東京大学JAXA社会連携講座シンポジウム

Sep/27/2012

超臨界圧における極低温流体混合現象の高精度数値モデリング

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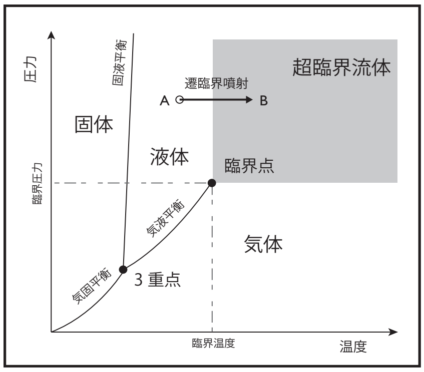
Backgrounds I



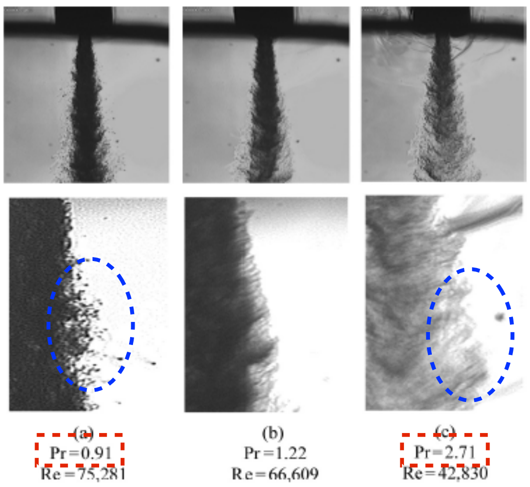
Pressure in rocket engine chamber

- 3~20 MPa: supercritical pressures

LE-7A engine

Mixing, followed by combustion

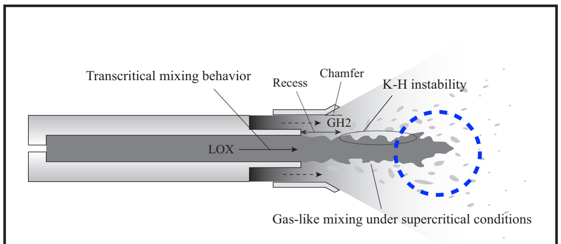
- Disappearance of surface tension and latent heat
- Stirring and diffusion process, rather than atomization: **Turbulent mixing**



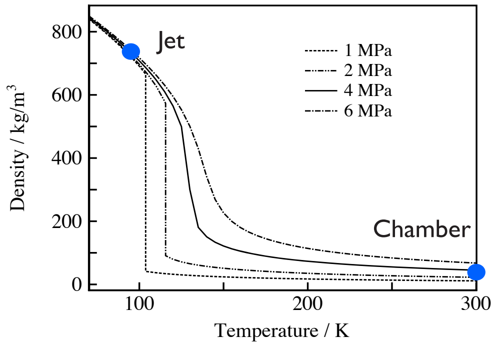
Chehroudi et al. (2002)

Backgrounds II

- Large difference of thermodynamic fluid properties: **cryogenic jet into supercritical fluids**



A schematic of atomization/mixing process in liquid rocket engine

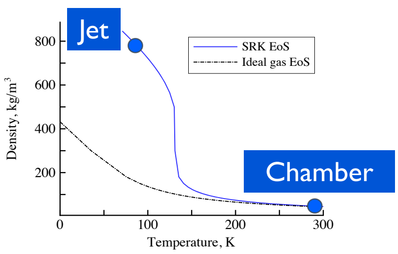


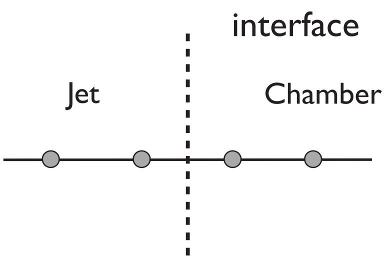
A diagram for nitrogen

- **Real fluid effects**
- **Turbulent flows**
- **Large density contrast**

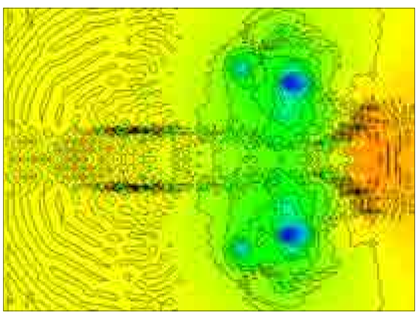
What the problem is

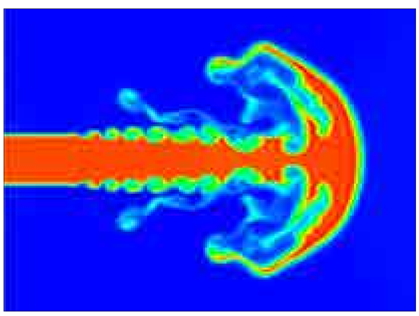
- **Turbulent flows** → High-order (central) schemes are preferred...,





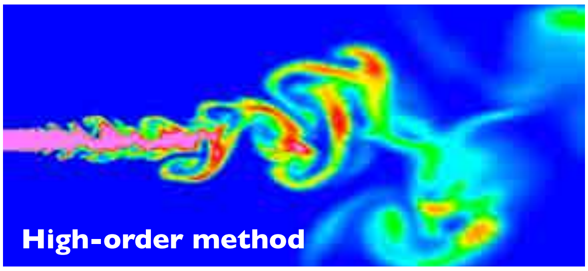
- **Large contrast:** gas-liquid-like interface → Computational instability





Superiority of high-order schemes

• To resolve a wide range of scales, acoustics, etc.,

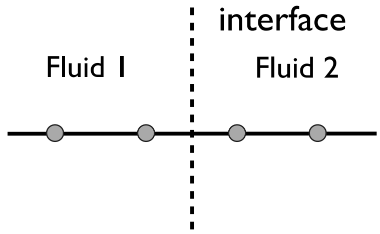


Objectives

• Propose an approach for simulating supercritical cryogenic fluids, while using high-order central differencing schemes and general EoS

• Explore some distinctive characteristics of supercritical cryogenic jet mixings

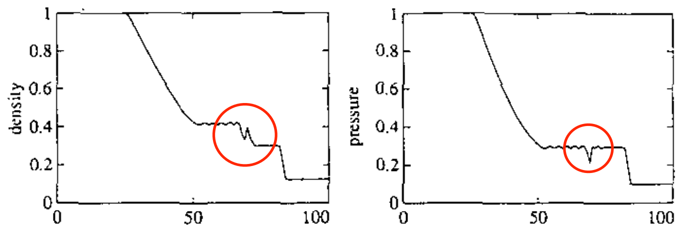
Present idea inspired by



1. Karni (JCP, 1994), Abgrall (JCP, 1996)

- maintaining velocity and pressure equilibriums at interface

- Spurious oscillations when using a conservative form in compressible multicomponent flows



Karni (JCP, 1994)

Two-component shock tube problem (calorically perfect gas EoS)

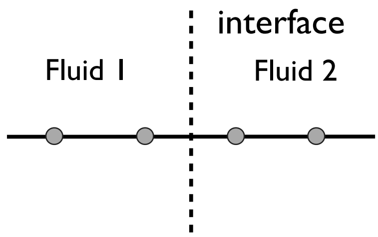
Discretization of the governing equations

- The Euler equations in an 1-D form
- Central difference discretization plus Numerical diffusion term

$$\rho_j^{n+1} = \rho_j^n - \frac{\Delta t}{\Delta x} D_j^c \left[\rho u - A_\rho\right]$$

$$(\rho u)_j^{n+1} = (\rho u)_j^n - \frac{\Delta t}{\Delta x}\left(D_j^c \left[\rho u u - A_{\rho u}\right] + D_j^c [p]\right)$$

$$E_j^{n+1} = E_j^n - \frac{\Delta t}{\Delta x} D_j^c \left[(E+p)u - A_E\right]$$



e.g.,

$D_j^c[f] = (f_{j+1} - f_{j-1})/2$: central differencing operator

$D_j^c[A.]$: numerical diffusion term

$$u_j^{n+1} = u_j^n = u$$

$$p_j^{n+1} = p_j^n = p$$

Velocity equilibrium

Considering the mass and momentum equations,

$$\rho_j^{n+1} = \rho_j^n - \frac{\Delta t}{\Delta x} u D_j^c \left[\rho - \frac{A_\rho}{u} \right]$$

$$(\rho u)_j^{n+1} = (\rho u)_j^n - \frac{\Delta t}{\Delta x} u u D_j^c \left[\rho - \frac{1}{u} \frac{A_{\rho u}}{u} \right]$$

$$\rightarrow \quad A_{\rho u} = u A_\rho$$

- The velocity and pressure are uniform across an interface at a time step

▸ The velocity is unchanged at the next time step (**oscillation-free**)

$$u_j^{n+1} = u_j^n = u$$

Pressure equilibrium

Considering the mass and energy equations,

$$\rho_j^{n+1} = \rho_j^n - \frac{\Delta t}{\Delta x} u D_j^c \left[\rho - \frac{A_\rho}{u} \right]$$

$$(\rho e + \rho \frac{uu}{2})_j^{n+1} = (\rho e + \rho \frac{uu}{2})_j^n - \frac{\Delta t}{\Delta x} \frac{uu}{2} u D_j^c \left[\frac{2}{uu} \rho e + \rho - \frac{2}{uu} \frac{A_E}{u} \right]$$

- The velocity and pressure are uniform across an interface at a time step

$$\rightarrow \quad A_E = A_{\rho e} + \frac{uu}{2} A_\rho$$

The energy equation is reduced to the internal energy equation:

$$\rightarrow \quad (\rho e)_j^{n+1} = (\rho e)_j^n - \frac{\Delta t}{\Delta x} u D_j \left[\rho e - A_{\rho e} \right]$$

Pressure equilibrium (*cont'd*)

with **a calorically perfect gas:** $p = (\gamma - 1)\rho e$

$$(\rho e)_j^{n+1} = (\rho e)_j^n - \frac{\Delta t}{\Delta x} u D_j \left[\rho e - A_{\rho e}\right]$$

↓ $A_{\rho e} = p A_\gamma$

$$\left(\frac{1}{\gamma - 1}\right)_j^{n+1} = \left(\frac{1}{\gamma - 1}\right)_j^n - \frac{\Delta t}{\Delta x} u D_j^c \left[\frac{1}{\gamma - 1} - A_\gamma\right]$$

&

$$A_E = \frac{uu}{2} A_\rho + p A_\gamma$$

- a well-known advection equation by Abgrall (JCP, 1996)

▸ The pressure is unchanged at the next time step (**oscillation-free**)

$$p_j^{n+1} = p_j^n = p$$

Summary of numerical diffusion terms (fluxes)

a calorically perfect gas

$$\begin{pmatrix} A_\rho \\ A_{\rho u} \\ A_E \end{pmatrix} = \begin{pmatrix} 1 \\ u \\ \frac{uu}{2} \end{pmatrix} A_\rho + \begin{pmatrix} 0 \\ 0 \\ p \end{pmatrix} A_\gamma$$

- serving as an interface-capturing
- velocity equilibrium
- pressure equilibrium

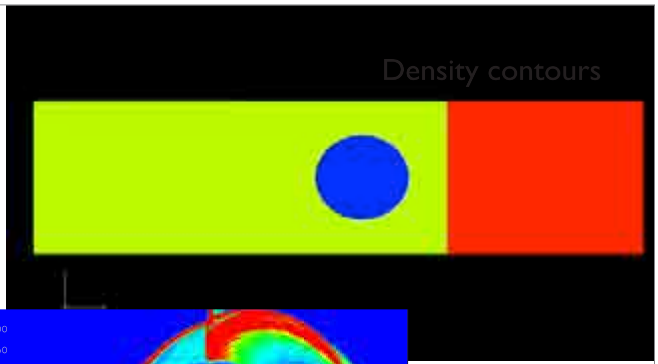
$$\left(\frac{1}{\gamma - 1}\right)_j^{n+1} = \left(\frac{1}{\gamma - 1}\right)_j^n - \frac{\Delta t}{\Delta x} u D_j^c \left[\frac{1}{\gamma - 1} - A_\gamma\right]$$

- pressure equilibrium

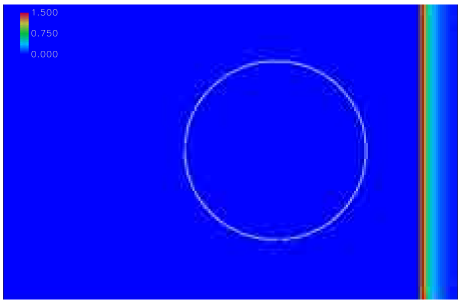
• A_ρ and A_γ modeled by extending the LAD method (Cook: JCP 2004, Kawai: JCP 2008)

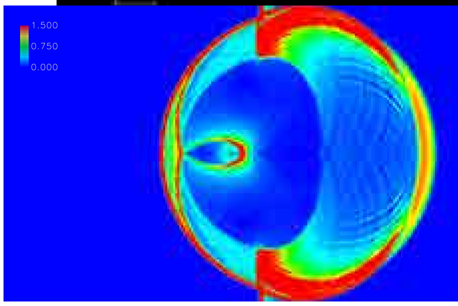
2-D shock-bubble interaction

- Experiment of Hass and Sturtevant (1987)
- 1300×361 with Δx=0.005

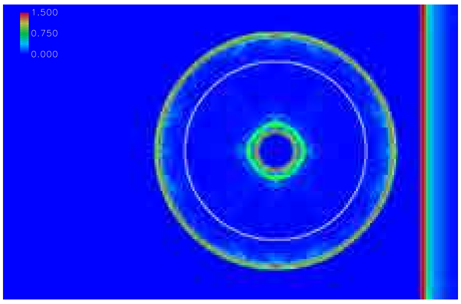


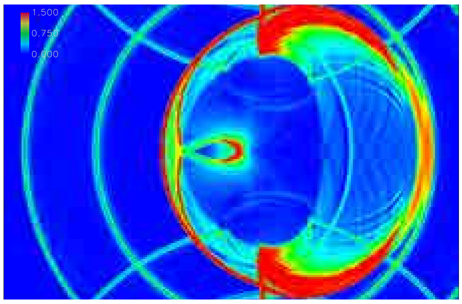
Present method Pressure gradient





FC method





Extend to general EoS: pressure equilibrium

$$(\rho e)_j^{n+1} = (\rho e)_j^n - \frac{\Delta t}{\Delta x} u D_j \left[\rho e - A_{\rho e}\right]$$

the calorically perfect gas !!

↓

$$\boxed{p = (\gamma - 1)\rho e} \longrightarrow \left(\frac{1}{\gamma-1}\right)_j^{n+1} = \left(\frac{1}{\gamma-1}\right)_j^n - \frac{\Delta t}{\Delta x} u D_j^c \left[\frac{1}{\gamma-1} - A_\gamma\right]$$

Considering a Mie-Gruneisen-type or a van der Waals equations of state,

$$\boxed{p(\rho, e, Y_i) = F(\rho, Y_i)\rho e + G(\rho, Y_i)}$$

$$\longrightarrow \quad \begin{aligned} (1/F)_i^{n+1} &= (1/F)_i^n - \frac{\Delta t}{\Delta x} u D_i \left[(1/F)\right] \\ (G/F)_i^{n+1} &= (G/F)_i^n - \frac{\Delta t}{\Delta x} u D_i \left[(G/F)\right] \end{aligned}$$

K.M. Shyue, JCP., 2001

- More complicated EOS

$$p = \frac{RT}{V - b_{srk}} - \frac{a_{srk}\alpha(T)}{V^2 + b_{srk}V}$$

: cubic EOS

$$p = \rho RT\left(1 + B(T)\rho + C(T)\rho^2 + \cdots\right)$$

: virial EOS

Look-up table-typed EOS

Attempting Abgrall's and Shyue's ideas seems to be difficult to general EOSs

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Pressure evolution equation

- Karni (1996), Fedkiw (2001)
- Single-species case considered

$$p = f(\rho, e)$$ -- (c-1)

$$\frac{Dp}{Dt} = \left(\frac{\partial p}{\partial \rho}\right)_e \frac{D\rho}{Dt} + \left(\frac{\partial p}{\partial e}\right)_\rho \frac{De}{Dt}$$

-- (c-2): Pressure evolution equation

$$\begin{aligned} &\frac{\partial p}{\partial t} + \boldsymbol{u}\cdot\nabla p \\ &= \left[\left(\frac{\partial p}{\partial \rho}\right)_e + \frac{p}{\rho^2}\left(\frac{\partial p}{\partial e}\right)_\rho\right](-\rho\nabla\cdot\boldsymbol{u}) + \left(\frac{\partial p}{\partial e}\right)_\rho\left(\frac{1}{\rho}\nabla\cdot(\boldsymbol{\tau}\cdot\boldsymbol{u} - \boldsymbol{q})\right) \\ &= -\rho c^2\nabla\cdot\boldsymbol{u} + \frac{\alpha_p}{c_v\beta_T}\left(\frac{1}{\rho}\nabla\cdot(\boldsymbol{\tau}\cdot\boldsymbol{u} - \boldsymbol{q})\right) \end{aligned}$$

-- (c-3)

$$c = \left(\frac{\partial p}{\partial \rho}\right)_s = \left(\frac{\partial p}{\partial \rho}\right)_e + \frac{p}{\rho^2}\left(\frac{\partial p}{\partial e}\right)_\rho$$

$$c_v = \left(\frac{\partial e}{\partial T}\right)_V \quad \alpha_p = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p \quad \beta_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T$$

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The proposed governing equations set

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

- Interface-capturing

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u} + p\boldsymbol{\delta} - \boldsymbol{\tau}) = \boxed{\nabla \cdot (\varrho_\rho (\boldsymbol{u} \otimes \boldsymbol{g}) \nabla \rho)},$$

- Velocity equilibrium

$$\boxed{\frac{\partial p}{\partial t} + \boldsymbol{u} \cdot \nabla p = -\rho c^2 \nabla \cdot \boldsymbol{u} + \frac{\alpha_p}{c_v \beta_T} \left(\frac{1}{\rho} \nabla \cdot (\boldsymbol{\tau} \cdot \boldsymbol{u} - \boldsymbol{q}) \right)},$$

- Pressure equilibrium

$$p = \frac{RT}{V - b_{srk}} - \frac{a_{srk}\alpha(T)}{V^2 + b_{srk}V}$$

$$\varrho_\rho = C_\rho \frac{c}{\rho} \overline{\left| \sum_{l=1}^{n_d} \frac{\partial^r \rho}{\partial x_l^r} \Delta_l^{r+1} \right|}$$

Disadvantage: the energy is not conserved, resulting in incorrect shock strength or speed, while the mass and momentum are conserved

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Numerical methods

- Sixth-order compact difference scheme
- Eighth-order low-pass filtering (a free-parameter: 0.495)
- Third-order TVD Runge-Kutta scheme

- CFL = 0.4
- One-point jump at initial condition

- FC method: conventional fully conservative method

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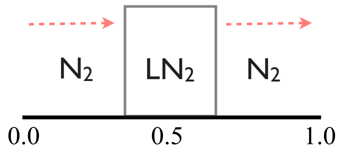
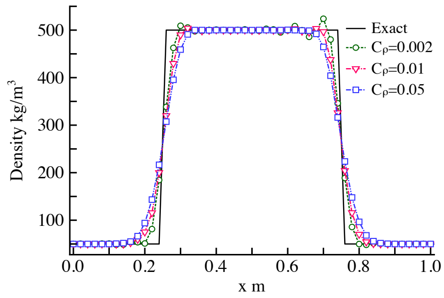
Advection of a contact discontinuity

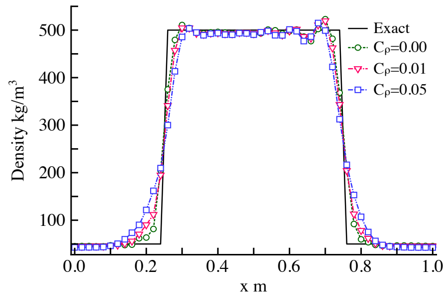
- 51 grid points with Δx=0.02
- Nitrogen single-species flow
- 5.0 MPa
- Density: 500/50, Temperature: 123/332

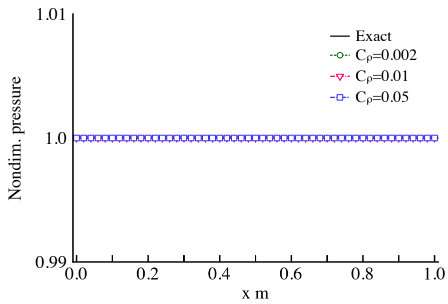


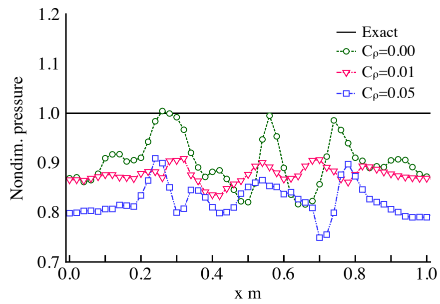
Present method

FC method





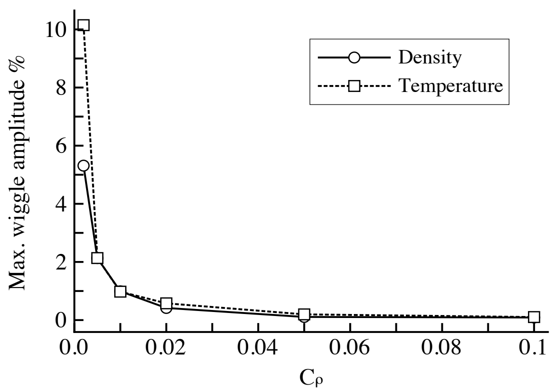


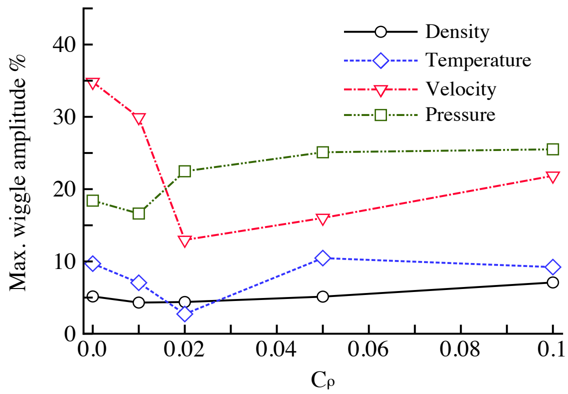


Unfavorable characteristics of a full conservation form

Present method

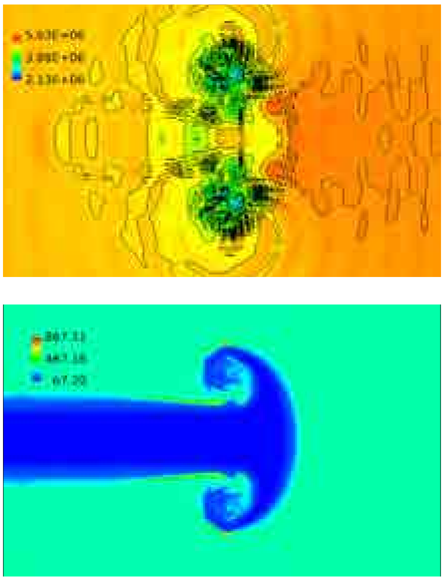
FC method



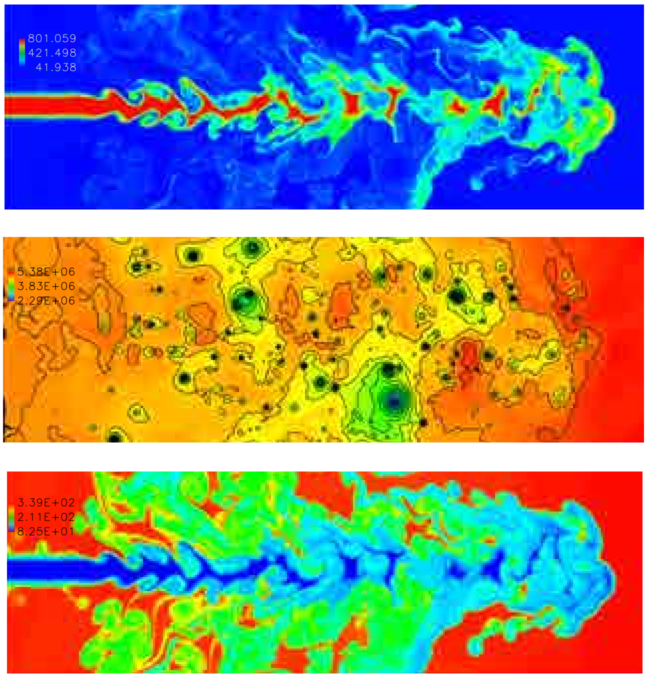


Performance of the proposed model

- Cryogenic nitrogen jet: Density: 800/50 kg/m^3, Temperature: 83/332 K, 5 MPa



Conventional (FC) method

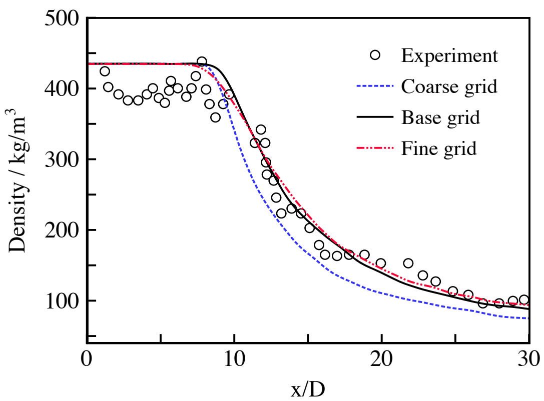


Proposed method

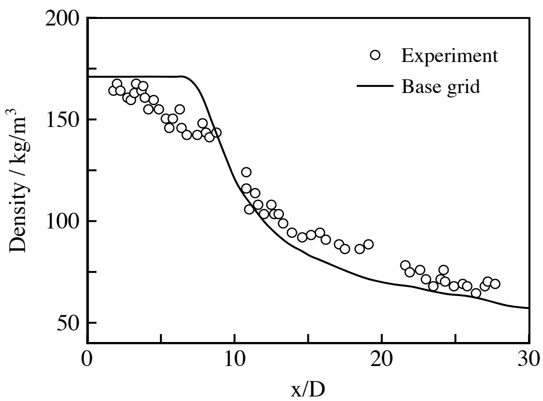
Validation of the proposed model

- Supercritical 3-D round jet in Mayer's experiment (Mayer et al., HMT 2003)

Case 3: T = 126 K, 4 MPa



Case 4: T = 137 K, 4 MPa

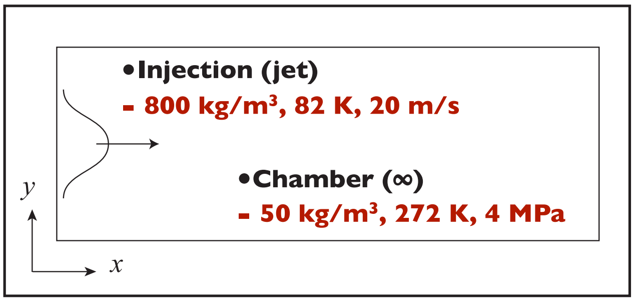


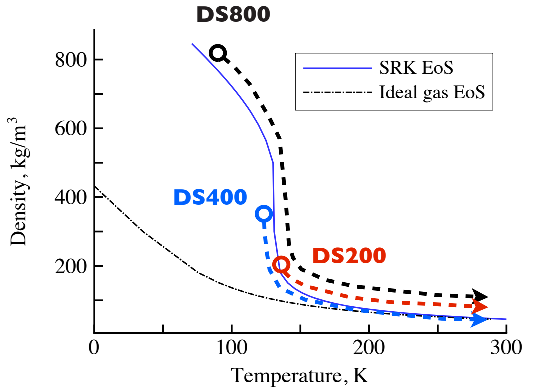
Density iso-surface and contours

Conditions

$p_{cr} = 3.4$ MPa, $T_{cr} = 126.2$ K, $\rho_{cr} = 313.3$ kg/m^3

- Two-dimensional planar N_2 (single-specie) jet in supercritical pressure conditions
- 4 and 8 MPa





*Pseudo-critical temperature: 128 K at 4 MPa

Table 1. Conditions for 4 MPa case.

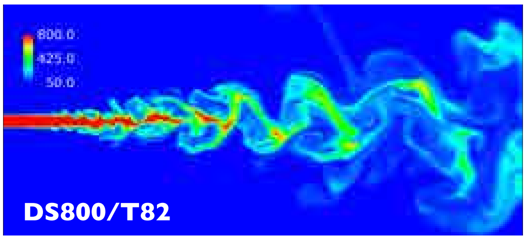
ρ_{jet} kg/m^3	u_{jet} m/s	T_{jet} K	Re$_{jet}$ $\times 10^5$	ρ_∞ kg/m^3	T_∞ K
800	20	82.1	1.2		
400	$20\sqrt{2}$	126.9	3.6	50.0	271.13
200	40	132.9	4.5		

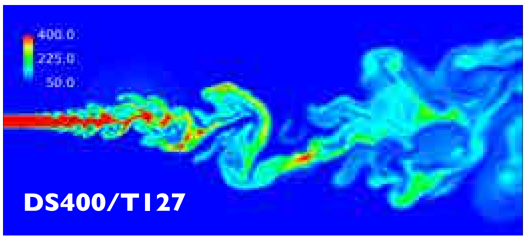
*the same momentum used for jet

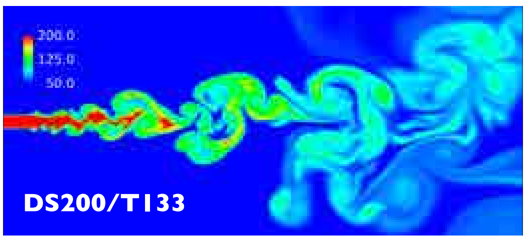
A unsteady jet mixing

T=100 K injection, 5 MPa

- Statistical data obtained over 10 ms

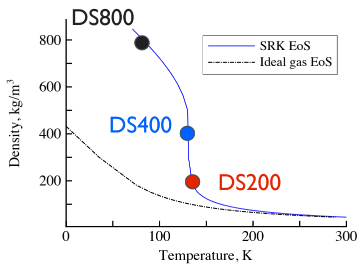


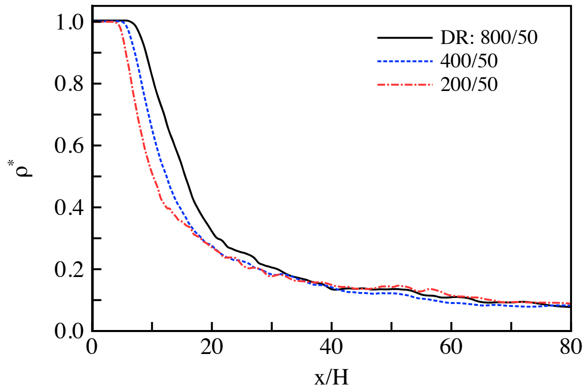


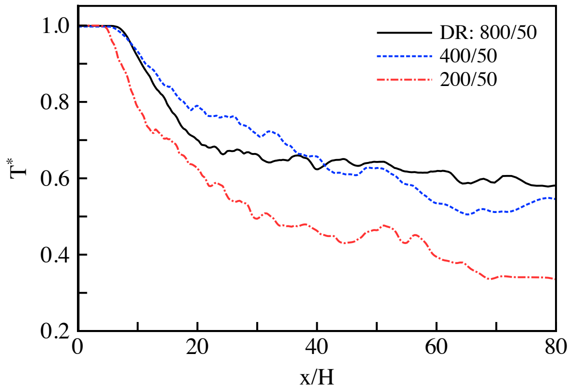


Results: mean properties on centerline

- 4 MPa



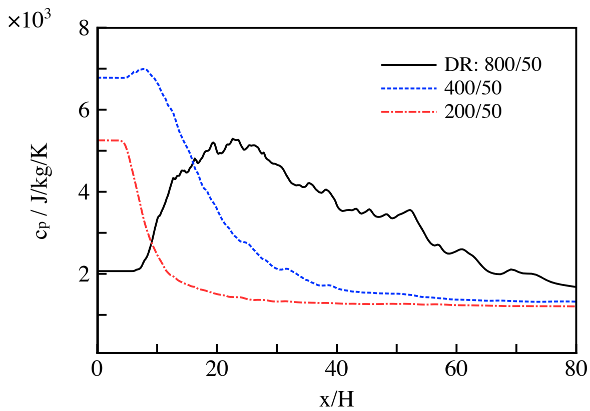


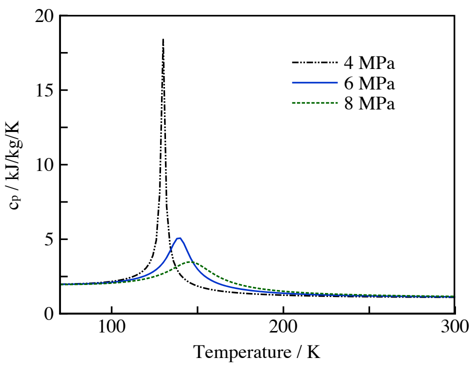


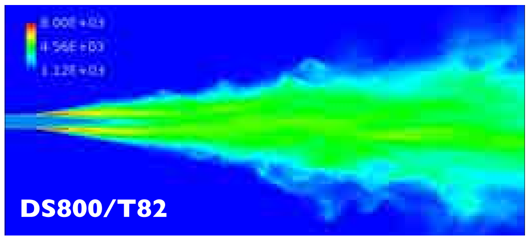
$$\rho^* = \frac{\rho - \rho_\infty}{\rho_{inj} - \rho_\infty}$$

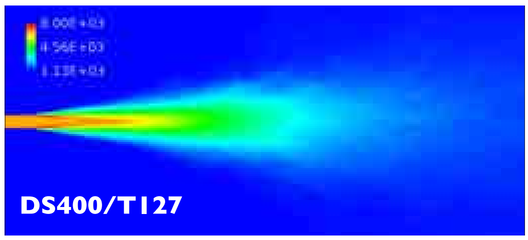
$$T^* = \frac{T - T_\infty}{T_{inj} - T_\infty}$$

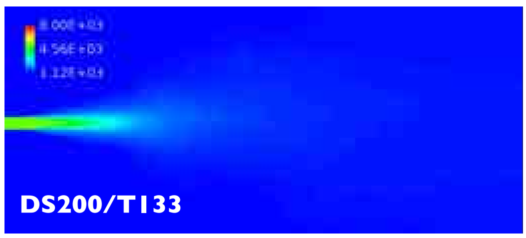
Why it happened: mean specific heat distributions



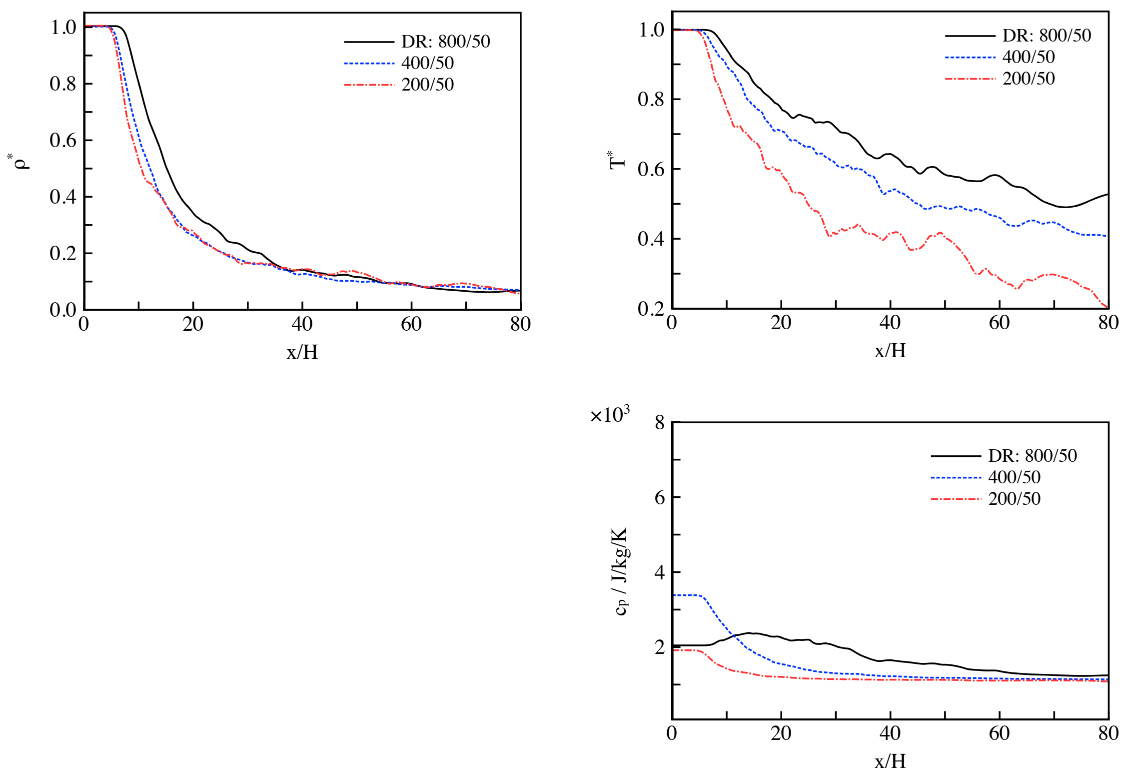








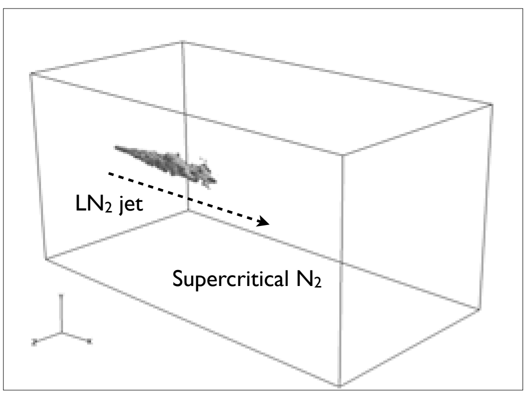
8 MPa case

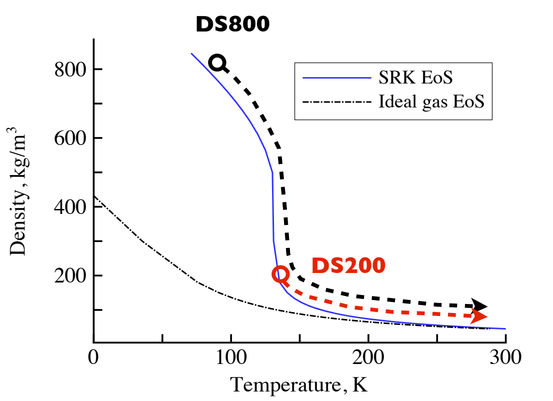


Demonstration on 3-D jet

$p_{cr} = 3.4$ MPa, $T_{cr} = 126.2$ K, $\rho_{cr} = 313.3$ kg/m^3

- Three-dimensional round N_2 (single-specie) jet in supercritical pressure conditions
- Injection geometry just changed: 2-D slit to 3-D circle, others are the same as the 2-D conditions
- Case1: 4 MPa, **82 K**, Case 2: 4 MPa, **133 K**





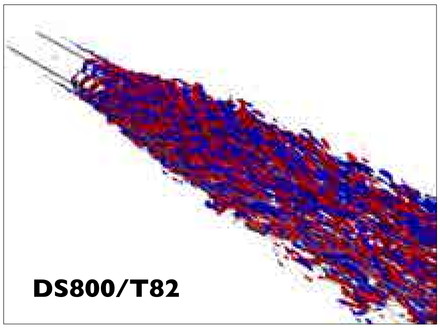
*Pseudo-critical temperature: 128 K at 4 MPa

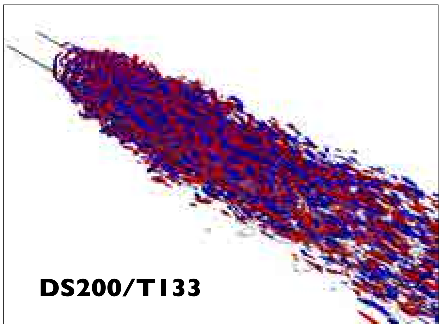
- 398×293×293 grid points used

3-D Results

$p_{cr} = 3.4\ \mathrm{MPa}, \quad T_{cr} = 126.2\ \mathrm{K}, \quad \rho_{cr} = 313.3\ \mathrm{kg/m^3}$

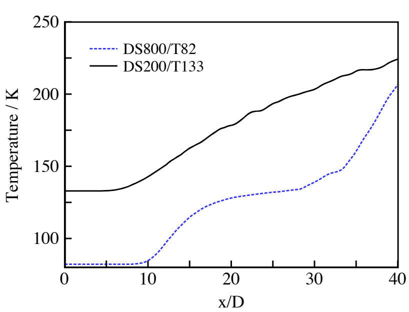
- There is no clear difference of vortical structures

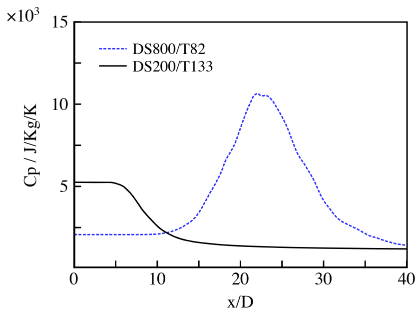




- Flattened temperature distribution appeared also in the 3-D round jet

*Pseudo-critical temperature: 128 K at 4 MPa





Summary

- A strategy for simulating gas-liquid-like flows under supercritical pressures proposed

Satisfying the pressure and velocity equilibriums is a key to robust application of high-order schemes to severe thermodynamic fluid conditions

Terashima and Koshi, J. Computational Physics, 231(2012)

- A unique characteristic of supercritical jets successfully explored

The distinctive features of temperature caused by the interaction of multiple factors: a very low temperature injection, a variation of the specific heat, and mixing process