"All-speed" reactive two-phase flow simulations with Basilisk

Hiroumi Tani

Japan Aerospace Exploration Agency
Massachusetts Institute of Technology

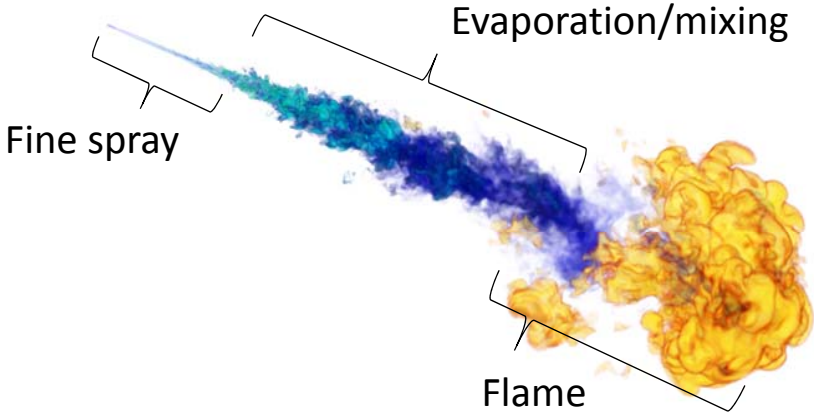
Motivation

Liquid propellant injection for space propulsion

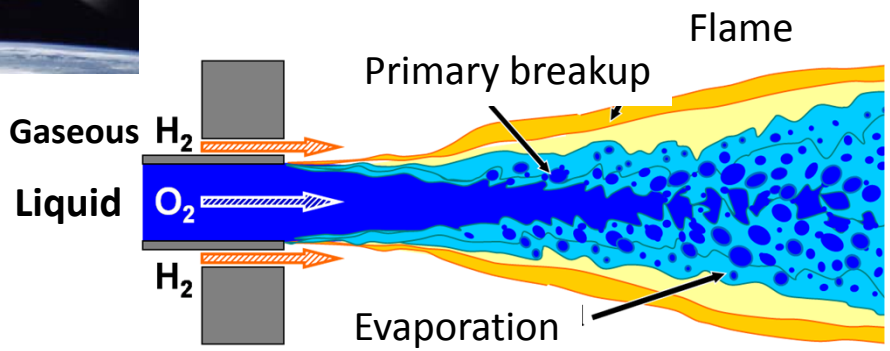
The atomization of liquid propellants in rocket and spacecraft engines is so poor that the primary breakup and flames interacts each other.

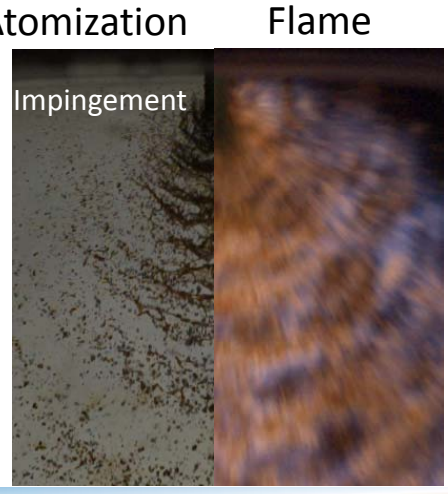
Two-phase flow (primary breakup) and chemical reaction (flame) should be modeled in a CFD code.

Automobile and gas turbine etc.



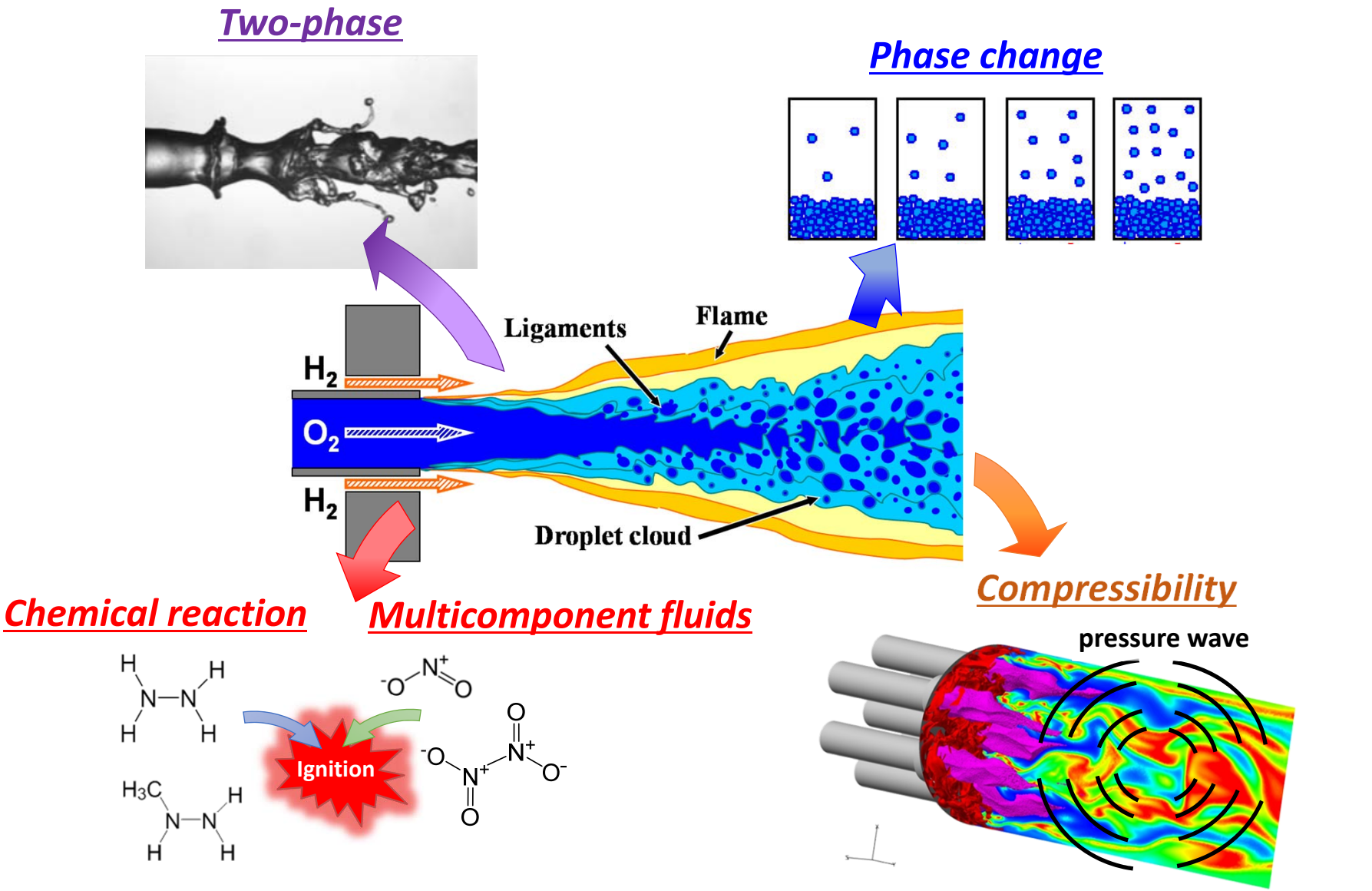
Rocket and spacecraft engines





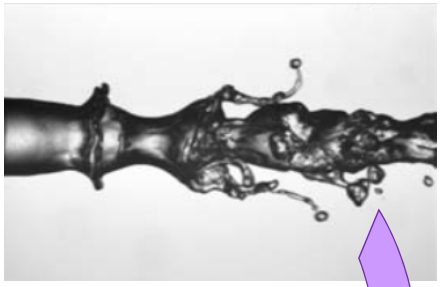
H. Tani, CNF 2017

Key physical models

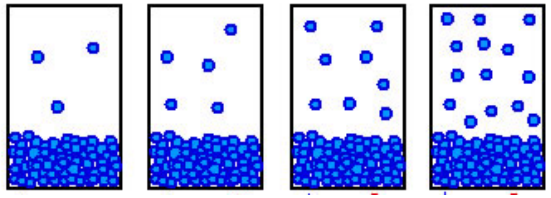


Key physical models

Two-phase

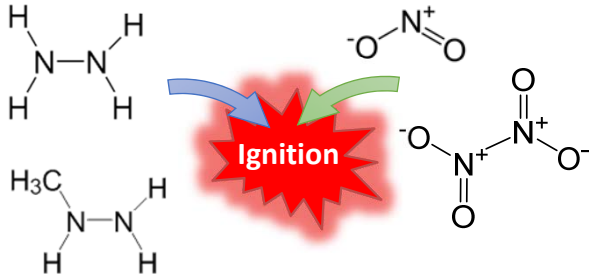


Phase change



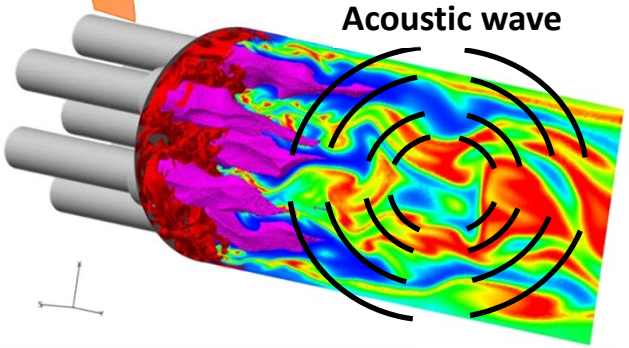
"All-speed" multiphase reactive flow simulator

Chemical reaction



Multicomponent fluids

Compressibility



N-S solver for all-speed flows

Density-based solver

Density fields are directly calculated by N-S eqns in the conservative form. Then, the pressure are expected by using a EoS.

Fully conservative

Fast calculation per one step

High-order scheme

Compressible (high-speed) flows

Simscale.com

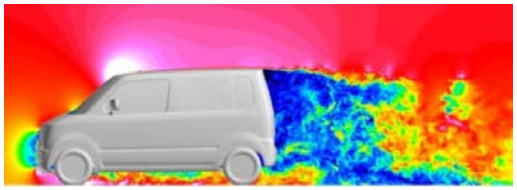
Pressure-based solver

N-S eqns are transformed to the non-conservative form. Pressure fields are extracted by solving a pressure eqn. which couples with velocity eqns.

Larger time step (Δt)

Easy to model two-phase flow

Incompressible (low-speed) flows



Supercomputer "Kei" 2016

TCUP method

Low-Mach number method
Preconditioning method

Governing equations

Non-consevartive forms of compressible N-S eqns.

$$\frac{\partial \rho}{\partial t} + (\boldsymbol{u}\cdot\nabla)\,\rho = -\rho\nabla\cdot\boldsymbol{u}$$

$$\rho\frac{\partial \boldsymbol{u}}{\partial t} + \rho\,(\boldsymbol{u}\cdot\nabla)\,\vec{u} = -\nabla p + \nabla : \boldsymbol{T}_\nu$$

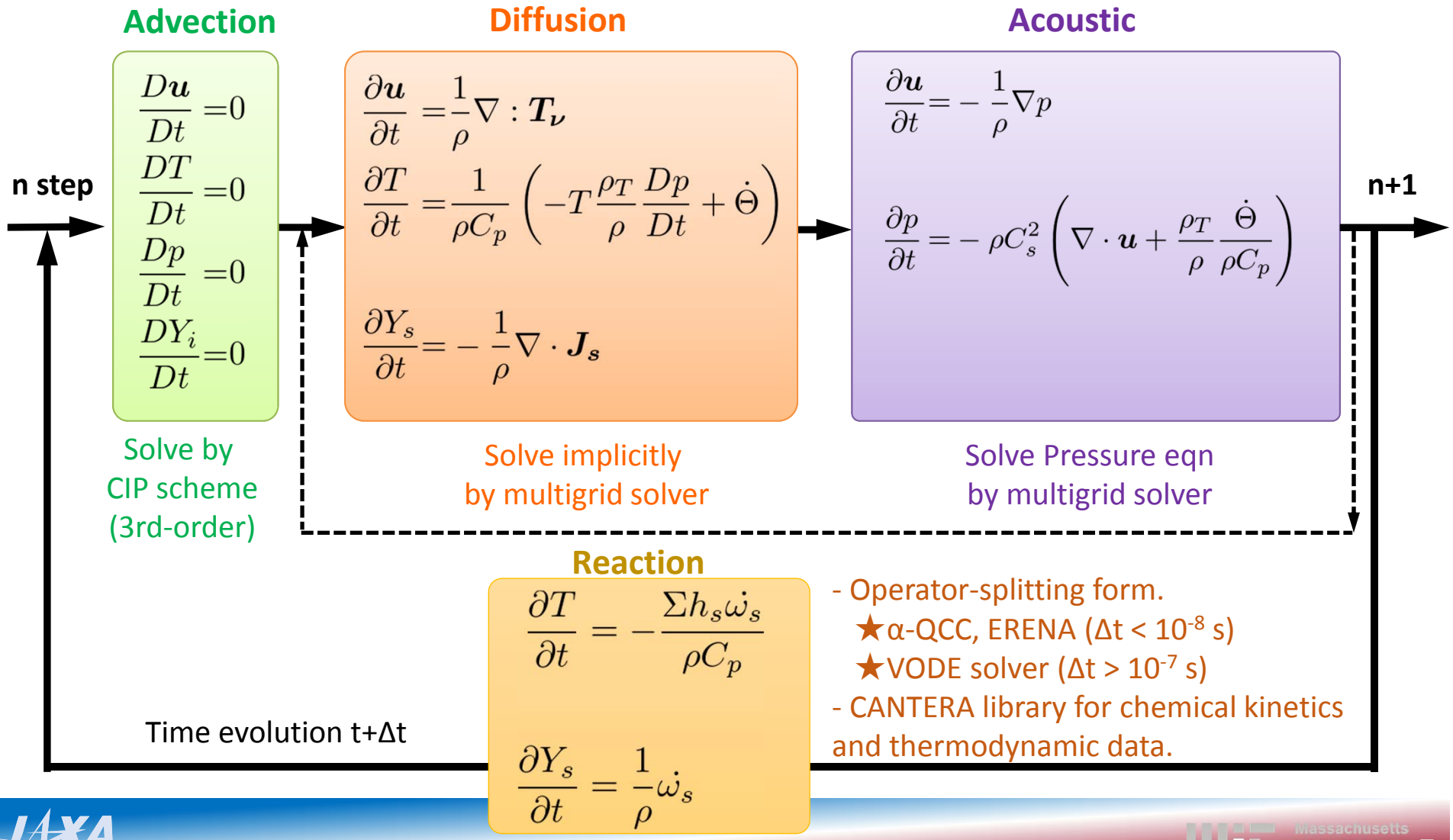
$$\rho\frac{\partial e}{\partial t} + \rho\,(\boldsymbol{u}\cdot\nabla)\,e = -p\nabla\cdot\boldsymbol{u} + \underbrace{(\boldsymbol{T}_\nu : \nabla)\cdot\boldsymbol{u} - \nabla\cdot(\boldsymbol{q_c}+\boldsymbol{q_d})}_{\dot{\Theta}}$$

$$\rho\frac{\partial Y_s}{\partial t} + \rho\,(\boldsymbol{u}\cdot\nabla)\,Y_s = -\nabla\cdot\boldsymbol{J_s} + \rho\dot{\omega}_s$$

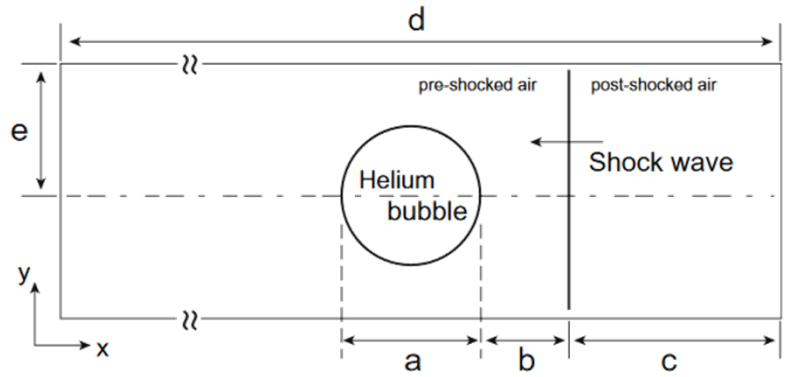
	Advection		Diffusion	Acoustic	Reaction
$\frac{\partial \boldsymbol{u}}{\partial t}$	$+(\boldsymbol{u}\cdot\nabla)\,\boldsymbol{u}$	$=$	$\frac{1}{\rho}\nabla : \boldsymbol{T_\nu}$	$-\frac{1}{\rho}\nabla p$	
$\frac{\partial T}{\partial t}$	$+(\boldsymbol{u}\cdot\nabla)\,T$	$=$	$\frac{1}{\rho C_p}\left(-T\frac{\rho_T}{\rho}\frac{Dp}{Dt}+\dot{\Theta}\right)$		$-\frac{\Sigma h_s\dot{\omega}_s}{\rho C_p}$
$\frac{\partial p}{\partial t}$	$+(\boldsymbol{u}\cdot\nabla)\,p$	$=$		$-\rho C_s^2\left(\nabla\cdot\boldsymbol{u}+\frac{\rho_T}{\rho}\frac{\dot{\Theta}}{\rho C_p}\right)$	
$\frac{\partial Y_s}{\partial t}$	$+(\boldsymbol{u}\cdot\nabla)\,Y_s$	$=$	$-\frac{1}{\rho}\nabla\cdot\boldsymbol{J_s}$		$+\dot{\omega}_s$

TCUP method

Temperature-Coupled Unified Procedure (TCUP) (Yabe et al. 1991, Himeno et al. 1999)

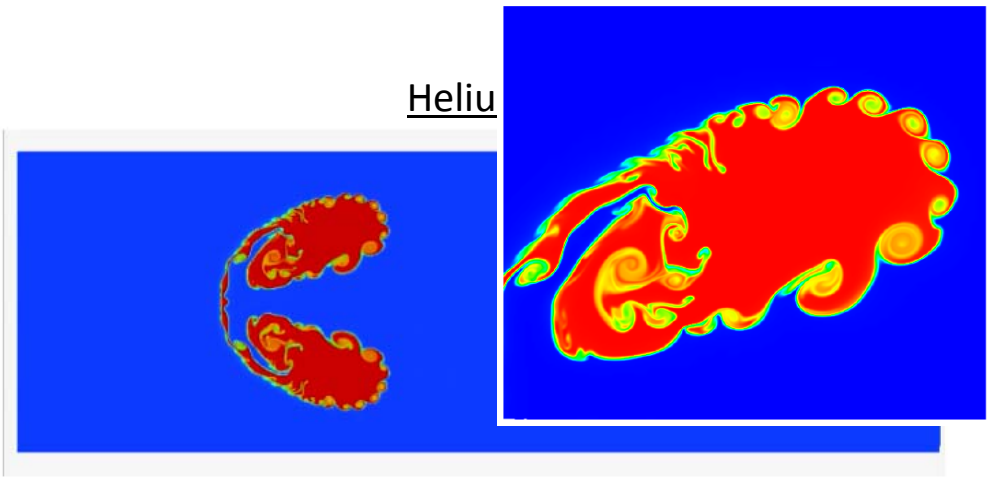


Shock-bubble interaction

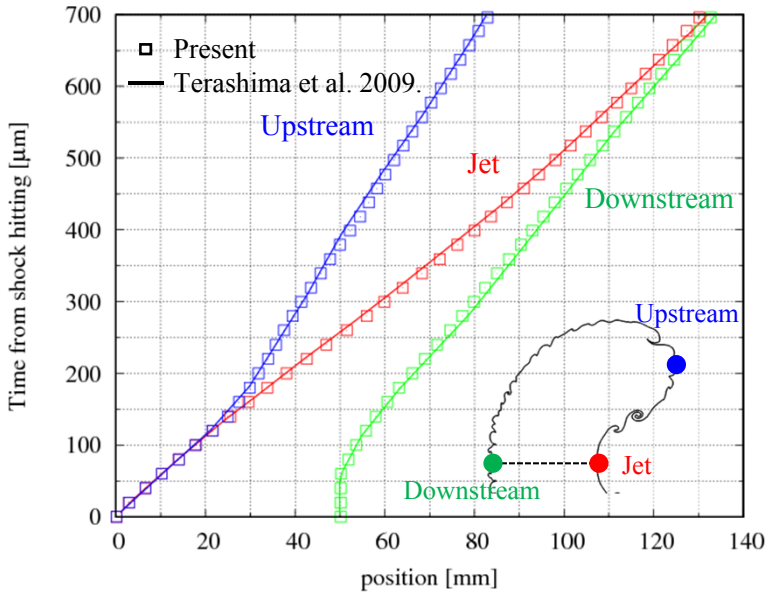


JCP 2009, H. Terashima et al.

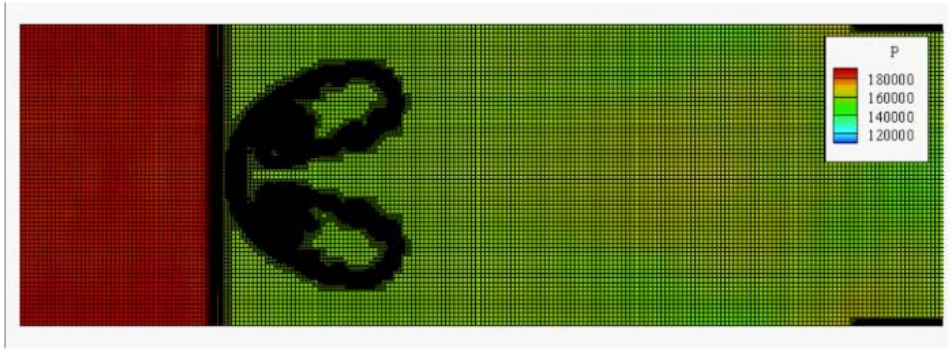
Heliu



Comparison with results of
a density-based solver

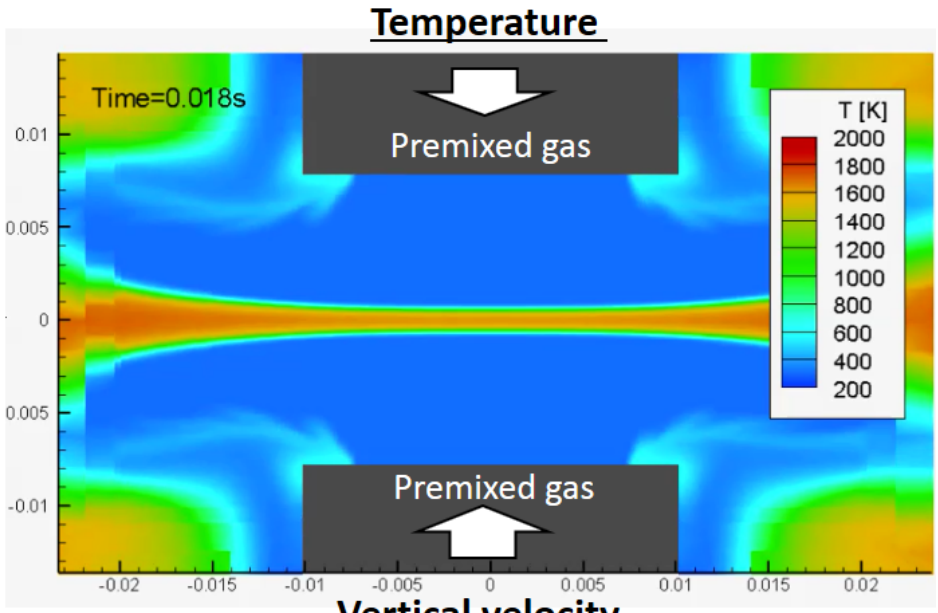


Pressure with meshes

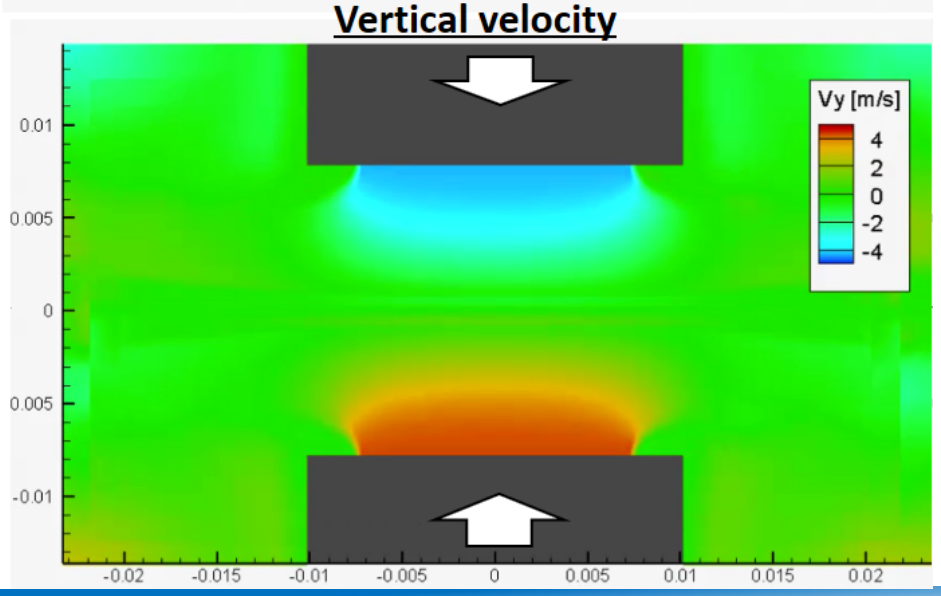


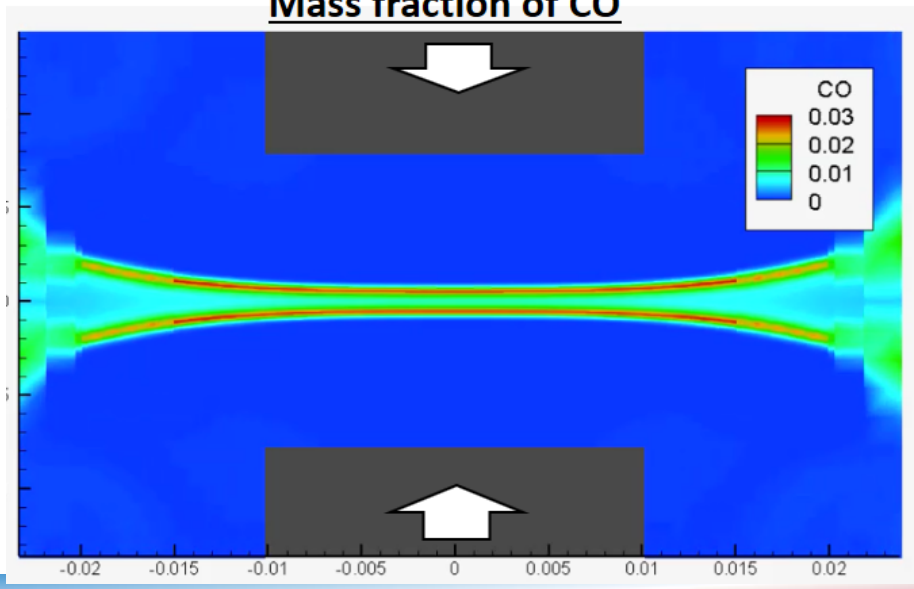
The present method can be adapted to supersonic (compressible) flows.

Extinction of premixed flame



- Investigated dominant chemical reactions in the flame extinction of premixed natural gases.
- A reaction model of 17 species and 58 reactions.





New CFD code

Two-phase

Phase change

"All-speed" multiphase reactive flow simulator

Chemical reaction

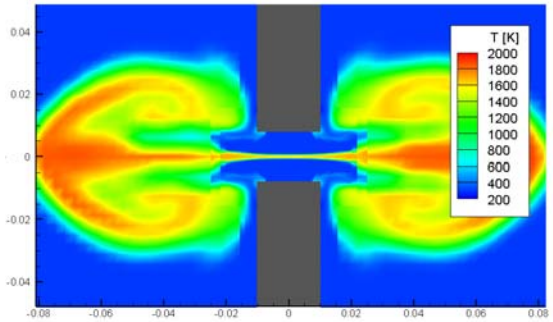
Operator-splitting

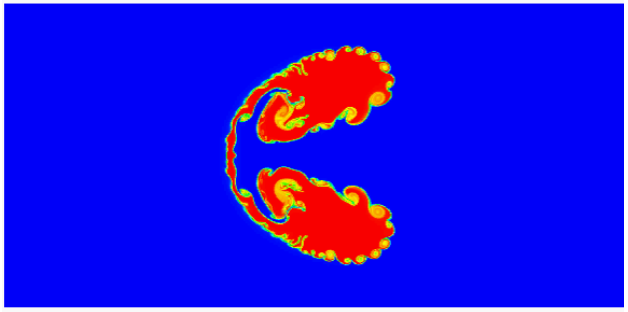
Multicomponent fluids

CANTERA

Compressibility

TCUP method





CLSVOF : Coupled Level-set and VOF

CLSVOF: Combination of Level-set and PLIC-VOF method

Volume of Fluid (VOF) *Hv*

$$\begin{aligned} \text{Liquid}: \quad & Hs = 0.5, \quad \phi > 0 \\ \text{Interface}: \quad & Hs = 0, \quad \phi = 0 \\ \text{Gas}: \quad & Hs = -0.5, \quad \phi < 0 \end{aligned}$$

$$\frac{\partial H_s}{\partial t} + (\vec{u_s} \cdot \nabla) H_s = 0$$

Solve cell-integrated form by PLIC-VOF method
(Mass conservation)

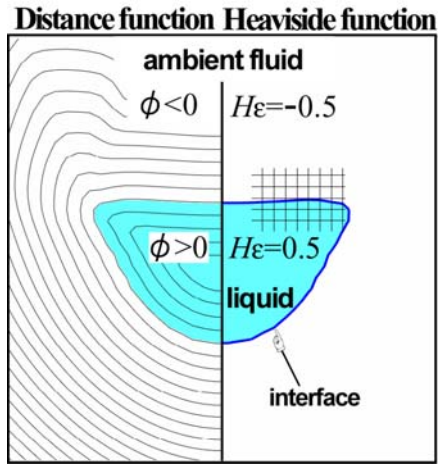
Level-set function ϕ

$$\frac{\partial \phi}{\partial t} + (\vec{u} \cdot \nabla) \phi = 0$$

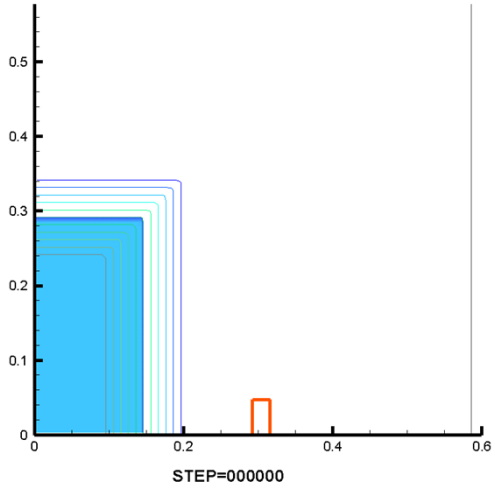
Solve by CIP method
(Sharpe interface)

Normal vector of interface

Reinitialization based on VOF



(Himeno et al. 1999)

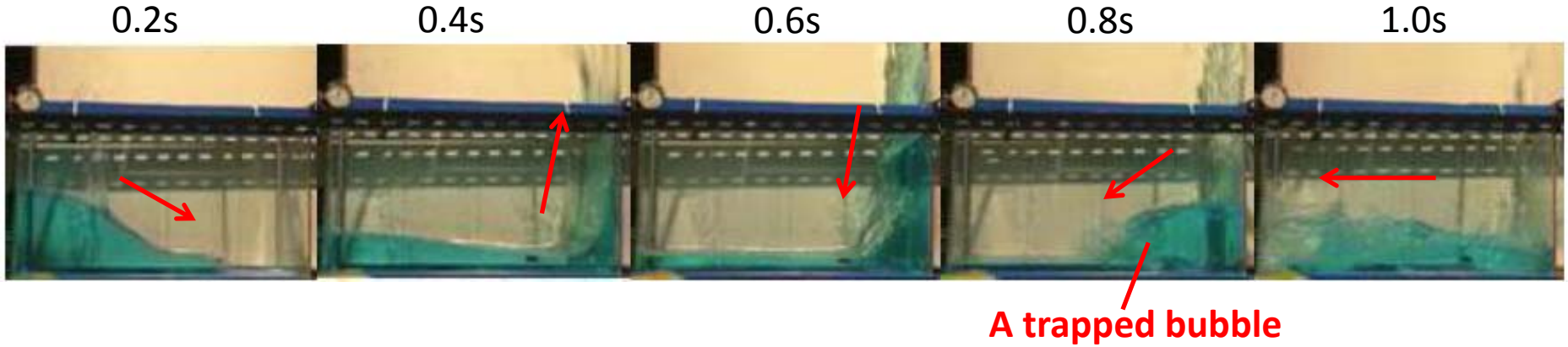


Calculation of thermodynamic properties

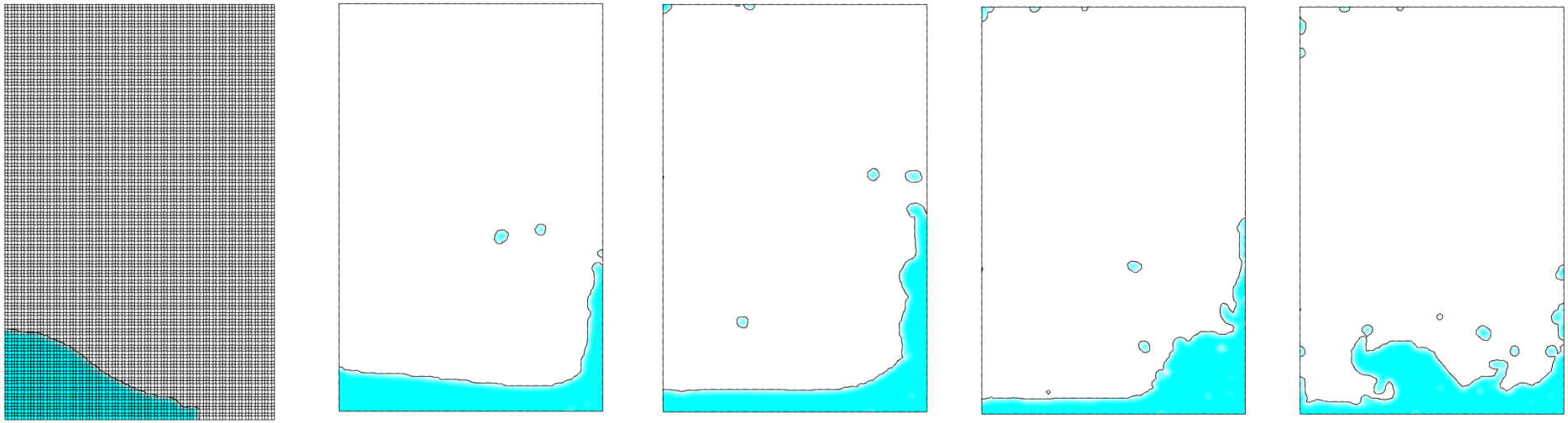
$$\rho = (0.5 - H_s)\rho_g + (0.5 + H_s)\rho_l$$

Dam break test (1/2)

Experiments (Koshizuka et al.)



Only VOF in 2D

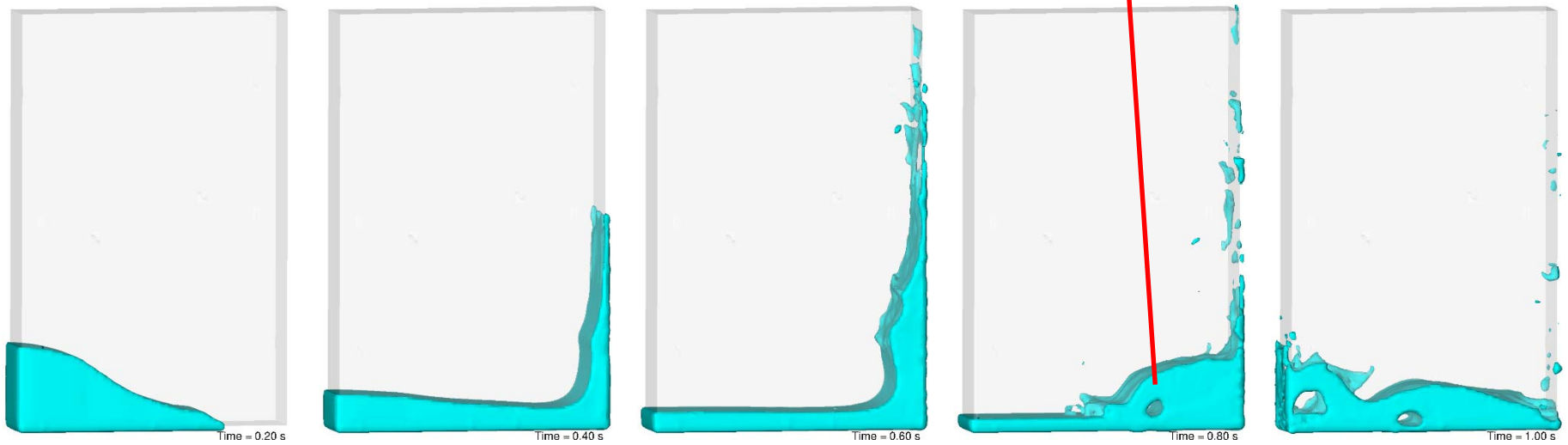


Dam break test (1/2)

Experiments (Koshizuka et al.)

CLSVOF in 3D

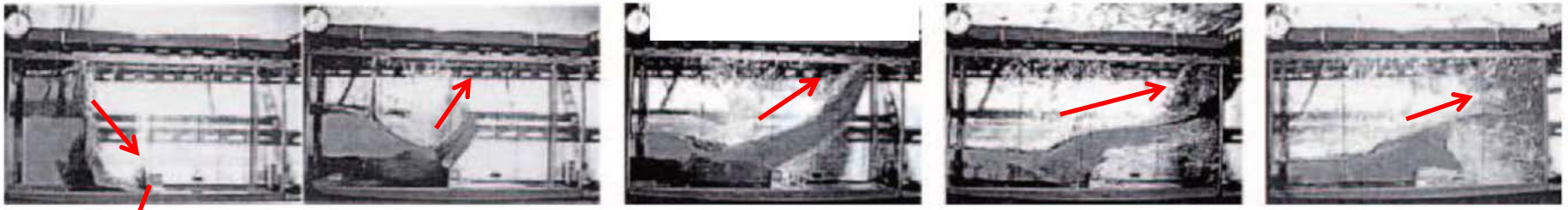
A trapped bubble



The present method well captured the dynamics of liquid surfaces

Dam break test (2/2)

Experiments (Koshizuka et al.)

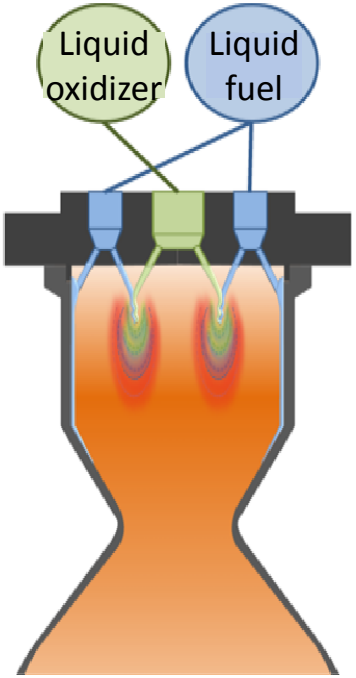


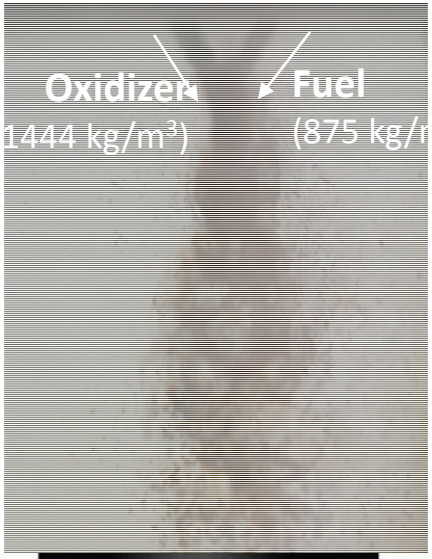
CLSVOF in 3D

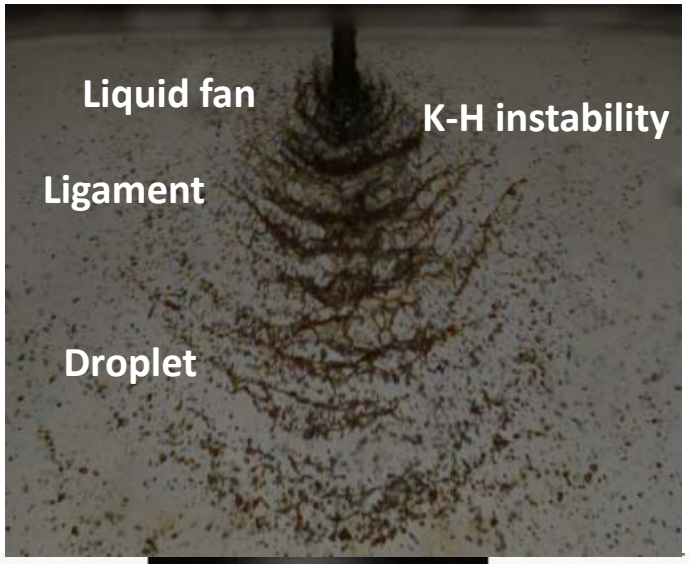
The present method precisely captured the dynamics of liquid-gas interfaces.

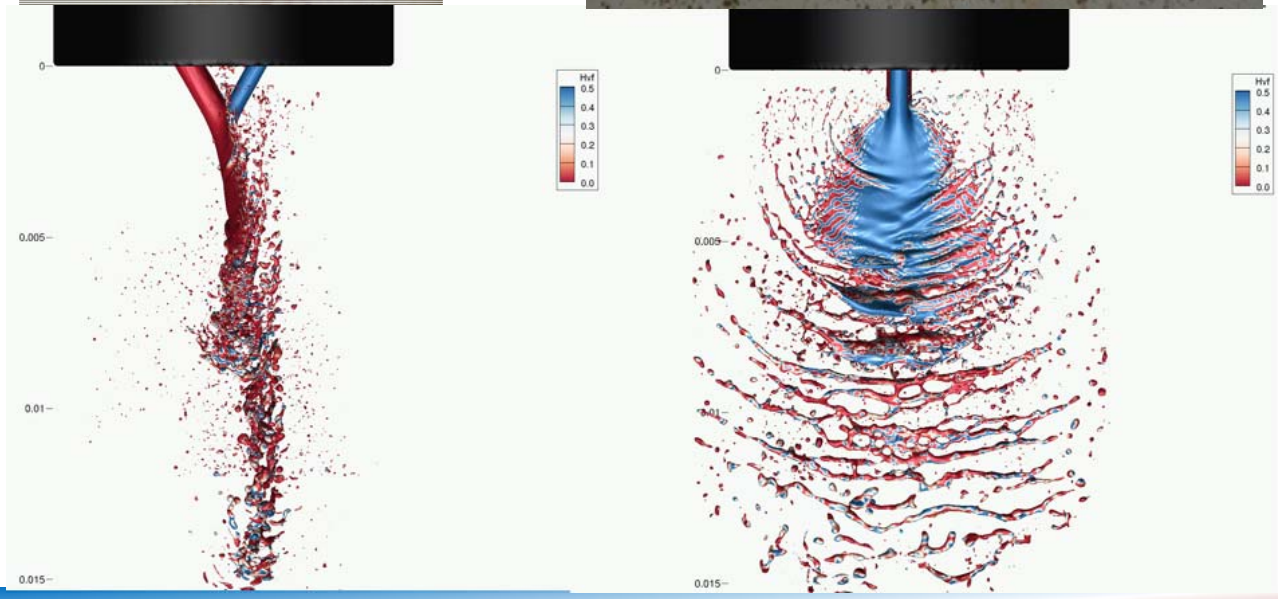
Breakup of impinging liquid jets

Impingement-type injector





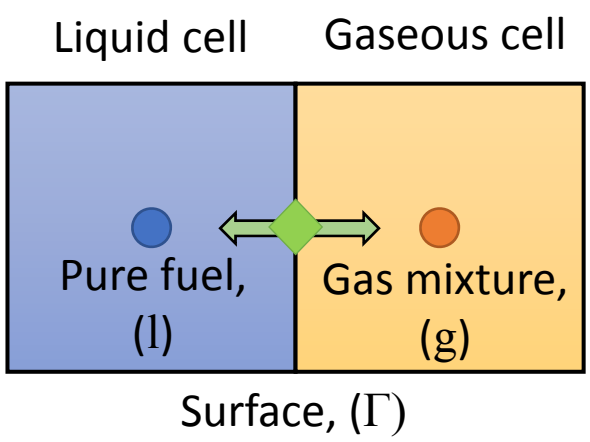




Phase change

Unknown variable : 2+N (Phase change rate, temperature and mass fractions on surface)

Constraint conditions : 2+N (Jump conditions, Phase equilibrium with Antoine eqn.)



Phase change rate : $\dot{m}$ [kg/(s・m^2)]

Latent heat : h_{lg}[J/kg]

Jump conditions (1+N eqns.)

$$\begin{cases} \dot{m}h_{lg} + (\lambda\nabla T)_l^\Gamma = (\lambda\nabla T)_g^\Gamma \\ \dot{m}Y_{l,s}^\Gamma + \boldsymbol{J}_{\boldsymbol{l,s}}^\Gamma = \dot{m}Y_{g,s}^\Gamma + \boldsymbol{J}_{\boldsymbol{g,s}}^\Gamma \end{cases}$$

$Y_{l,s}$=1 only when s=fuel

Phase equilibrium (1 eqn.)

Clausius-Clapeyron

$$\frac{p_{g,fuel}^\Gamma}{p_{g,tot}^\Gamma} = \exp\left[\frac{h_{lg}M_{fuel}}{R}\left(\frac{1}{T^B} - \frac{1}{T^\Gamma}\right)\right]$$

Partial pressure

$$\frac{p_{g,fuel}^\Gamma}{p_{g,tot}^\Gamma} = X_{g,fuel}^\Gamma\left(Y_{g,1}^\Gamma, Y_{g,2}^\Gamma, Y_{g,3}^\Gamma \cdots\right)$$

T_B is a saturated temperature of pure fuel at the total pressure.

Antoine eqn. $T_B = \dfrac{B}{A - \log_{10}(p_{g,tot})} - C$

$$p_{g,tot}^\Gamma = p_{g,tot}$$

Assumption and solution

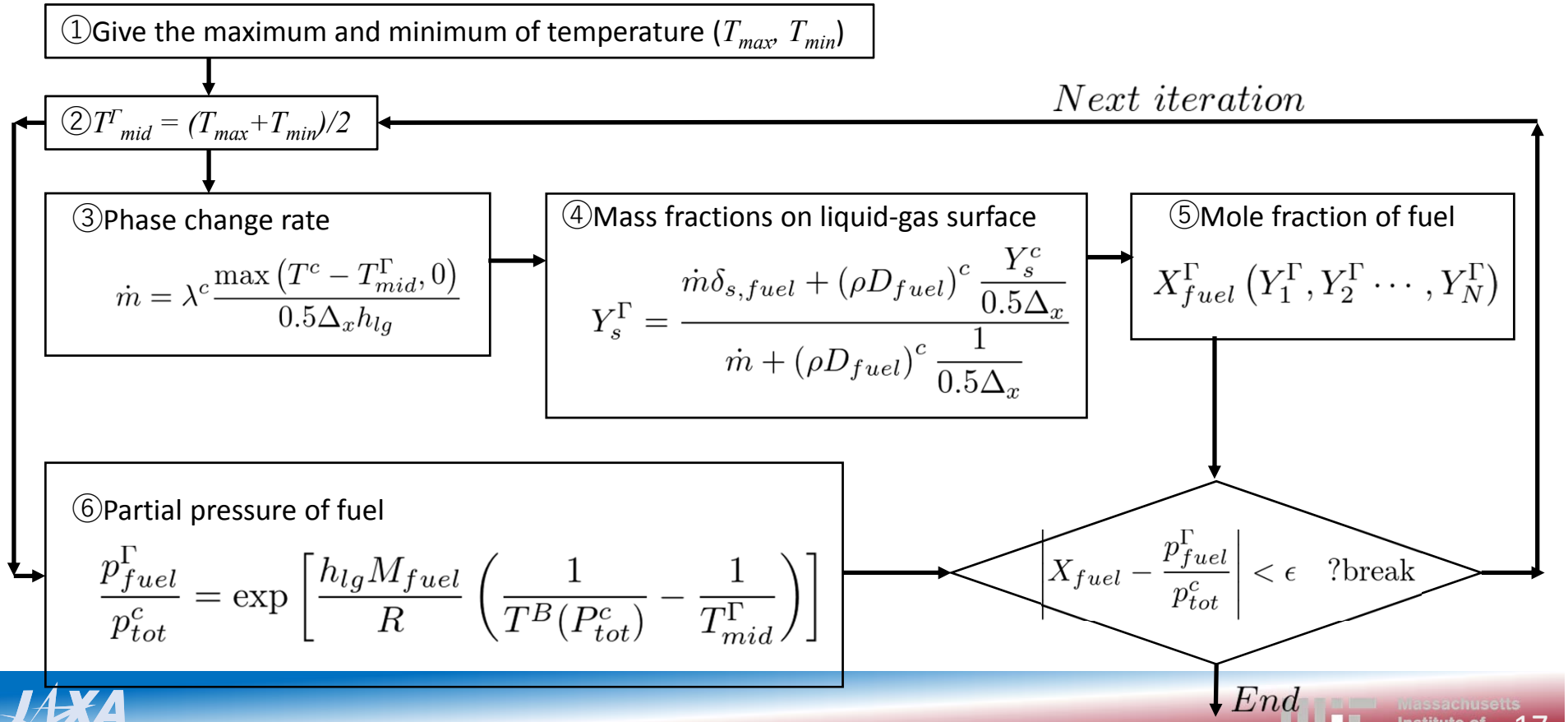
- Transport coefficients are directly interpolated from those on cell center.

$$\lambda = \lambda^c, \quad D_s = D_s^c$$

- Diffusion coefficients of all species are equal to the mixture-averaged diffusion coefficient of liquid species.

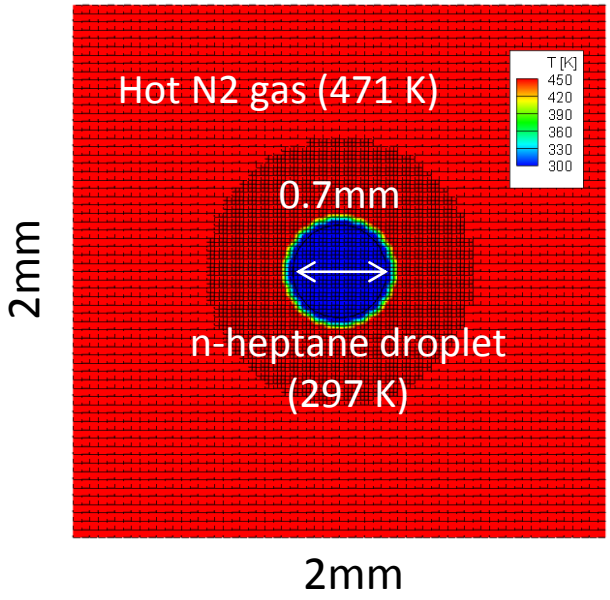
$$D_1 = D_2 = \cdots = D_N = D_{fuel}$$

Then, unknown variables can be solved by using the bisection method.

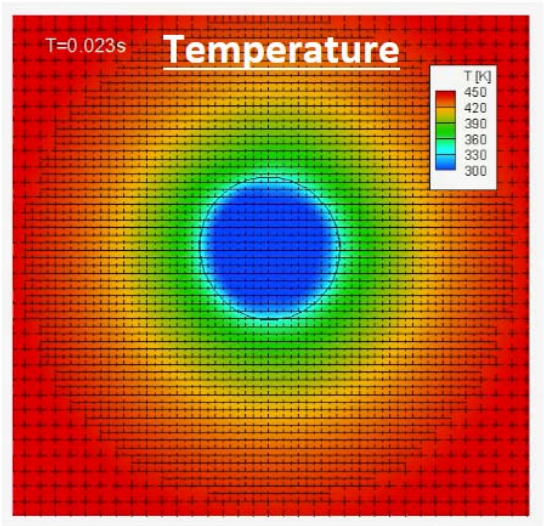


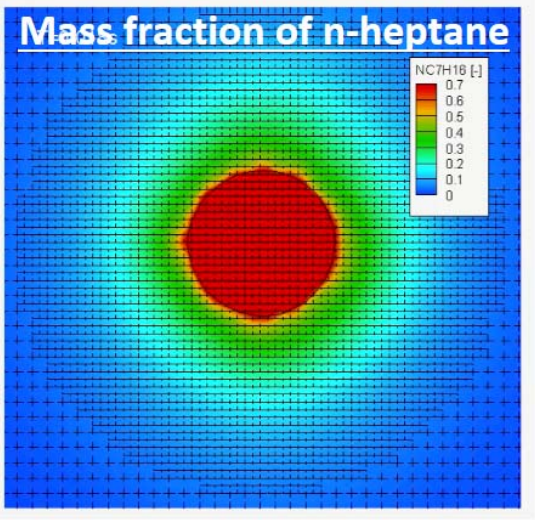
Evaporation of n-heptane droplet

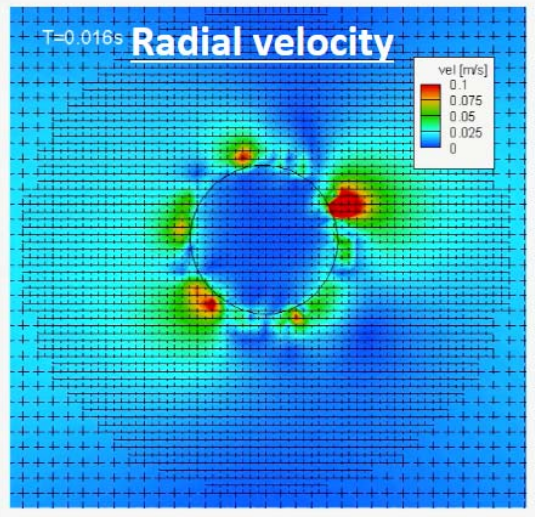
Initial conditions



The evaporation was induced by the mass diffusion near the liquid surfaces.

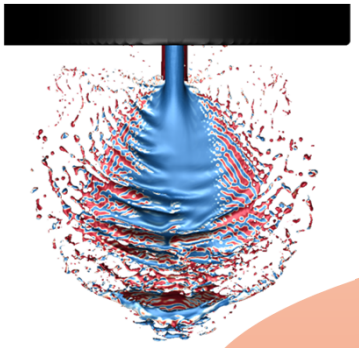






New CFD code

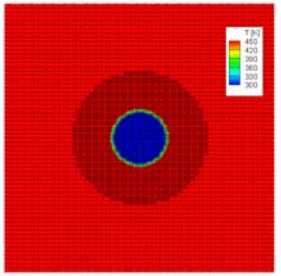
Two-phase



CLSVOF

Jump conditions & Phase equilibrium

Phase change



"All-speed" multiphase reactive flow simulator

Chemical reaction

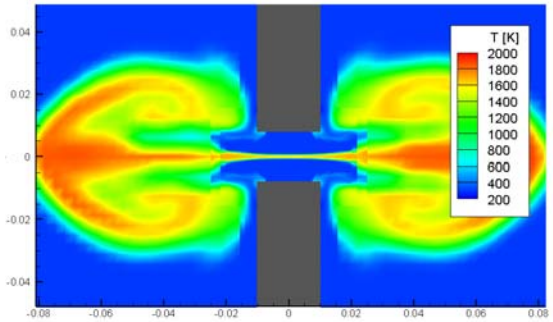
Operator-splitting

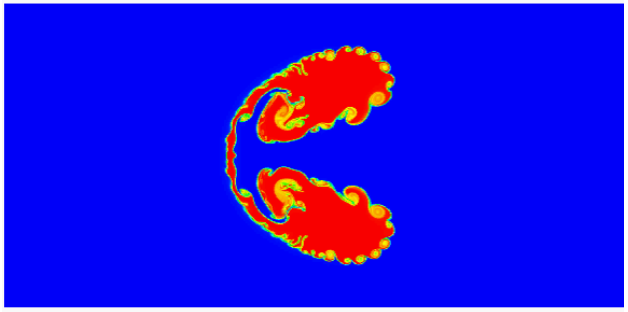
Multicomponent fluids

CANTERA

Compressibility

TCUP method





Summary

An all-speed CFD code is being developed to simulate the interaction between the primary breakup and flames in spacecraft engines.

The TCUP method was programed in Basilisk. Also, CLSVOF, chemical reaction and phase change model were implemented. The new code showed the advantages of the present algorism for compressible/incompressible, two-phase and reactive flow simulations.

Future works,

- Find a way to relax the pulsatile velocity increase due to the phase change and validate the phase change model.
- Apply the new code to simulations of a burning liquid droplet or jet.