RECENT DEVELOPMENTS OF THE MULTI-PHYSICS SOLVER
CHAMPS-ICE

Mohamad Karim Zayni, Maxime Blanchet, Éric Laurendeau
Mechanical Engineering, Polytechnique Montréal, Montréal, Québec, H3T 1J4, Canada

Abstract—This paper presents recent improvements in CHAMPS (Chapel Multi-Physics Software) developed at Polytechnique Montréal with emphasis on the aero-icing capabilities. This software, written in the Chapel language, is designed to simulate two-dimensional and three-dimensional multi-physics phenomena involving aerodynamics such as ice accretion and fluid-structure interactions through an Unstructured Finite-Volume Unsteady Reynolds-Averaged Navier-Stokes (URANS) realm. It is programmed using the open-source Chapel language, which facilitates parallel computing on laptops, desktops and High-Performance Computing (HPC) platforms. The basic approach to model ice shapes involves several modules with a segregated strategy: aerodynamic, droplet, thermodynamic and geometric. Four newly implemented state-of-the-art features expand the aero-icing suite, CHAMPS-ICE. A first feature is the implementation of a transitional turbulence model to enhance the physical representation of the boundary layer state near the airfoil (1). Furthermore, a local ice roughness model is added (2) to properly quantify the position of the laminar-turbulent transition which influences the surface convective heat transfer. As for the droplet module, it considers the first and second-order effects of Supercooled Large Droplets (SLD) such as droplet splashing and deformation (3). This extension brings the collection efficiency amplitude and impingement limits closer to experimental data. Another development addresses the stochasticity of the ice accretion process using an advancing front technique (4). Those newly implemented features are discussed and validated on 2D and 3D rime and glaze ice cases taken from the American Institute of Aeronautics and Astronautics (AIAA) Ice Prediction Workshops and the European Ice Genesis project.

Keywords-component—Computational Fluid Dynamics; Aircraft Icing

I. INTRODUCTION

In the last years, a growing amount of research has been devoted to in-flight ice accretion. Aircraft icing usually occurs when aircraft fly through a low-temperature moist cloud. When the unfrozen water droplets hit the aircraft, and if the thermal conditions are right, this promotes ice accumulation on the vulnerable wet surfaces of the aircraft [1]. This phenomenon is of interest because it might affect the aerodynamic configuration of the aircraft and thus, the safety of the flight. In America, from 1990 to 2000, 12% of all aircraft accidents caused by severe weather conditions were related to ice accretion [2]. Polytechnique Montréal is devoted to the numerical simulation of these phenomena, which play a key role in the certification of an aircraft, as it is not always possible to predict the ice shapes foreseen by the conditions of the FAR part 25 Appendix C [3] with in-flight or wind tunnel tests.

Ice accretion is a complex multi-physical phenomenon. It involves computing the airflow around an aircraft, the impingement of the supercooled water droplets on the geometry, the thermodynamic exchanges and the ice growth. Numerical simulations are performed using an unstructured RANS software named CHapel Multi-Physics Simulation (CHAMPS-ICE) [4]. The latter is programmed using the Chapel programming language [5] and uses a cell-centered finite volume approach. This paper presents the aero-icing suite CHAMPS-ICE while underlining the key features recently implemented. The following section presents an overview of the CHAMPS-ICE’s ice accretion workflow. Section III describes the transitional and turbulence models used to compute the airflow. Section IV continues with an overview of the droplet solvers used in CHAMPS-ICE. It is followed by the introduction of the local roughness model used in the thermodynamic module in Section V. The implementation of a stochastic advancing front technique is featured in Section VI.
II. CHAMPS-ICE’S ACCRETION PROCESS

The ice accretion process is divided into five main stages. Each can be simulated individually in a steady state using the quasi-steady nature of ice accretion [6]. The multi-layer process is illustrated in Figure 1. First, the continuous phase of the fluid is simulated. The airflow is the main driver for the droplets impingement, the convective heat transfer, and the water runback on the aircraft geometry [7]. CHAMPS-ICE uses a state-of-the-art RANS solver to compute the airflow around the geometry. It is capable of modeling compressible effects in addition to viscous and turbulent mechanisms. The dispersed phase of the droplets is then transported by the previously simulated airflow. The droplet impingement map is a key element for the ice accretion process. Droplet trajectories can be modeled by two means. A Lagrangian method that solves the equation of motion for each droplet individually [8] and an Eulerian method that solves partial differential equations considering the dispersed phase as a continuous one [9].

Once the droplet impingement map is obtained, and the convective heat transfer is prompted by the airflow, thermodynamic exchanges are computed on the surface of the geometry. The resolution mainly involves balancing mass and momentum exchanges which can be set as decaying turbulence. For a laminar-turbulent purpose, both models can be coupled with the $\gamma - \tilde{Re}_{\theta t}$ extension developed by Langtry and Menter [17]. The model uses the intermittency $\gamma$ to control the production of turbulence in the boundary layer. The intermittency is triggered by the transition momentum thickness Reynolds number $\tilde{Re}_{\theta t}$. The turbulence model is used only in turbulent regions, i.e. when $\gamma$ is superior to zero. The two additional transport equations are given below:

$$\frac{\partial \gamma}{\partial t} + u_j \frac{\partial \gamma}{\partial x_j} = P_\gamma - E_\gamma + \frac{\partial}{\partial x_j} \left[ \left( \frac{\mu + \mu_t}{\sigma_f} \right) \frac{\partial \gamma}{\partial x_j} \right]$$  \hfill (2)

$$\frac{\partial \tilde{Re}_{\theta t}}{\partial t} + u_j \frac{\partial \tilde{Re}_{\theta t}}{\partial x_j} = P_{\theta t} + \frac{\partial}{\partial x_j} \left[ \sigma_{\theta t} (\mu + \mu_t) \frac{\partial \tilde{Re}_{\theta t}}{\partial x_j} \right]$$  \hfill (3)

The production terms and the boundary conditions are given in [17]. The turbulence intensity is computed with the following equation for the $k\omega\gamma - \tilde{Re}_{\theta t}$ model:

$$Tu = 100 \frac{\sqrt{2k/3}}{U}$$  \hfill (4)

where $k$ is the turbulence kinetic energy and $U$ is the norm of the local flow velocity. Whereas it is assumed to be constant for the $SA$ turbulence model. The implementation of such transition models enables the reduction of the skin friction coefficient, and thus of the heat transfer coefficient for the laminar region near the stagnation point. The effect on the predicted ice shapes will be discussed in Section V.

III. TRANSITIONAL TURBULENCE MODELS

The convective heat transfer at the wall contributes tremendously to the icing process. It is a crucial term in the energy balance previously discussed. However, it is a difficult task to correctly model these thermodynamic exchanges. In order to do so, the convective heat flux at the wall can be obtained from the laminar viscosity ($\mu$) and the turbulent eddy viscosity ($\mu_t$) normally computed in RANS codes:

$$\dot{Q}_{wall} = c_p \left( \frac{\mu_t}{Pr_t} + \frac{\mu}{Pr_l} \right) \frac{\partial T}{\partial n} \bigg|_{wall}$$  \hfill (1)

where the term $\partial T/\partial n$ is determined using the temperature gradient. The ratio of momentum diffusivity to thermal diffusivity varies in the viscous sublayer. The values are normally assumed to be $Pr_l = 0.9$, which is the value in the logarithmic region [14] and $Pr_r = 0.707$. The convective heat flux is influenced by the state of the boundary layer and how accurately the latter is modeled. Therefore, the implementation of specific transitional and turbulence models can enhance the accuracy of the already existing workflow. SA [15] and SST [16] turbulence models are implemented in CHAMPS-ICE. The former provides high accuracy, though it is a computationally expensive scheme. The SST model is more accurate for shear and separated flows as well as decaying turbulence. For a laminar-turbulent purpose, both models can be coupled with the $\gamma - \tilde{Re}_{\theta t}$ extension developed by Langtry and Menter [17]. The model uses the intermittency $\gamma$ to control the production of turbulence in the boundary layer. The intermittency is triggered by the transition momentum thickness Reynolds number $\tilde{Re}_{\theta t}$. The turbulence model is used only in turbulent regions, i.e. when $\gamma$ is superior to zero. The two additional transport equations are given below:

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$$\frac{\partial \tilde{Re}_{\theta t}}{\partial t} + u_j \frac{\partial \tilde{Re}_{\theta t}}{\partial x_j} = P_{\theta t} + \frac{\partial}{\partial x_j} \left[ \sigma_{\theta t} (\mu + \mu_t) \frac{\partial \tilde{Re}_{\theta t}}{\partial x_j} \right]$$  \hfill (3)

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IV. DROPLET SOLVER

A droplet impingement map, necessary for the assessment of the ice accretion is obtained through the droplet trajectories. This can be achieved with two approaches: Lagrangian and Eulerian. A Lagrangian method solves the equation of motion for each particle individually and can be used as stipulated in Eq. (5) [8]:

$$\frac{du}{dt} = \frac{f}{m} + g = F(v - u) + g$$  \hfill (5)

where $v$ is the flow velocity, $u$ is the droplet velocity and $f$ is the exerted force on the droplet. This source term considers the drag force due to the fluid flow and the gravity term due to the droplet mass. The scalar function $F$ can be found using the droplet local Reynolds number based on the relative velocity $||v - u||$ and the droplet diameter. This leads to a force coefficient:

$$F = \frac{C_D \frac{1}{2} \rho ||v - u||^2 A}{m ||v - u||} = \frac{3C_D \rho ||v - u||}{4 \rho_w D}$$  \hfill (6)
where $C_D$ is the drag coefficient of the droplet, $\rho_a$ is the air density, $\rho_w$ is the water density and $D$ is the droplet diameter. The computational cost of such a method is significant. CHAMPS-ICE uses the approach in [8], which relies on the mesh used for the airflow in order to compute the droplet trajectories based on the nearest facet intersection of a fluid cell. Therefore, it makes the computations more efficient. An eulerian approach considers the dispersed phase as dense enough that can be modeled as a continuous phase [9]. Thus, the RANS mesh used for the fluid flow can be reused for the droplet trajectories, extending by the process any parallelism done for the flow solver. The governing equations for the conservation of mass and momentum of the droplets are written in Eq. (7):

$$\begin{align*}
\frac{\partial \rho_a}{\partial t} + \nabla \cdot (\rho_a \mathbf{u}) &= 0 \\
\frac{\partial \rho_w}{\partial t} + \mathbf{u} \cdot \nabla \rho_w &= C_D \frac{Re_a}{24K} (\mathbf{v} - \mathbf{u}) + \left(1 - \frac{\rho_w}{\rho_a}\right) \frac{1}{Fr} g
\end{align*}$$

(7)

where $\alpha$ is the non-dimensionalized volume fraction of water, $Fr$ is the Froude number based on the chord length and $K$ is the inertia parameter. CHAMPS-ICE extends both methods to account for the first and second-order effects of supercooled large droplets (SLD) according to [18]. This relies purely on semi-empirical formulations that adjust the droplet trajectories and the mass loss due to impact. Droplet deformation is considered by modifying the drag coefficient formulation of Eq. (8). Typically, droplets are assumed to have a perfectly spherical shape, which is true for small droplets. However, [19] shows that large droplets witness a deformation due to the inertial forces applied by the fluid flow. This can be modeled by assuming a combination of a spherical-shape drag coefficient and a disk-shape drag coefficient. The weight $\epsilon$ is calculated based on the local Reynolds and Weber numbers.

$$C_D = (1 - \epsilon)C_{D, sphere} + \epsilon(C_{D, disk})$$

(8)

Droplet's bouncing, splashing and rebound are complex phenomena that occur for large droplet impacts. Modeling the interface of the droplet upon impact is complicated and needs large computational assets. Current models tend to extract semi-empirical formulations from experimental data [18]. These models are based on the normal component of the droplet impact velocity and the angle of impact. CHAMPS-ICE uses two approaches. The first approach is proposed by [20], defining the sticking rate $\epsilon$:

$$\epsilon = g\left(\frac{\theta}{\theta_c}\right)f\left(\frac{K_n - K_0}{K_0}\right)$$

(9)

where $\theta$ represents the impact angle, $\theta_c$ is a critical angle computed based on the capillary number of the droplet, $K_n$ is the Cossali number and $K_0$ is the threshold between full deposition and splashing regime. A second definition is used in LEWICE 3.2 [21]:

$$\epsilon = 1 - 0.7(1 - \sin(\theta_0))(1 - e^{-0.0992(K_{L,n}-200)})$$

(10)

where $\theta_0$ is the impact angle and $K_{L,n}$ is the normal component of the splashing onset. This affects directly the collection efficiency $\beta$ of the geometry for the droplets upstream:

$$\beta = \frac{\epsilon}{(1 - \epsilon) dy/\epsilon}$$

(11)

with $\epsilon = 1$ meaning that the droplet is fully deposited on the geometry. Employing these approaches have a significant impact on the computed collection efficiency, by bringing its amplitude and limits closer to the experimental data. This is illustrated in Figure 2 when comparing experimental results from [22] on a NACA23012 case. Without considering SLD effects (Figure 2a), the computed collection efficiency is significantly higher than the experience. Using Eq. 9 (Figure 2b) tends to underpredict the $\beta$ at the stagnation point but manages to depict more accurately the regions near the limits of impingement. It is the opposite case for Eq. 10 as shown in Figure 2c.

V. LOCAL ROUGHNESS

The eddy viscosity can be enhanced by the surface roughness in the flow solver. The aim is to have a heat transfer that increases when the surface roughness does, to improve the accuracy of the predicted ice shapes. Ice accretion has a great influence on the roughness of the surface depending on the type of ice being formed. Glaze ice is distinctly hard to predict because not all impinging droplets freeze upon impact. Since the heat transfer is not sufficient, the unfrozen water film tends to run back from the stagnation point and freezes forming a horn shape. The roughness on the surface can be linked mainly to beads and rivulets growing or being torn on the surface. The roughness is minimal in
the film region, and increases in the beads/rivulets region [23]. Considering the lack of experimental data on ice surface roughness, a global roughness entry is usually imposed on the considered geometry. However, this single value cannot capture the non-homogeneous nature of ice roughness. For hydrodynamically rough surfaces, the roughness height increases the shear stress at the wall. Therefore, a correction needs to be applied in the turbulence models. Typically, RANS codes take into account the equivalent sand grain roughness, as proposed by Nikuradse [24]. The challenge remains to transform the surface roughness into a sand grain equivalent roughness. Many methods ([25]–[30]) have been developed to provide an approximate of the global roughness, but they are not enough to define the ice roughness and do not hold in 3D cases. The ice shape may not be accurately predicted by the process. Consequently, local roughness models are a great addition for computing accurately the heat convective transfer.

CHAMPS-ICE employs a model proposed by McClain [31]. The root-mean-square of the roughness scale (mean deviation of the roughness height) is presented in Eq. (12).

\[
R_q = \frac{LWC \cdot U \cdot \Delta t_{\text{ice}}}{\rho_{\text{ice}}} \beta(0.7(1.0 - C_p)) \left( 0.34 + \frac{\Delta T_{\text{ice}}^2}{T_{S}^2} \right)
\]  

where \(LWC\) is the liquid water content, \(U\) is the freestream air velocity, \(\Delta t_{\text{ice}}\) is the accretion time, \(\rho_{\text{ice}}\) is the ice density, \(\beta\) is the collection efficiency, \(C_p\) is the local pressure coefficient, \(T_S\) is the stagnation supercooling temperature. Eq. (13) is proposed by McClain to include the local freezing fraction \(n\).

\[
R_q = n \frac{LWC \cdot U \cdot \Delta t_{\text{ice}}}{\rho_{\text{ice}}} \beta(0.7(1.0 - C_p)) \left( 0.34 + \frac{\Delta T_{\text{ice}}^2}{T_{S}^2} \right)
\]  

Finally, the correlation from Flack and Schultz [32] can be used to obtain the equivalent sand grain roughness used in most of the turbulence models as seen in Eq. (14). They linked the mean deviation of the roughness height with the skewness of the roughness elevation, \(s_k\), which is assumed to be zero because of the lack of information on its value.

\[
K_s = 4.43R_q \cdot (1 + s_k)^{1.37}
\]

Those local roughness correlations can be combined with the turbulence and transition models. When a transition model is used, an additional transport equation is employed to consider the effect of the roughness on the upstream shift of the transition location [33]. In this work, the effects of the integration of the diverse models are studied in comparison with experimental data generated in the NASA IRT [34]. The differences between the computed results and the experimental ice shapes are assessed. The airfoil used is a NACA0012 with a \(385 \times 257\) 2D O-grid mesh. Multiple experimental data at several spanwise sections are collected for the test case. A monodispersed droplet size distribution is used. The angle of attack is \(0^\circ\), the chord is \(0.5334\) m, the freestream velocity is \(102.8\) m/s, the LWC is \(0.55\) g/m³, the MVD is \(20\) µm and the icing time is 7 minutes. Figure 3 shows the ice shape comparison between the different roughness and turbulence models when Eq. (13) is employed for the local roughness model.

In Figure 3, the IRT experiments are illustrated by the dotted curve. Using the transitional model (orange and green curves) moves the horns away from the stagnation point. The effect is complemented by the use of the local roughness model, which computes a low roughness value near the stagnation point and increases it in the horn region. By doing so, the predicted ice shapes are in better agreement with the experimental values. Figure 4 illustrates the comparison between the local roughness models of Eq. (12) (identified as 1) and Eq. (13) (identified as 2). As anticipated, using Eq. 13 creates horns closer to the stagnation point because the value of the freezing fraction is close to zero in this region. The results are farther from the experimental data.

VI. STOCHASTIC ICE ADVANCING FRONT

Ice accretion is chaotic in nature. The deterministic approach previously presented cannot capture small morphologies (e.g. rime ice feathers) or even strong ice morphologies...
Figure. 3: Ice shapes obtained for the NASA IRT case 403 with the SA turbulence and transition models, comparison of the global and local roughness models (6 layers, $k_s/c = 600 \mu$)

Figure. 4: Ice shapes obtained for the NASA IRT case 403 with the SA turbulence and transition models, comparison of the local roughness models (6 layers, $k_s/c = 600 \mu$)

(e.g. scallops formation on swept wings). The continuous nature of the model limits the evolution of the ice front developing on the geometry. Hence, a non-deterministic approach is needed. CHAMPS-ICE stochastic model features an unstructured advancing front technique. The mesh is dynamically created by generating triangular (or tetrahedral) elements based on the impact positions of the droplets. Droplets are randomly seeded from a plane upstream. They are gathered in clusters in order to reduce the computational cost. Droplet trajectories are then extracted from the Eulerian droplet velocity field via the streamline technique proposed by [8]. Upon impact, and if the freezing fraction is equal to unity, the cluster completely freezes and a new element of ice is generated. If not, the remaining mass moves downstream on the iced geometry. These steps are repeated until the targeted mass of accumulated ice is reached. Stochasticity is introduced via the random insertion of the cluster in the computational domain. The initial position is generated using a pseudo random number on the seeding plane. The diameter of the cluster is obtained randomly from the droplet size distribution. The ice elements are generated successively via an unstructured advancing front technique based on the methodology proposed by [35]:

1) The initial front is formed using the boundaries of the geometry. It is then uniformly discretized rather than using the RANS non-uniform surface distribution. This allows a more precise control of the size of the newly generated element. The order of treatment is defined using the intersection between the trajectory of the impinging cluster of droplets and the active front.

2) A front facet is then selected to generate a new element based on already existing front nodes or newly created ones. The created element must be validated by checking intersections with existing elements. If it is the case, new front nodes must be created.

3) The initial front is then updated by removing the current facet and adding the newly created ones.

4) The previous steps are repeated until there is no more facets to be treated.

As shown in Figure 5, the stochastic model helps to represent ice feathers in the lower region, which could not be achieved using only one layer and the standard node displacement technique. However, no ice horns can be specifically identified using the stochastic model and no blatant distinctions can be identified using or not the transitional and roughness models. In [36], ice horns are predicted for other icing cases.
CONCLUSION

In this paper, improvements in the multi-layer icing framework of CHAMPS-ICE are presented. The use of Chapel language makes the framework of the code more flexible and easier to implement. The flow module is enhanced by adding the $\gamma - \tilde{R}_{\text{eff}}$ transition model. The latter has a direct effect on the heat transfer coefficient through the skin friction coefficient. It can be combined with a local roughness model in order to predict the state of the boundary layer. This has a strong effect on the position, orientation, and shape of horns developed under glaze conditions. First and second-order effects of supercooled large droplets are added to the droplet solver. The collection efficiency of water droplets takes into account the mass loss due to droplet’s bouncing, splashing and rebounding upon impact. The resulting collection is closer to experimental data for big droplets. Finally, a stochastic front advancing technique is presented. It is based on an unstructured advancing front technique. It enables the dynamic generation of new elements depending on the impinging positions of the randomly seeded cluster of droplets. This approach leads to obtaining different, less dense, ice shapes than the ones obtained via the traditional deterministic approach while capturing different ice morphologies.

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