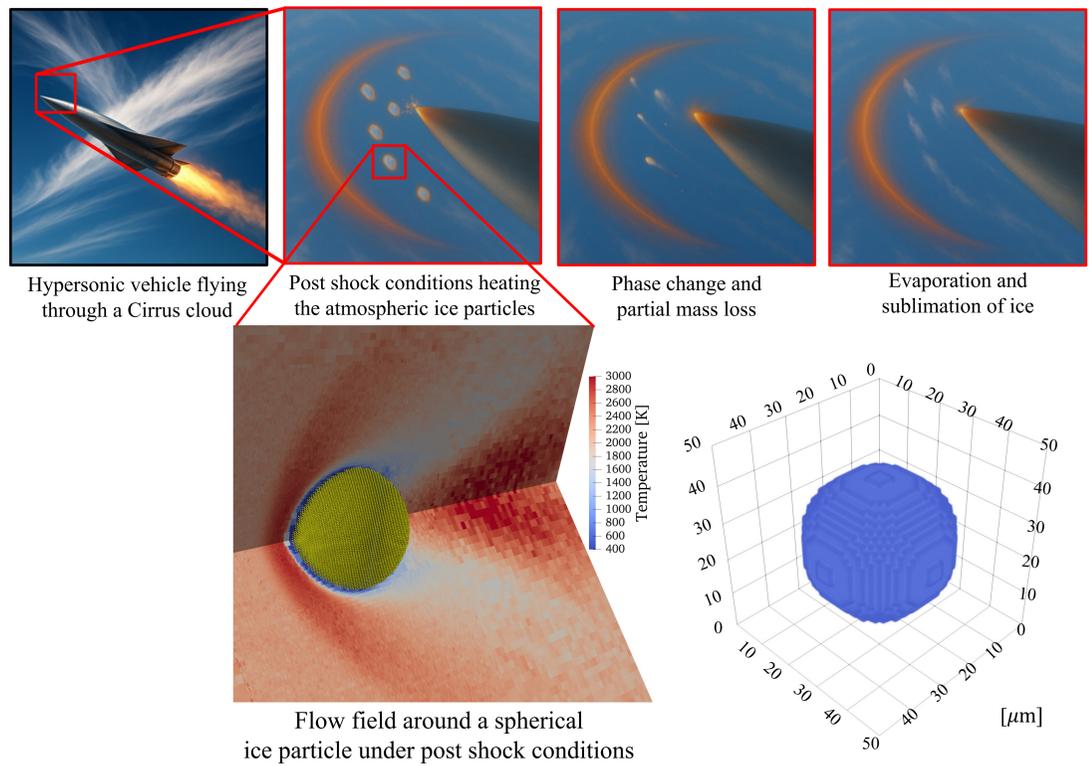
Introduction

The presence of residual metallic molecules originating from decommissioned spacecraft components, mineral dust from deserts, and meteorites are responsible for ice nucleation within the atmosphere of Earth, growing mainly by water vapor deposition. Atmospheric ice formation is dynamic and happens on hourly time scales. The process of ice crystallization happens in distinct shapes, such as hexagonal and plate-like geometries.

At hypersonic velocities, surfaces that receive high-velocity impingement can suffer plastic deformation when constantly exposed to impacts. For any hypersonic vehicle flying at the same altitude as Cirrus clouds, the ice particles become a naturally formed obstacle, interacting with the post-shock environment. One of the possible post-shock scenarios for the ice particle is a partial or total mass loss caused by phase-change processes. Numerical analyses that address these phase-change processes (including melting and evaporation processes) are being conducted to quantify the thermal-fluid response of ice particles. The unified numerical fluid-thermal framework called LBM is capable of compute the phase-change processes of ice particles of any shape is being developed. The framework quantify the melting by the total enthalpy-based lattice Boltzmann model (ELBM), and the fluid flow is calculated using the direct simulation Monte Carlo (DSMC) method.

Results obtained by the LBM framework are compared with results obtained by the OLB framework, which is a modified version of the open source OpenLB code, which was verified by analytical formulations for temperature for a longer 3D-1D slab case (Figure 1, and Figure 3). The comparisons for the numerical temperature distributions between frameworks are shown by Figure 2, and Figure 4.

Hypersonic vehicle flying through a Cirrus cloud

Post shock conditions heating the atmospheric ice particles

Phase change and partial mass loss

Evaporation and sublimation of ice

Flow field around a spherical ice particle under post shock conditions

Methods and framework

Melting is calculated by the ELBM numerical scheme, where the collision term is modeled using a two-relaxation-time (TRT) model for the enthalpy equation.

$$\partial_t \left(\rho_0 C_p T\right) + \nabla \cdot \left(\rho_0 C_p T \mathbf{u}\right) = \nabla \cdot (\lambda \nabla T) - \partial_t \left(\rho_0 L f_l\right) - \nabla \cdot (\rho_0 L f_l \mathbf{u})$$

$$\frac{\partial (\rho H)}{\partial t} = -\nabla \cdot \left(\rho c_p T \boldsymbol{u}\right) + \nabla \cdot (\lambda \nabla T)$$

$$g_i^*(\mathbf{x},t) = g_i(\mathbf{x},t) - \frac{\Delta t}{\tau_g^+}\left(g_i^+(\mathbf{x},t) - g_i^{eq+}(\mathbf{x},t)\right) - \frac{\Delta t}{\tau_g^-}\left(g_i^-(\mathbf{x},t) - g_i^{eq-}(\mathbf{x},t)\right)$$

$$g_i^{\text{eq}} = \begin{cases} H - C_{p,ref}T + \omega_i C_p T\left(\frac{C_{p,ref}}{C_p} - \frac{\mathbf{I:uu}}{2c_s^2}\right), & i = 0 \\ \omega_i C_p T\left[\frac{C_{p,ref}}{C_p} + \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_i\mathbf{e}_i - c_s^2\mathbf{I}):\mathbf{uu}}{2c_s^4}\right], & i \neq 0 \end{cases}$$

$$T = \begin{cases} T_s - \frac{H_s - H}{C_{p,s}}, & H \leq H_s \\ \frac{H_l - H}{H_l - H_s}T_s + \frac{H - H_s}{H_l - H_s}T_l, & H_s < H < H_l \\ T_l + \frac{H - H_l}{C_{p,l}}, & H \geq H_l \end{cases}$$
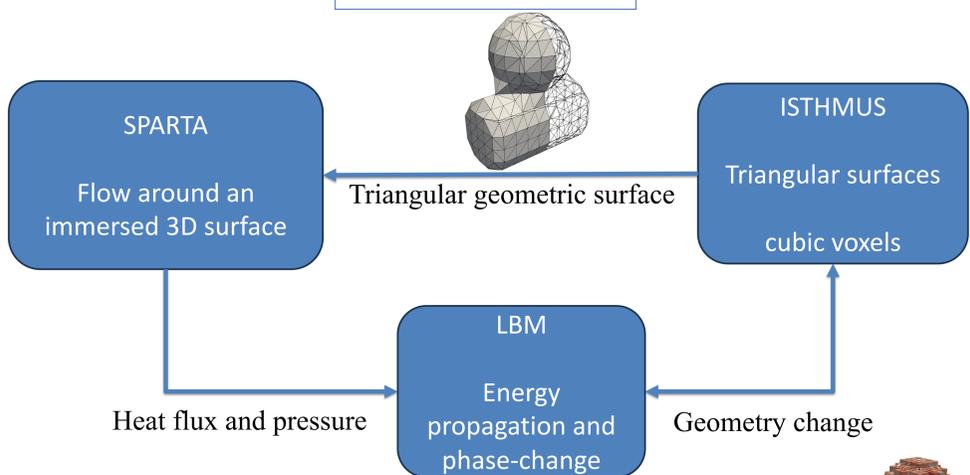
To create a unified framework between the ice particle and the fluid flow domain, the ELBM solver melts the ice particle, and the flow field is generated by an open-source code developed at Sandia National Laboratories called SPARTA, modified at the University of Kentucky, where the flow field around the ice particle imposes the boundary conditions for the ELBM framework.

The numerical results are compared to analytical solutions for the temperature profile of a two-phase melting problem, as well as the interface between phases (given below)
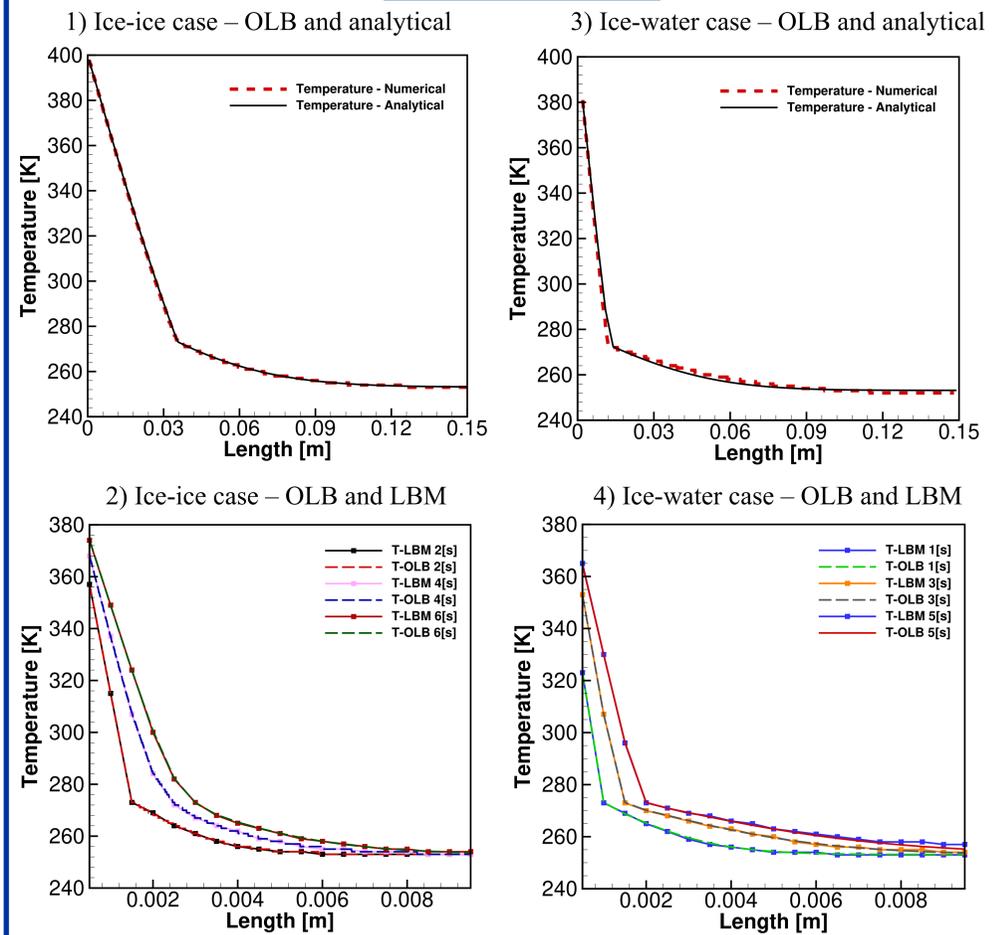
$$T(\mathbf{x},t) = \begin{cases} T_h - \frac{T_h - T_m}{\text{erf}(k)}\,\text{erf}\left(\frac{x}{2\sqrt{\lambda_l/(\rho_0 C_{p,l})\,t}}\right), & 0 \leq x \leq X_i(t)\ \text{(liquid)}, \\ T_0 + \frac{T_m - T_0}{\text{erfc}\left(k/\sqrt{R_\alpha}\right)}\,\text{erfc}\left(\frac{x}{2\sqrt{\lambda_s/(\rho_0 C_{p,s})\,t}}\right), & x > X_i(t)\ \text{(solid)}, \quad X_i(t) = 2k\sqrt{\lambda_l/(\rho_0 C_{p,l})\,t} \end{cases}$$

$$\frac{Ste_l}{\exp\left(k^2\right)\text{erf}(k)} - \frac{Ste_s\sqrt{R_\alpha}}{\exp\left(k^2/R_\alpha\right)\text{erfc}\left(k/\sqrt{R_\alpha}\right)} = k\sqrt{\pi}$$

Numerical scheme

SPARTA — Flow around an immersed 3D surface

Triangular geometric surface

ISTHMUS — Triangular surfaces — cubic voxels

LBM — Energy propagation and phase-change

Heat flux and pressure

Geometry change

Results

1) Ice-ice case – OLB and analytical

- Temperature - Numerical
- Temperature - Analytical

3) Ice-water case – OLB and analytical

- Temperature - Numerical
- Temperature - Analytical

2) Ice-ice case – OLB and LBM

- T-LBM 2[s]
- T-OLB 2[s]
- T-LBM 4[s]
- T-OLB 4[s]
- T-LBM 6[s]
- T-OLB 6[s]

4) Ice-water case – OLB and LBM

- T-LBM 1[s]
- T-OLB 1[s]
- T-LBM 3[s]
- T-OLB 3[s]
- T-LBM 5[s]
- T-OLB 5[s]

Conclusions

Four cases were analyzed to examine the influence of thermophysical properties on the phase-change process. In the first and second cases, the liquid and solid domains have the same thermophysical properties, fixed for ice. The third and fourth cases are analogous to the first case; however, each phase has its actual thermophysical values for ice and liquid water, called the ice-water cases. The first and third had their temperature profiles, and the interface between phases is compared against analytical predictions, showing a good agreement for both temperature profile and interface position, despite small fluctuations when mixing thermophysical properties is considered.

Cases two and four also show the temperature profile for the phase-change process. Here, only the numerical solutions obtained by both frameworks are compared against each other, showing a good agreement for multiple timestamps.

Future work

With the correct marching of the solid-liquid interface and the temperature profile, the next step is to account for additional energy absorption for the evaporation process. Future work will focus on integrating the Nusselt-Langmuir method into the current framework, allowing the consumption of voxels and the dynamic allocation of boundary conditions appropriate for changing geometries.

Acknowledgments