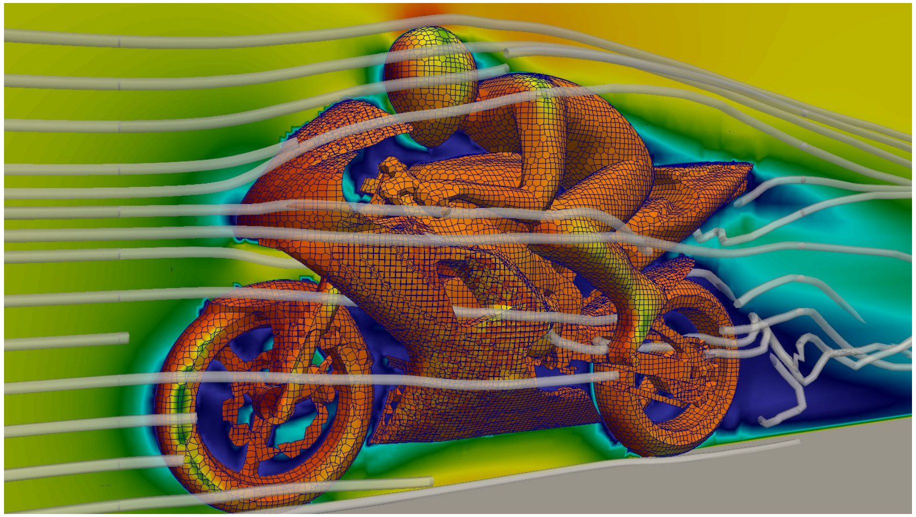
Open Source Computational Fluid Dynamics



An MSc course to gain extended knowledge in Computational Fluid Dynamics (CFD) using open source software.

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Multiphase flows

We can discuss VOF (Volume of fluid method) only.

- only one momentum equation is solved for mixture
- indicator function: e.g. alpha1 = 1 for liquid, alpha1 = 0 for gas

$$\sum_i \alpha_i = 1$$

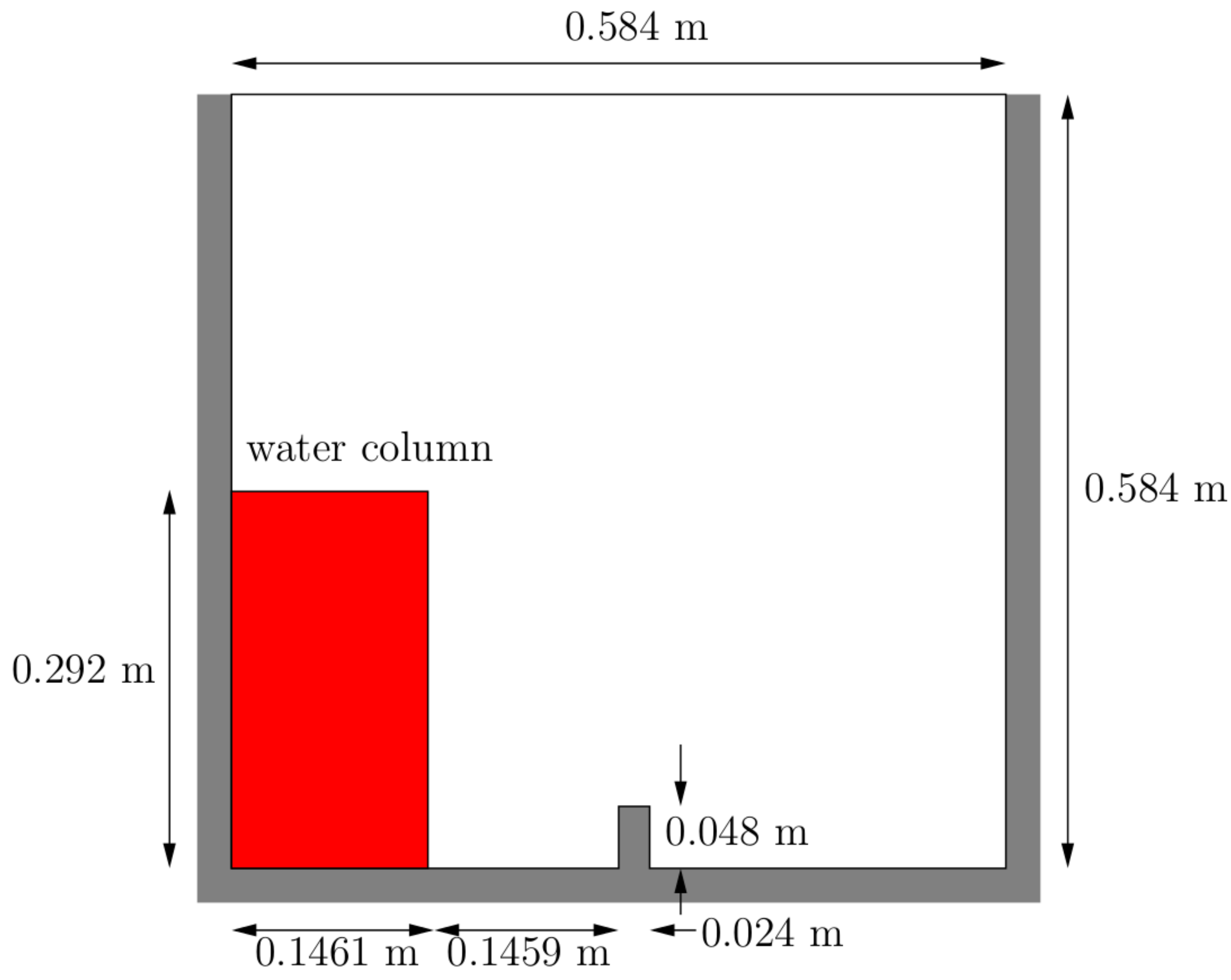
- advection equation for indicator function:

$$\frac{\partial \alpha_i}{\partial t} + \nabla \cdot (U \cdot \alpha_i) = 0$$

- transport properties: weighted averages based on characteristic functions

$$\rho = \sum_i \alpha_i \rho_i$$

Breaking of a dam



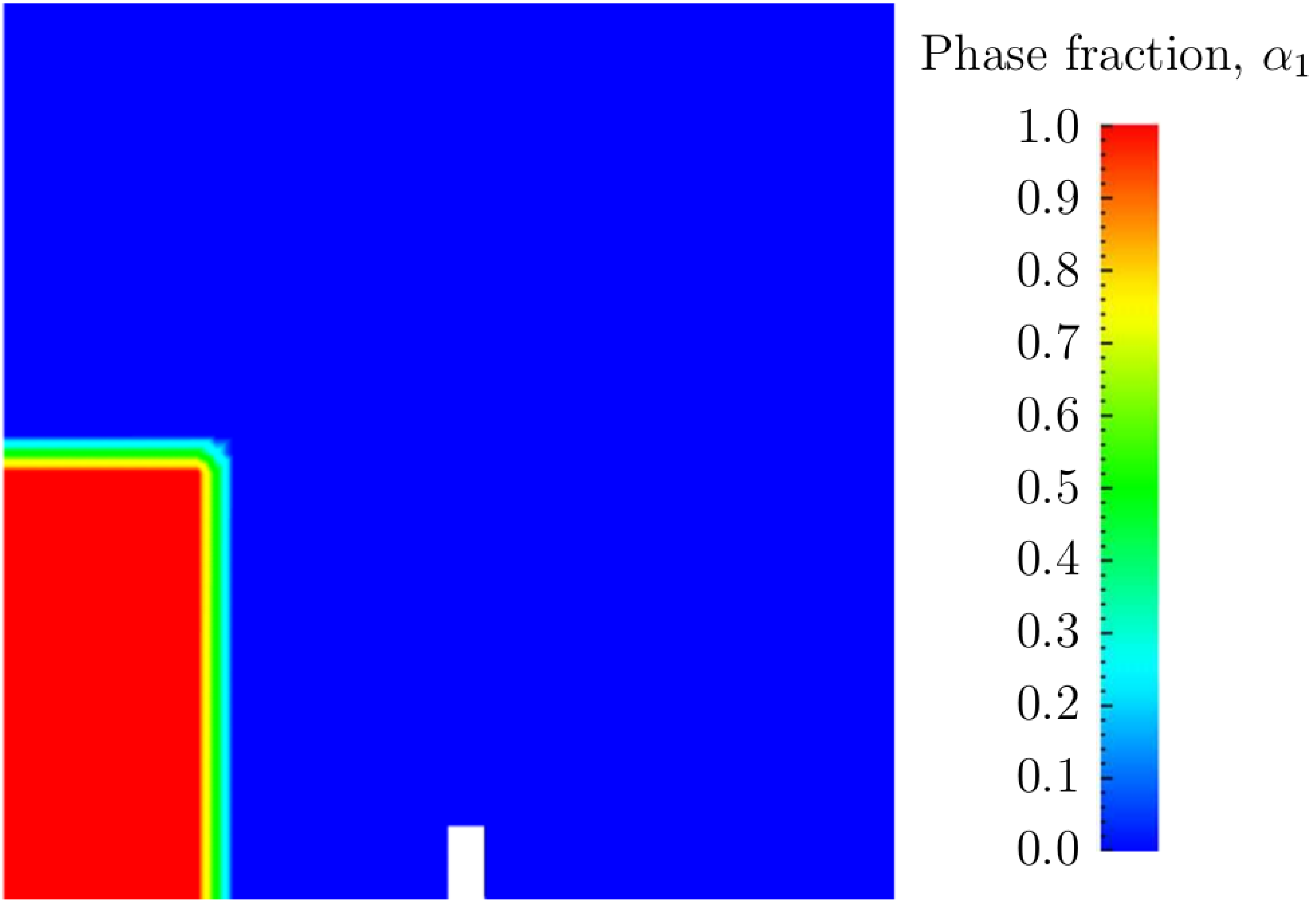
Breaking of a dam

system/setFieldsDict:

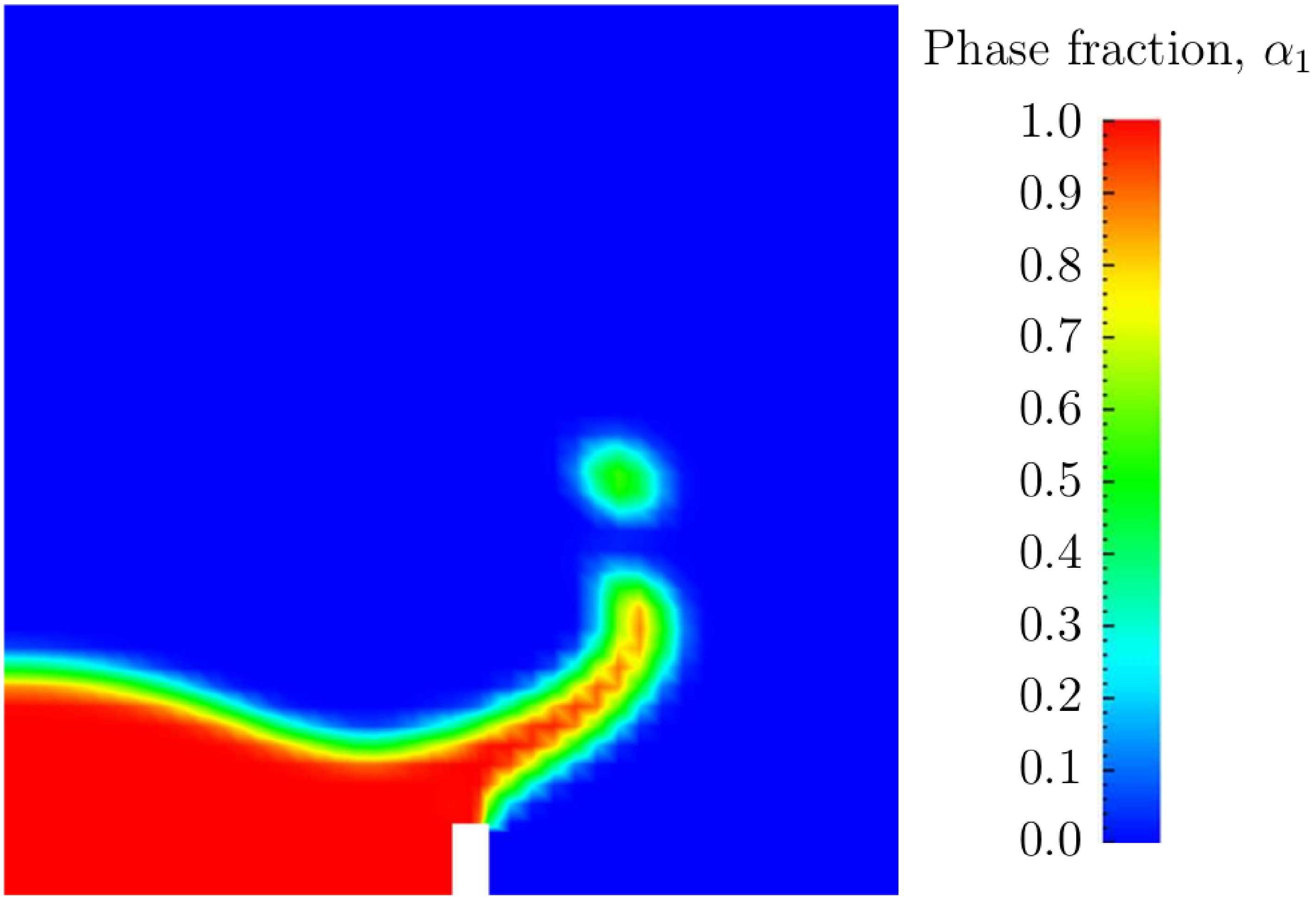
```
defaultFieldValues
(
    volScalarFieldValue alpha1 0
);

regions
(
    boxToCell
    {
        box (0 0 -1) (0.1461 0.292 1);
        fieldValues
        (
            volScalarFieldValue alpha1 1
        );
    }
);
```

Breaking of a dam



Breaking of a dam



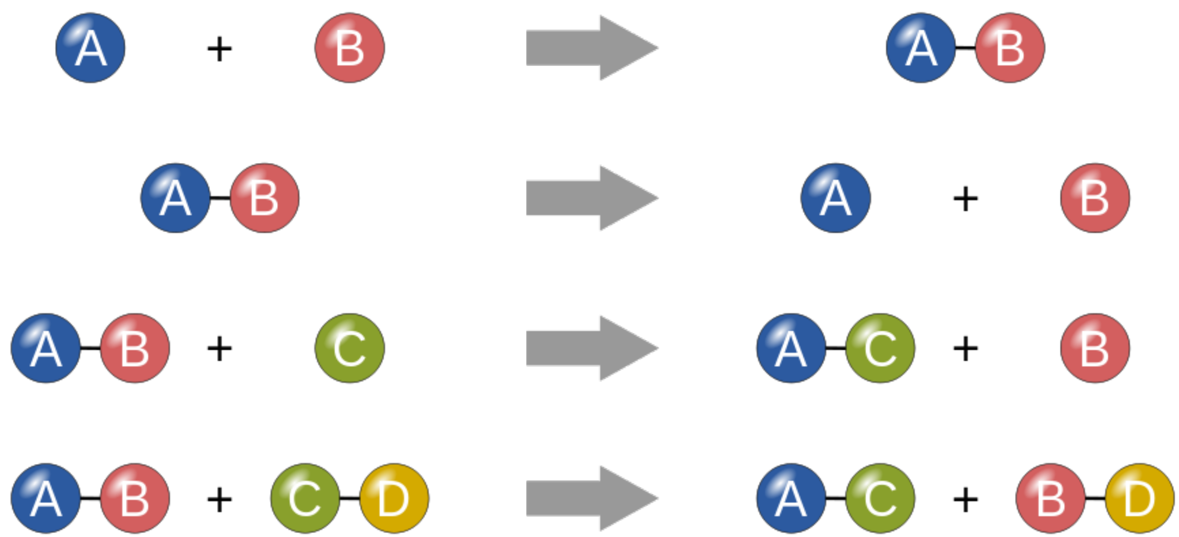
(a) At $t = 0.25$ s.

Reactive flows

Conservation equation for chemical specie *i*:

$$\frac{\partial \rho y_i}{\partial t} + \nabla \cdot (\rho y_i U) + \nabla j_i = R_i$$

- y_i : mass fraction of specie
- j_i : mass diffusion-flux of specie (relative to U)
- R_i : source/sink due to chemical reactions



Four basic chemical reactions types: synthesis, decomposition, single replacement and double replacement.

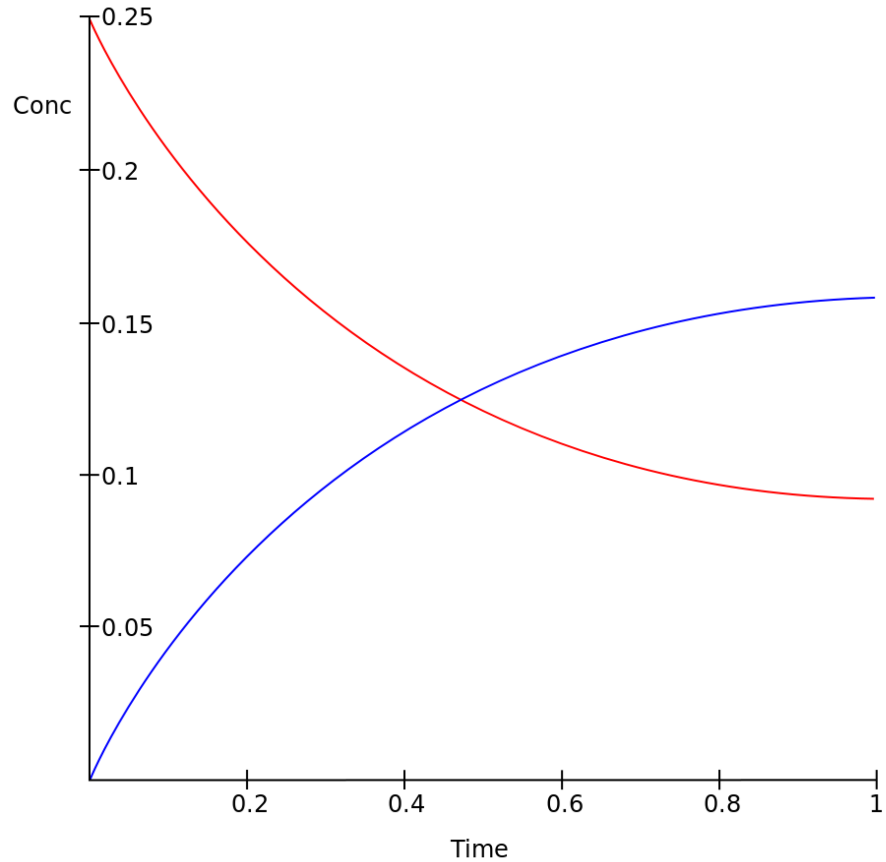
Chemical kinetics

A system of ODEs are solved for every reactions in every cells:

$$\frac{-d[C]}{dt} = k \cdot [C]^n$$

Arrhenius reaction rate:

$$k = A \cdot \exp\left(\frac{-E_a}{RT}\right)$$



Multicomponent transport

```
H2O
{
    specie
    {
        nMoles          1;
        molWeight       18.0153;
    }
    thermodynamics
    {
        Tlow            200;
        Thigh           5000;
        Tcommon         1000;
        highCpCoeffs    ( 2.67215 0.00305629 -8.73026e-07 1.201e-10 -6.39162e-15 -29899.2 6.86282 );
        lowCpCoeffs     ( 3.38684 0.00347498 -6.3547e-06 6.96858e-09 -2.50659e-12 -30208.1 2.59023 );
    }
    transport
    {
        As              1.67212e-06;
        Ts              170.672;
    }
}
```

Sutherland (dynamic) viscosity [Pa-s]:

$$\mu = \frac{A_s \sqrt{T}}{1 + T_s / T}$$

Multicomponent transport

NASA polynomials for heat capacity and enthalpy:

$$\frac{Cp}{R} = a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4$$
$$\frac{H}{RT} = a_0 + \frac{a_1 T}{2} + \frac{a_2 T^2}{3} + \frac{a_3 T^3}{4} + \frac{a_4 T^4}{5} + \frac{a_5}{T}$$

Note: R is the universal gas constant here!