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25th July 2018

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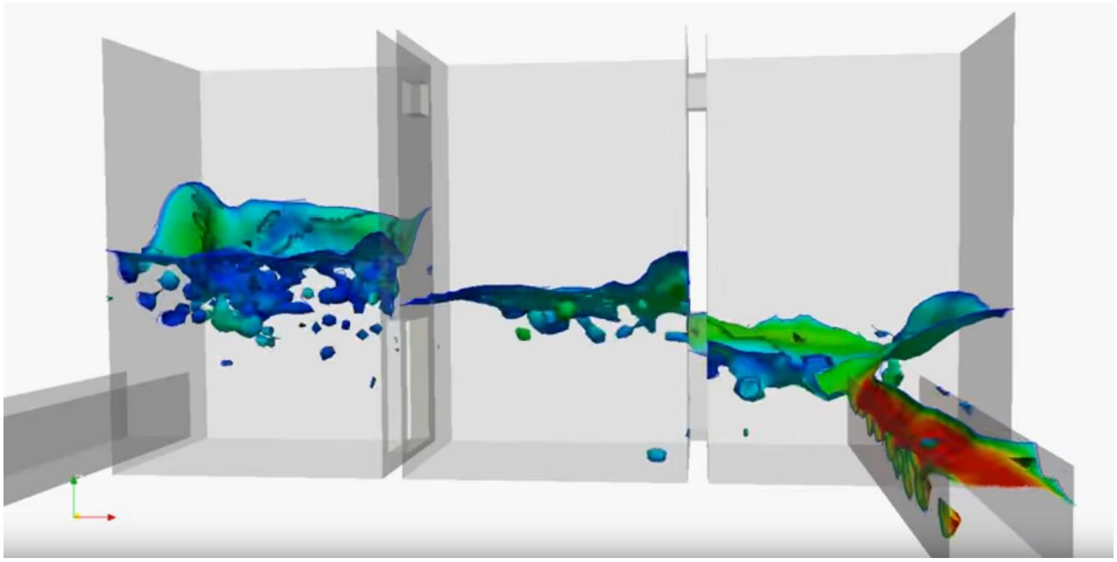
WHY Wildkatze Solver?
Volume of Fluid



This document gives few software insights regarding the VOF model. In our software, several interface tracking schemes are provided:

HRIC

The High Resolution Interface Capturing scheme (HRIC) is based on a blending of the Bounded Downwind and Upwind schemes (UD), with the aim of combining the compressive property of the DD scheme with the stability of the UD scheme.

CICSAM

The CISCAM scheme of Ubbink was formulated based on the idea of the donor-acceptor formulation such, that the discretization depends on the interface velocity direction and the angle it makes with the integration cell face. However, rather than choosing as base schemes, the downwind and upwind scheme, it blends between the ULTIMATE QUICKEST scheme of Leonard and the Hyper C scheme. The Hyper C scheme being used when the cell face is directed perpendicular to the interface normal vector and the ULTIMATE_QUICKEST scheme is used when the face normal vector is aligned with the normal to the interface.

The Upwind Cell Framework

The major drawback of unstructured grid implementation of various schemes is that the upwind cell is not available as compared to Cartesian grid solvers, where the upwind cell is always available.
It is noted that the construction of the upwind cell value plays a very important role for interface tracking accuracy. The situation is made worse, by the fact that in case of locally refined hexa-meshes or simply Cartesian meshes, this cell is there but never used by the solver.
To remove this drawback, Wildkatze has a framework, where solver can access this upwind cell and uses its exact value whenever possible. If it is not possible to exactly use this cell value, then the interpolation using this upwind cell values is used.
Note that it takes more memory and more parallel field exchanges to make these values available to the physics models.

HRIC U2

This is a HRIC implementation using the upwind cell values from upwind cell (from mesh) rather than calculating them by standard computation method of unstructured meshes.

CICSAM SHARPER

This is a version of CICSAM scheme, again the upwind cell values are from upwind cells from mesh and not from a virtual upwind cell.

Interface Capturing Enhancement

Is provided as “convection enhancement” option in the simulation tree for VOF model. For many applications where the interface has to be very sharp, the interface tracking provided by above mentioned schemes is not enough. For such applications **THINC** (Tangent of Hyperbola for Interface Capturing) scheme based on work of Yokoi Kensuke is provided.
This scheme is further enhanced by flux computed by one of the above mentioned schemes. Final flux to be used is then blended between the flux computed by **THINC** scheme and by one of the base schemes (HRIC, HRIC-U2, CICSAM, CICSAM-SHARPER).

THINC scheme due to its superior performance is suggested whenever possible to use. Since the interface is very sharp, this results in sharp change in density and viscosity. This could result in instability problems in some calculations. For this purpose, it is possible to limit the maximum fraction of THINC flux that is used.
Please consult **“Efficient implementation of THINC scheme: A simple and practical smoothed VOF algorithm”** by Yokoi Kensuke for details on THINC scheme.

Time stepping for VOF

Time integration is performed by following methods:

- **Explicit Euler**
- **Second Order TVD Runge Kutta**
- **Third Order TVD Runge Kutta**

Other than using one of the three methods user can further divide the time-step into multiple smaller inner steps. This is achieved by setting **inner-iterations** to a value more than 1.

Surface Tension

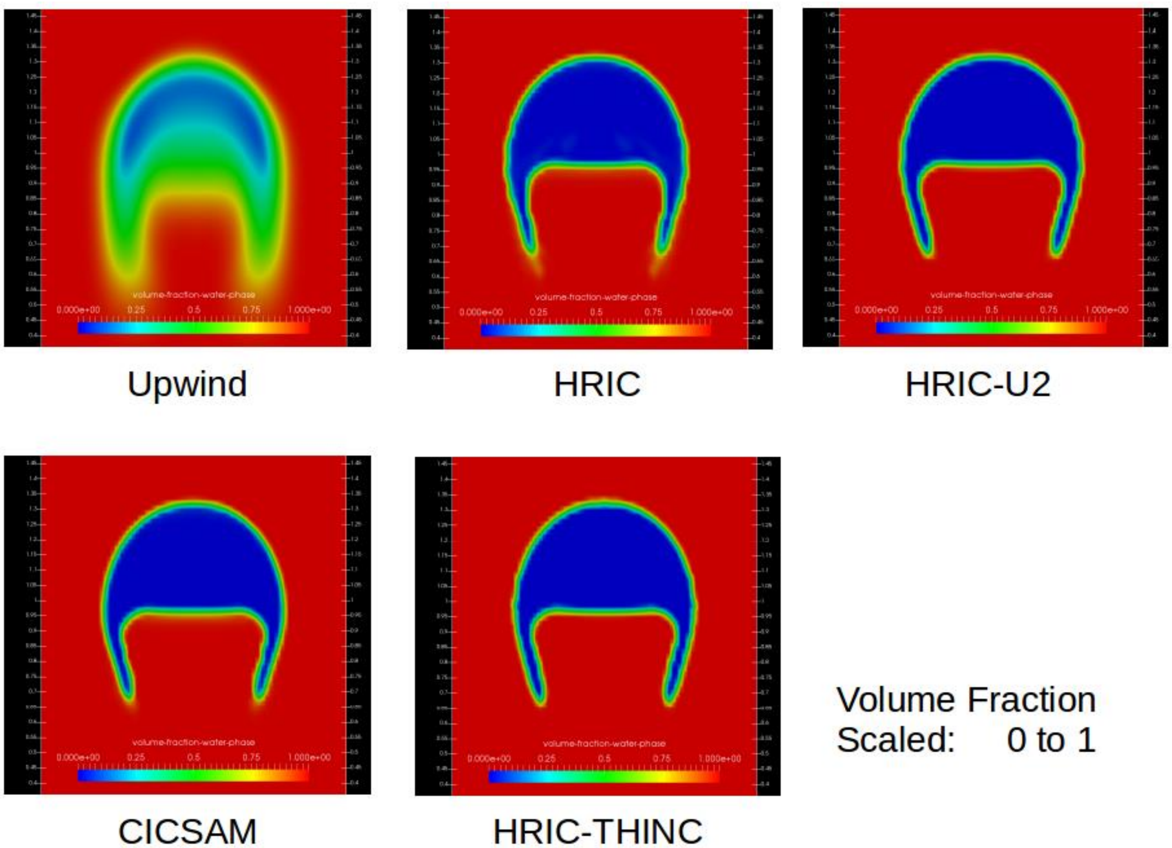
Surface Tension could be modeled by one of the two models provided:

- **Continuum Surface Stress**
- **Continuum Surface Force**

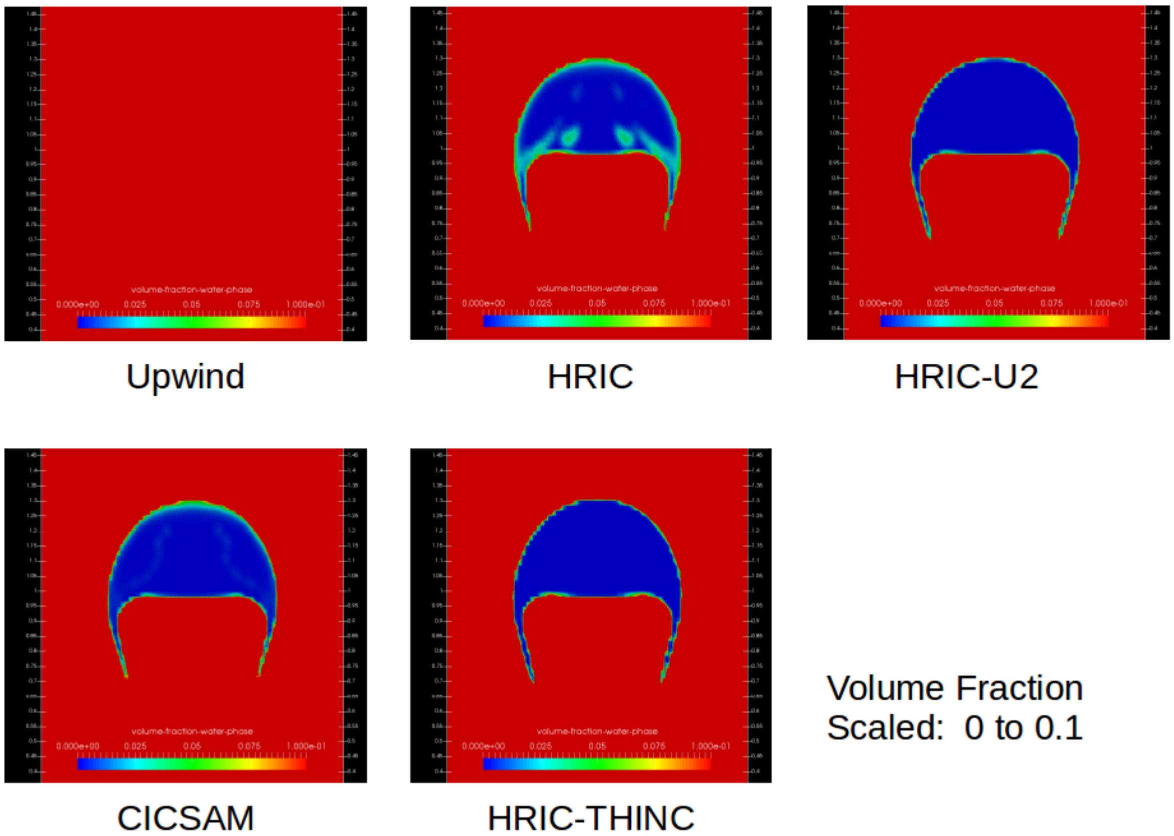
Continuum Surface Stress model avoids calculation of curvature needed for Continuum Surface Force model and it performs better near walls with sharp angles.

Bubble rising in a bubble column

To demonstrate various methods we presented, the bubble rising validation case is set up and run for 3 *seconds*. At the end of this simulation (t = 3*sec*), following comparison is obtained:



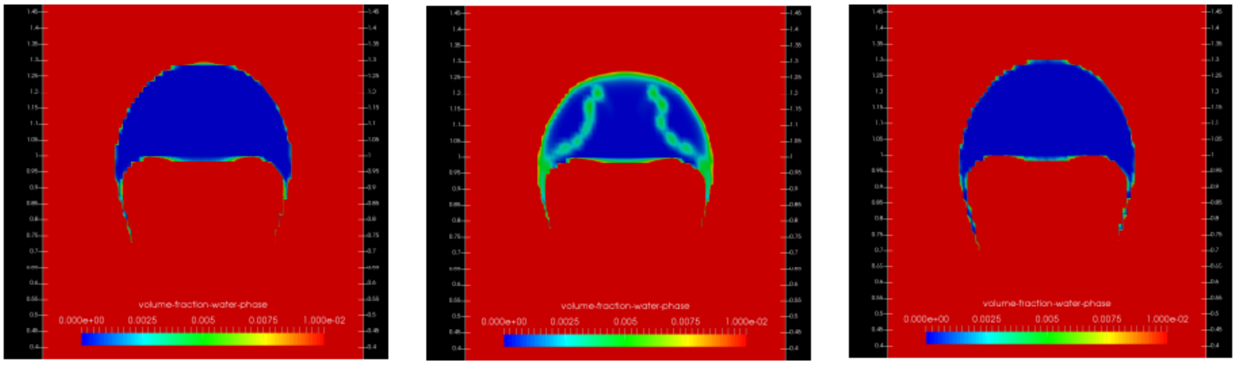
As one can see, the upwind scheme is not suitable for interface tracking. It can be noticed that there are some dissipative errors in case of HRIC scheme. When the contour is scaled from 0 to 0.1, these errors are easier to notice:



From above given comparison following conclusions could be made for this case:

- HRIC-U2 performs much better than the original HRIC scheme. The availability of upwind cell does play an important role as expected.
- CICSAM performs better than HRIC scheme as expected.
- THINC scheme is very sharp, even though it is blended with original HRIC scheme (that on its own performed the worse among VOF schemes).

The scale of Contour plot is further changed from 0 to 0.01 to reveal smaller changes as follows:



HRIC-U2 CICSAM HRIC-THINC

Volume Fraction Scaled: 0 to 0.01

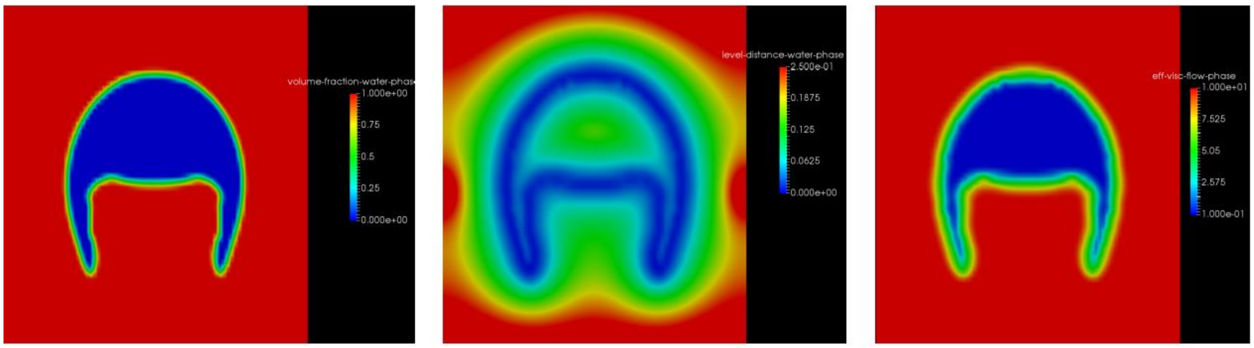
It can be seen that HRIC-U2 and HRIC-THINC performs the best for this test case.
Note that based on experience, THINC schemes remain very sharp over long periods of iterations, whereas HRIC based schemes alone, usually do not remain this sharp over very long iteration periods (say after 200000 time steps).

Level Distance Coupled VOF

Wildkatze solver provides newly developed Level Distance Coupled VOF model which is based on similar ideas to Level Set Coupled VOF model. The major difference with standard Level Set method is that in this method a transport equation for distance function is solved, where the iso-surface of volume fraction = 0.5 is assumed to be 0 distance, whereas in standard Level Set method signed distance function is solved.

Following the ideas from standard Level Set method, the density, viscosity and surface tension forces are computed from the level distance function.

To illustrate this method, following picture shows volume fraction, level distance function and the viscosity calculated from the level distance function for the benchmark problem of bubble rising in liquid. (CICSAM method for interface capturing)



Volume Fraction | Distance Function | Viscosity from Distance Function

Advantages over standard Level Set method:

- Level Set method requires accurate calculation of iso-surface of volume fraction = 0.5 and often this calculation is done by geometric methods. These geometric methods are difficult to code and take efforts to get it right. Whereas in Level Distance model this step is simply taken care by one line of code in discretization of Level Distance equation.
- One needs to solve wall distance equation once, unlike the Level Set re-initialization equation that has to be solved few times until it converges.
- Level distance method is always stable as long as there is volume fraction variation. The same is not true for Level Set re-initialization equation, which requires careful implementation to make it stable.

Hybrid Time Stepping

Multiphase simulations are mostly transient simulations. For fast transient multi-phase simulations, Wildkatze provides a **Hybrid Time Stepping** method with combined implicit and explicit methods. This can reduce the computation time more than two or three times in most cases.

Reactive Mold Filling

In reactive molding simulation, the reactive mold is tracked by an interface tracking method like Volume of Fluid (VOF), while flow is solved by SIMPLE method.

Flow properties are obtained based on reaction state of the mold (for example amount of gas produced and mold temperature). Energy is solved by using simplified energy equation. Fluid properties are computed based on state of reaction components.

Polyurethane expansion

Polyurethane expansion is an example of reactive mold filling that is directly available to user as a physics model. Here the mold filling reactions could be mainly divided into two groups (see **"Numerical simulation of 3D polyurethane expansion during manufacturing process"** of J. Bikard et. al.):

- **Gelling Reaction**

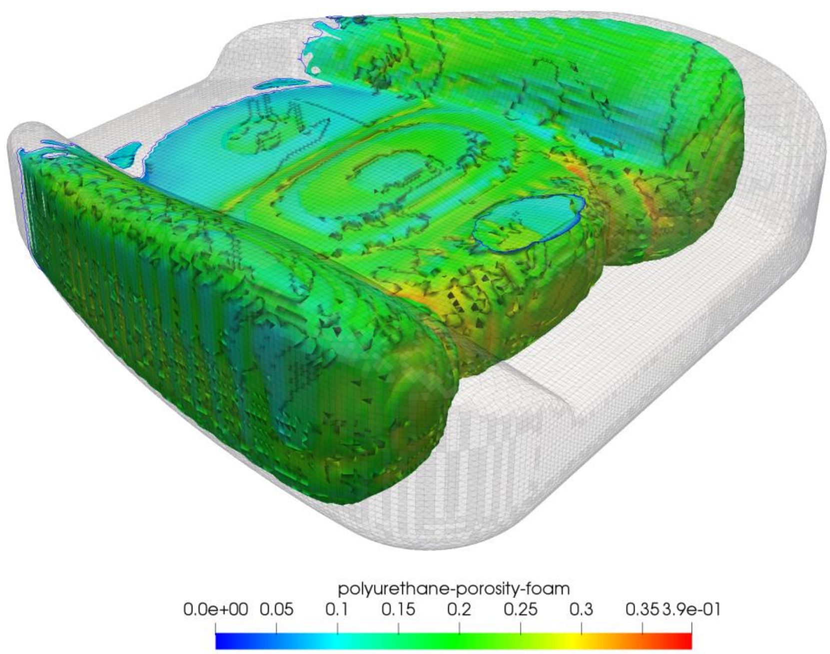
$$\frac{d\beta}{dt} = \frac{1}{\tau_\beta}\beta^{m_\beta}\ (1-\beta)^{n_\beta}$$

$$\text{with}\ \beta = \beta_0 \quad \text{at} \quad t = t_0$$

- **Blowing reaction**

$$\frac{d\alpha}{dt} = \frac{1}{\tau_\alpha}\alpha^{m_\alpha}(1-\alpha)^{n_\alpha}$$
$$\text{with} \quad \alpha = \alpha_0 \quad \text{at} \quad t = t_0$$

Below picture demonstrates this method implemented in Wildkatze:



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