

Numerical Approach on Hydrogen Detonation: Fundamentals and Applications -Part 1-

2007.08.02

Nobuyuki TSUBOI
ISAS/JAXA, Japan



Overview

1. Motivations

2. Numerical simulation for compressible
high speed flow

(1) Scalar equations

(2) System equations

(3) System equations with chemical reactions

3. Summary

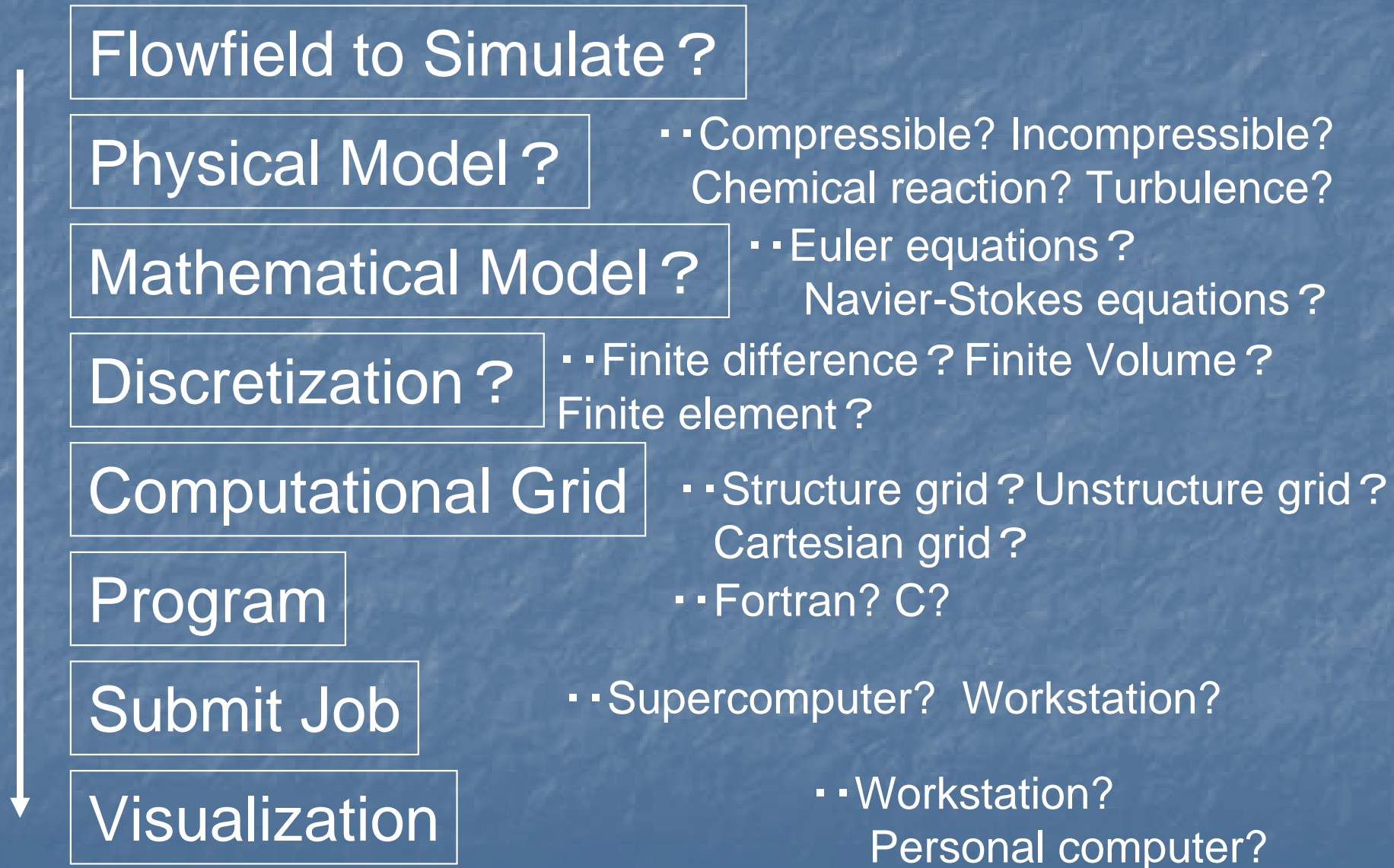
Motivations

1. Hydrogen/air mixture: detonable gas
2. Detonation: shock induced combustion
 - Pressure behind detonation increases about 10 times ambient pressure
3. Closed environment such as a tunnel causes serious accident.

Numerical Simulations

1. Detonation as well as thermal and gas dynamic phenomena of airplane and aerospace plane are elucidated numerically.
2. Main issues
 - (1) Robust numerical scheme for high pressure and temperature
 - (2) Stiff problem: chemical characteristic time is much faster than the fluid characteristic time
 - (3) Chemical reaction model for high pressure combustion
 - (4) Unsteadiness, turbulence, and three-dimensional problems

Flow Chart of Numerical Simulations



Numerical Model

Mathematical Model	Target	Level
Panel Method Potential Eq.	w/o separation less turbulence	Conceptual design
Euler Eq.	Shock	Conceptual design
RANS(Reynolds averaged Navier- Stokes Eq.)	Boundary layer, separation	Academic research, Detailed design
LES(Large Eddy Simulation)	Solve scale vortices smaller than grid	Academic research
DNS(Direct Numerical Simulation)	Solve all vortices	Academic research

Computational Grids

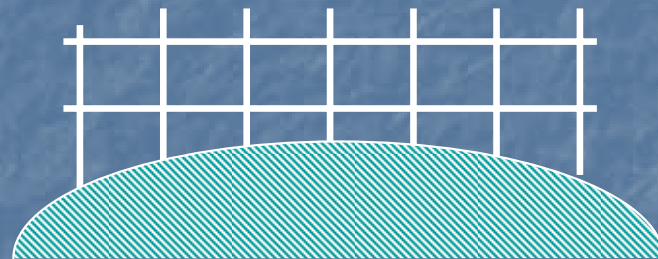
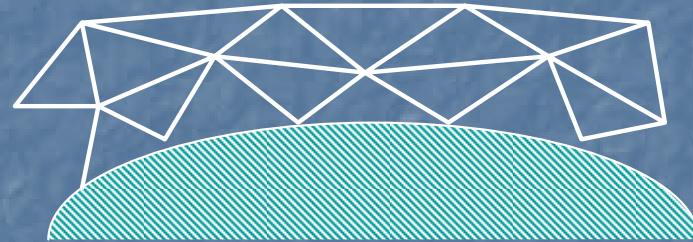
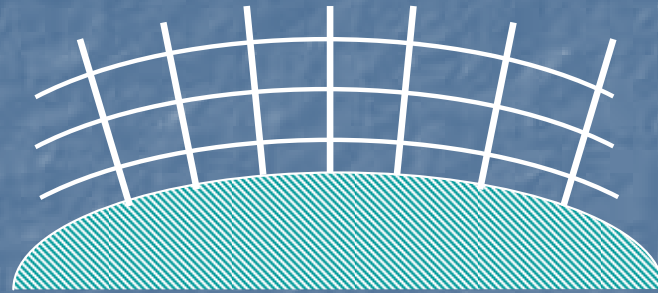
Structured grid ?

Unstructured grid ?

Cartesian grid ?

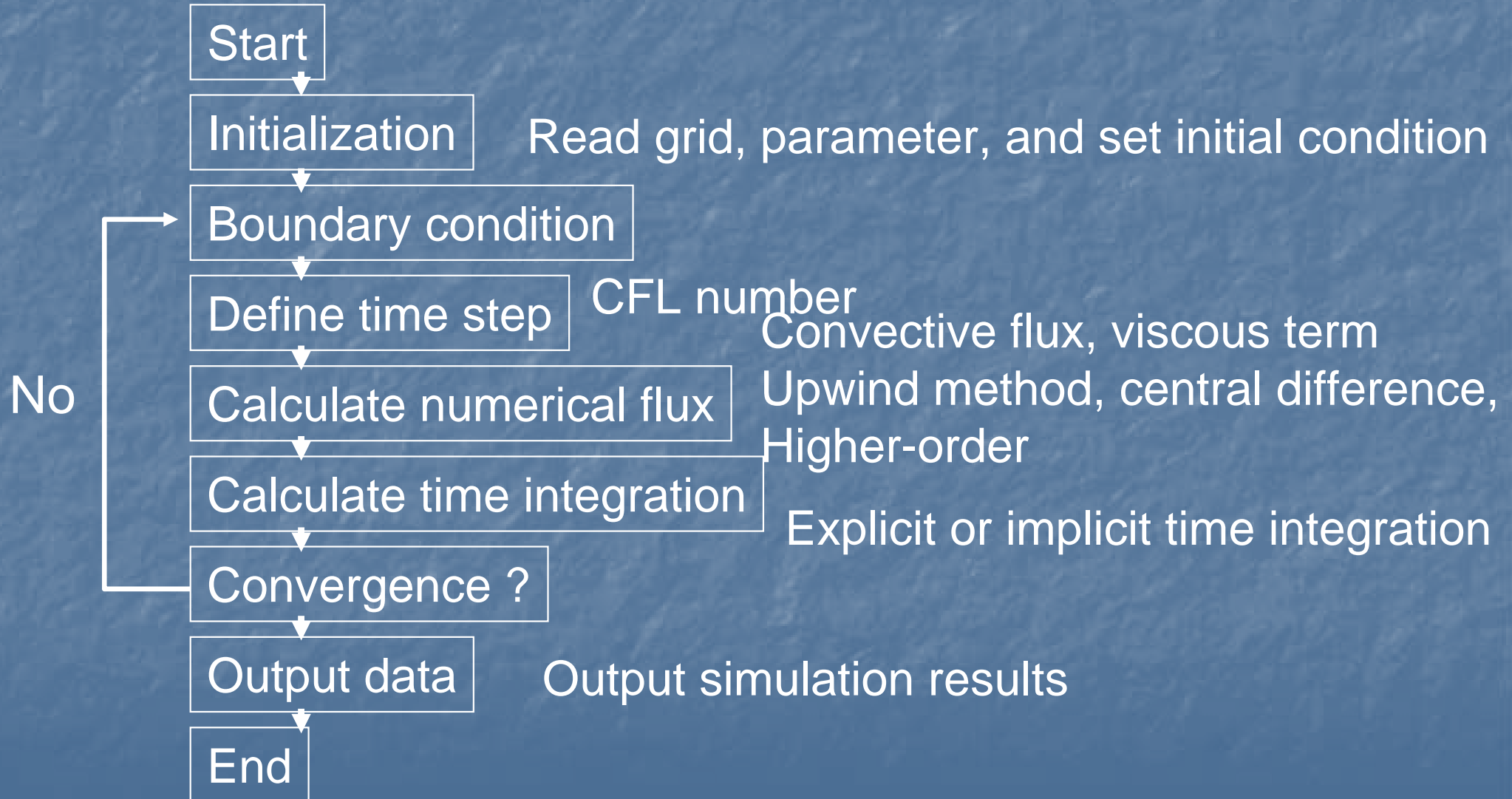
How to make grids ?

- Commercial software ?
- Make by oneself ?



Numerical analysis for fluid: finite different method

Flowchart of program is defined after discretization and grid are decided

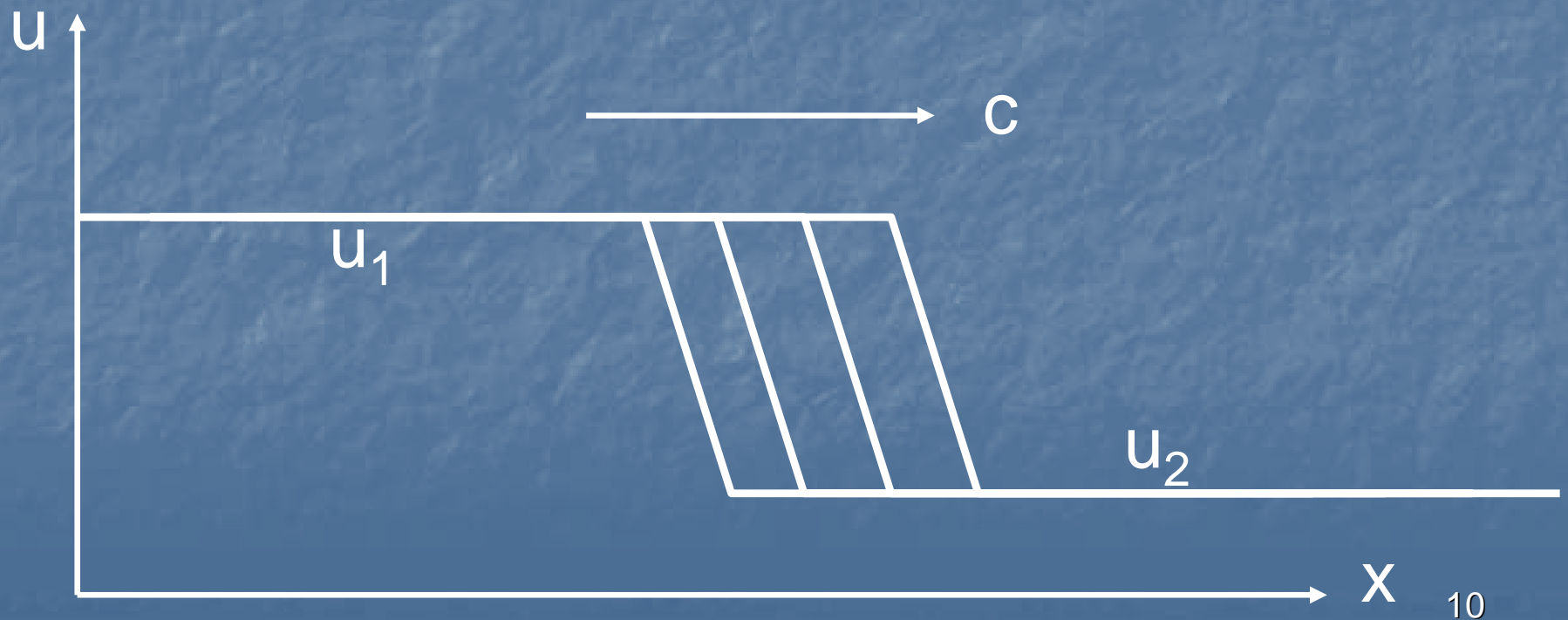


Scalar Equation

Finite Difference for Scalar Equation

Wave equation ▪▪ wave propagates with speed, c

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0$$



$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0$$

FTCS (Forward in Time and Central Difference in Space)

$$u_j^{n+1} = u_j^n - \frac{c}{2} \left(\frac{\Delta t}{\Delta x} \right) (u_{j+1}^n - u_{j-1}^n)$$

- Explicit+central difference:unstable
- CFL number: parameter to govern numerical stability

$$v = c \left(\frac{\Delta t}{\Delta x} \right)$$

Lax method

$$u_j^{n+1} = \frac{1}{2} (u_{j-1}^n + u_{j+1}^n) - \frac{c}{2} \left(\frac{\Delta t}{\Delta x} \right) (u_{j+1}^n - u_{j-1}^n)$$

More stable than FTCS
Large numerical dissipation

Lax-Wendroff method 2nd order in space and time

$$u_j^{n+1} = u_j^n - \frac{c}{2} \left(\frac{\Delta t}{\Delta x} \right) (u_{j+1}^n - u_{j-1}^n) + \frac{c^2}{2} \left(\frac{\Delta t}{\Delta x} \right)^2 (u_{j+1}^n - 2u_j^n + u_{j-1}^n)$$

First-order upwind method (Upwind difference)

$$u_j^{n+1} = u_j^n - c \left(\frac{\Delta t}{\Delta x} \right) (u_j^n - u_{j-1}^n)$$

- Find direction which wave propagates and use upwind data only

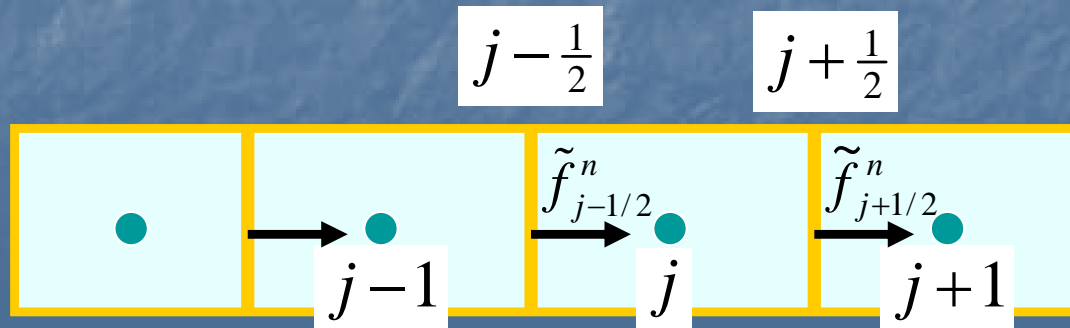
Pseudo-finite volume method

- **Conservation form**

- Non-linear equation with discontinuous wave can be calculate and discreted
- Compressible equations is based on this concept

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0, \quad \underline{f = cu} \quad \text{Flux}$$

$$u_j^{n+1} = u_j^n - \left(\frac{\Delta t}{\Delta x} \right) \left(\tilde{f}_{j+1/2}^n - \tilde{f}_{j-1/2}^n \right) \quad \tilde{f}_{j+1/2}^n : \text{Numerical flux}$$



$$u_j^{n+1} = u_j^n - \left(\frac{\Delta t}{\Delta x} \right) \left(\tilde{f}_{j+1/2}^n - \tilde{f}_{j-1/2}^n \right)$$

For example, FTCS is applied,

$$\begin{aligned} u_j^{n+1} &= u_j^n - \frac{c}{2} \left(\frac{\Delta t}{\Delta x} \right) (u_{j+1}^n - u_{j-1}^n) \\ &= u_j^n - \frac{1}{2} \left(\frac{\Delta t}{\Delta x} \right) \left\{ (cu_{j+1}^n + cu_j^n) - (cu_j^n + cu_{j-1}^n) \right\} \\ &= u_j^n - \left(\frac{\Delta t}{\Delta x} \right) \left(\tilde{f}_{j+1/2}^n - \tilde{f}_{j-1/2}^n \right) \end{aligned}$$

Therefore

$$\tilde{f}_{j+1/2}^n = \frac{1}{2} (f_{j+1}^n + f_j^n) = \frac{c}{2} (u_{j+1}^n + u_j^n)$$

There exist many numerical schemes, however, these schemes are designed how to estimate numerical flux $\tilde{f}_{j+1/2}^n$

FTCS

$$\tilde{f}_{j+1/2}^n = \frac{1}{2}(f_{j+1}^n + f_j^n) = \frac{c}{2}(u_{j+1}^n + u_j^n)$$

Lax

$$\tilde{f}_{j+1/2}^n = \frac{c}{2}(u_{j+1}^n + u_j^n) - \frac{1}{2}\left(\frac{\Delta x}{\Delta t}\right)(u_{j+1}^n - u_j^n)$$

Lax-Wendroff

$$\tilde{f}_{j+1/2}^n = \frac{c}{2}(1 + \nu)u_j + \frac{c}{2}(1 - \nu)u_{j+1} = c\left[u_j + \frac{1}{2}(1 - \nu)(u_{j+1} - u_j)\right]$$

1st order upwind difference

$$\tilde{f}_{j+1/2}^n = \frac{c}{2}(u_{j+1}^n + u_j^n) - \frac{c}{2}(u_{j+1}^n - u_j^n) = cu_j^n = f_j^n$$

$$\nu = c\left(\frac{\Delta t}{\Delta x}\right)$$

1st order upwind difference

$$\tilde{f}_{j+1/2}^n = \frac{c}{2}(u_{j+1}^n + u_j^n) - \frac{c}{2}(u_{j+1}^n - u_j^n) = cu_j^n = \underline{f_j^n}$$

When sign of c is unclear, summarized as follows:

$$\tilde{f}_{j+1/2}^n = \begin{cases} f_j^n, & 0 \leq c \\ f_{j+1}^n, & c \leq 0 \end{cases}$$

$$\begin{aligned} \tilde{f}_{j+1/2}^n &= \frac{c - |c|}{2} u_{j+1} + \frac{c + |c|}{2} u_j \\ &= \frac{1}{2} [(cu_{j+1} + cu_j) - |c|(u_{j+1} - u_j)] \\ &= \frac{1}{2} [(f_{j+1} + f_j) - |c|(u_{j+1} - u_j)] \end{aligned}$$

TVD (Total Variation Diminishing) Method

1st order upwind
difference

$$\tilde{f}_{j+1/2}^n = cu_j^n$$

Lax-Wendroff

$$\begin{aligned}\tilde{f}_{j+1/2}^n &= \frac{c}{2}(1+v)u_j + \frac{c}{2}(1-v)u_{j+1} \\ &= c\left[u_j + \frac{1}{2}(1-v)(u_{j+1} - u_j)\right]\end{aligned}$$

L-W scheme = 1st order upwind + modified flux
→ 2nd order

$$\tilde{f}_{j+1/2}^n = c \left[u_j + \frac{1}{2} (1 - \nu) (u_{j+1} - u_j) \right]$$

$$\sigma(c) \cong \frac{1}{2} c (1 - \nu)$$

modified flux

L-W scheme generates numerical oscillation.
Another scheme added non-linear flux is introduced.

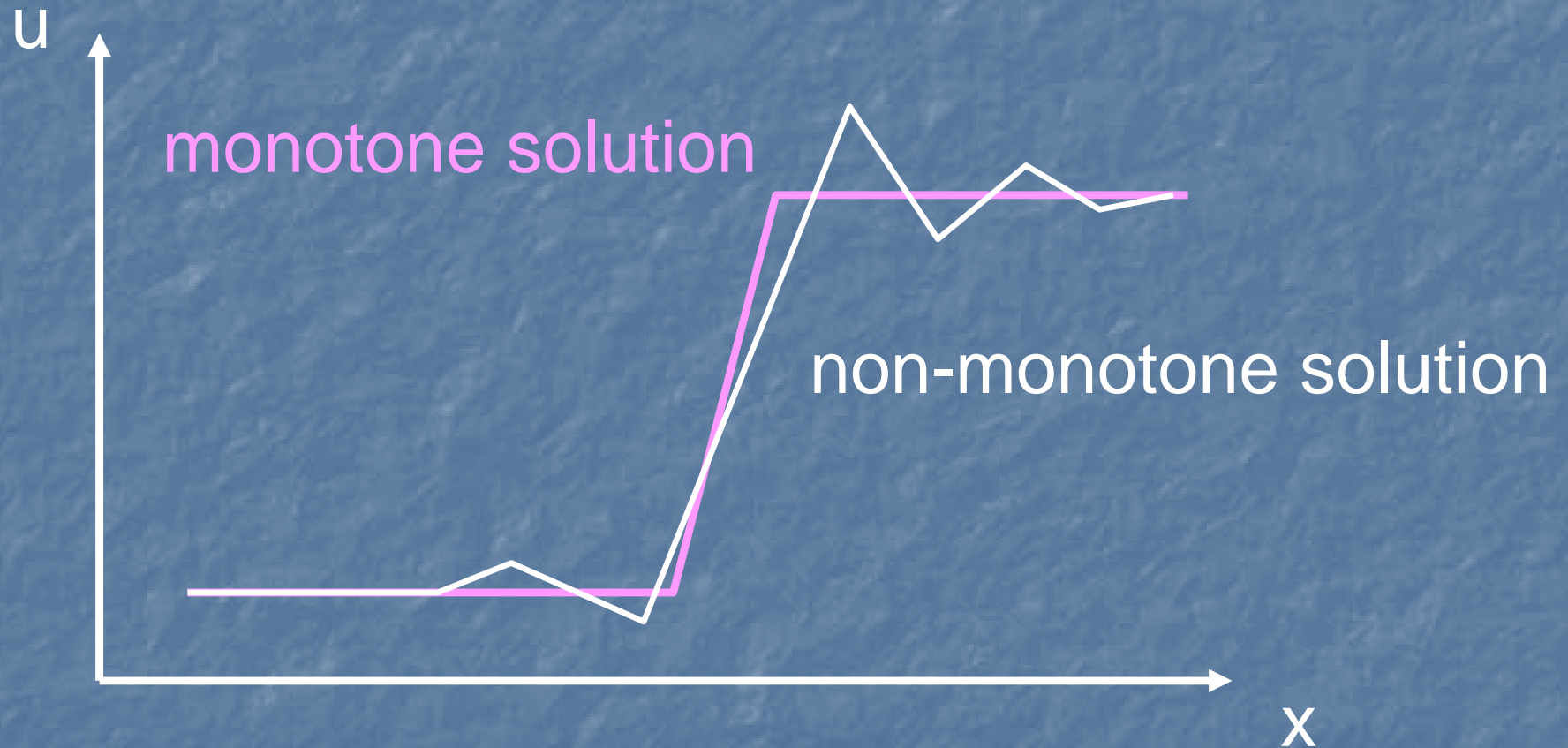
$$\tilde{f}_{j+1/2}^n = c \left[u_j + \frac{1}{2} B_{j+1/2} (1 - \nu) (u_{j+1} - u_j) \right]$$

flux limiter function

When B select well, monotone scheme, which is almost higher order and becomes 1st order near discontinuity, can be created

- Modified flux method proposed by Harten

What is monotone scheme?



Monotone imply a property to become 1st order near discontinuity

TVD(Total Variation Diminishing) Method

Total variation in space at a time defines as follows:

$$TV(u^n) = \sum_j |u_{j+1}^n - u_j^n| \quad : \text{Total variation}$$

TV stability: Total variation decrease with time (diminishing) • • TVD condition

$$TV(u^{n+1}) \leq TV(u^n)$$

Scheme which is satisfied this condition is called TVD scheme.

TVD(Total Variation Diminishing) Method

TVD scheme means to preserve monotone profile

$$u_j^{n+1} = u_j^n + \frac{\Delta t}{\Delta x} [c_{j+1/2}^- (u_{j+1} - u_j) + c_{j-1/2}^+ (u_j - u_{j-1})]$$

In order to preserve monotone,

CFL condition

$$c_{j+1/2}^- > 0, \quad c_{j-1/2}^+ > 0, \quad \frac{\Delta t}{\Delta x} (c_{j+1/2}^- - c_{j-1/2}^+) \leq 1$$

For example, 1st order upwind difference is TVD scheme.

monotone
TVD scheme

Higher order Numerical Flux

$$\tilde{f}_{j+1/2}^n = \begin{cases} f_j^n = cu_j^n, & 0 \leq c \\ f_{j+1}^n = cu_{j+1}^n, & c \leq 0 \end{cases}$$

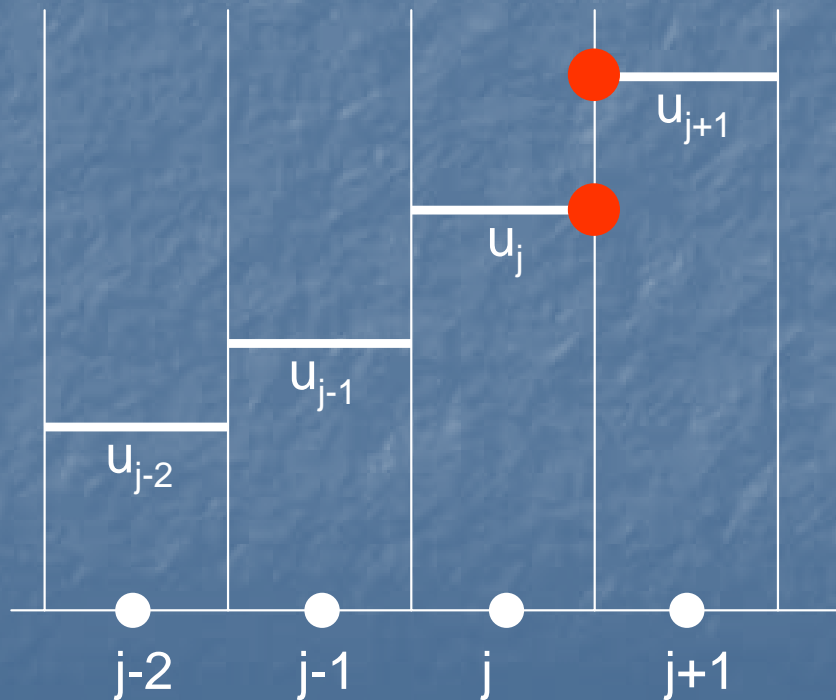
From

piecewise constant in cell

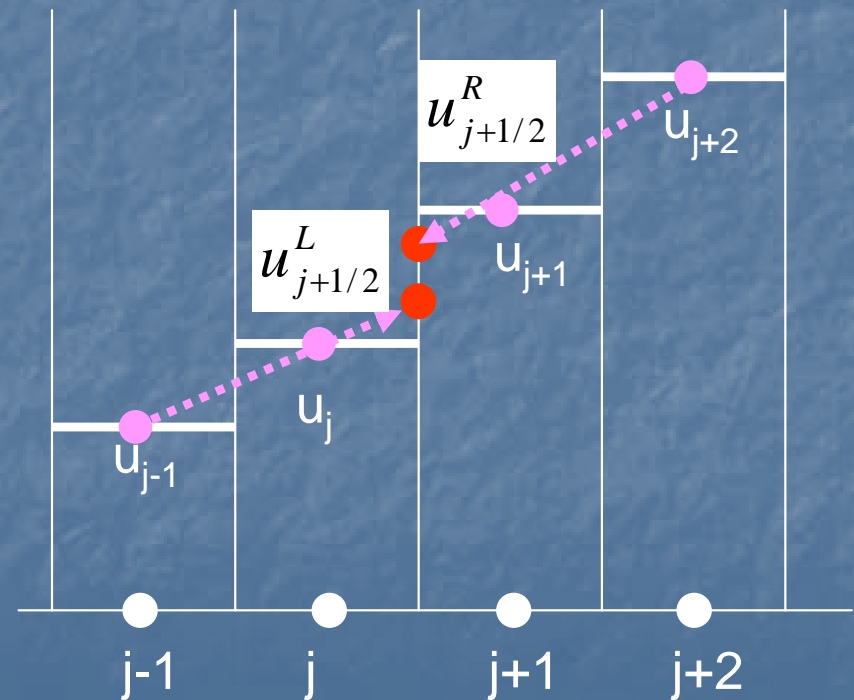
to

piecewise linear in cell

- • cause oscillate solutions!

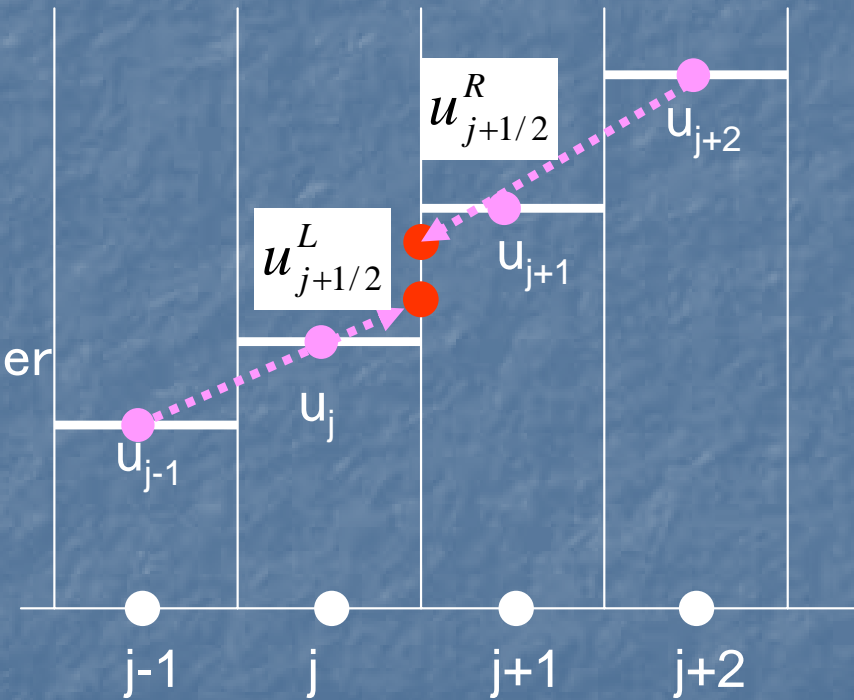
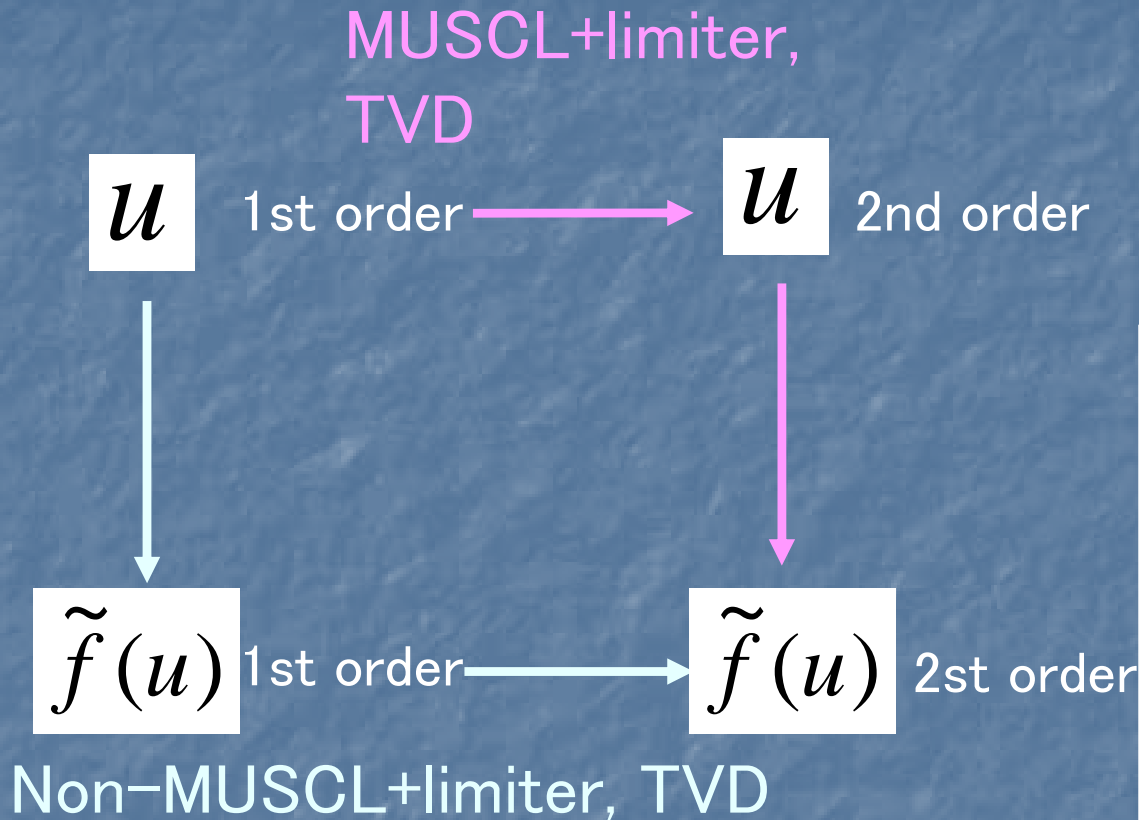


piecewise constant



piecewise linear

Higher order Numerical Flux

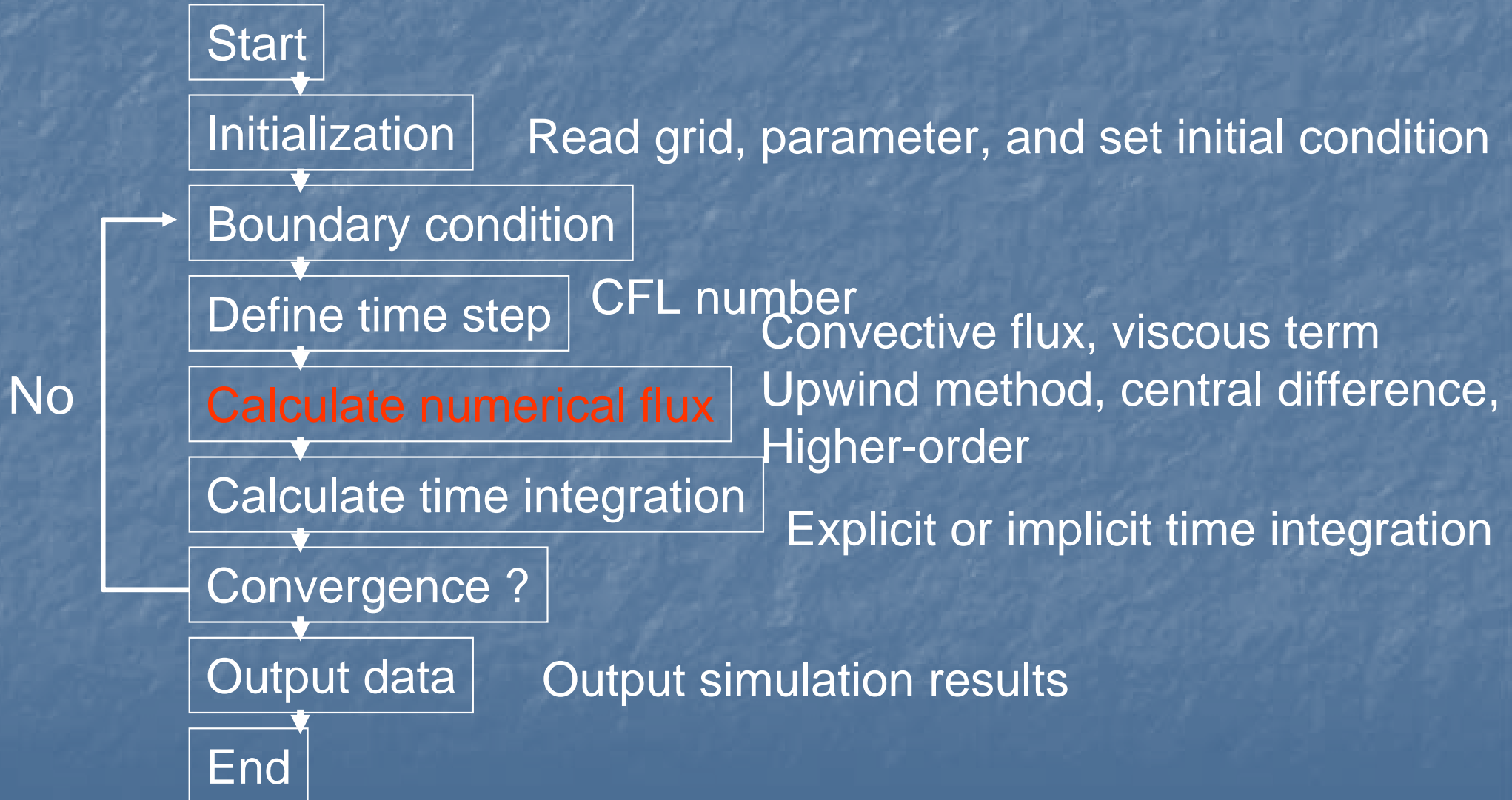


MUSCL: Monotone Upstream-centred Schemes for Conservation Laws

System Equation

Numerical Analysis for Fluid: Finite Different Method

Define flowchart of program after discretization and grid are decided



Solution of scalar equation

- Non-linear
 - Previous discussion assumed as linear equation
- Simultaneous equations
 - Difficult to find the upwind direction

Therefore,

- Linearization is necessary
- Decompose to some wave equations in order to define the upwind direction

Solution of system equations

Discretization of System Equations

1-D Compressible Euler Equations

Mass
conservation

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0$$

Momentum
conservation

$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = 0$$

Energy
conservation

$$\frac{\partial e}{\partial t} + \frac{\partial ((e + p)u)}{\partial x} = 0$$

Equation of State
(Ideal Gas)

$$p = \rho R T$$

where

$$e + p = h = \rho H$$

Enthalpy per unit mass

where, (ideal gas)

$$e = \rho \left(E + \frac{u^2}{2} \right) = \frac{P}{\gamma - 1} + \frac{1}{2} \rho u^2$$

Internal energy per unit mass

$$E = \frac{1}{\gamma - 1} \frac{p}{\rho} = \frac{1}{\gamma - 1} RT = C_v T$$

Enthalpy per unit mass

Enthalpy per unit volume

$$H = \frac{h}{\rho} = \frac{e + p}{\rho} = \frac{1}{\rho} \left(\frac{p}{\gamma - 1} + \frac{1}{2} \rho u^2 + p \right)$$
$$= \frac{\gamma}{\gamma - 1} \frac{p}{\rho} + \frac{1}{2} u^2 = \frac{\gamma}{\gamma - 1} RT + \frac{1}{2} u^2 = C_p T + \frac{1}{2} u^2$$

Vector form of governing equations:

1-D

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} = 0$$

$$Q = \begin{pmatrix} \rho \\ \rho u \\ e \end{pmatrix}, E = \begin{pmatrix} \rho u \\ p + \rho u^2 \\ (e + p)u \end{pmatrix}$$

2-D

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = 0$$

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{bmatrix}, E = \begin{bmatrix} \rho u \\ p + \rho u^2 \\ \rho uv \\ (e + p)u \end{bmatrix}, F = \begin{bmatrix} \rho v \\ \rho vu \\ p + \rho v^2 \\ (e + p)v \end{bmatrix}$$

Governing equation is linearized

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} = 0 \quad \longrightarrow \quad \frac{\partial Q}{\partial t} + A \frac{\partial Q}{\partial x} = 0$$

$$A = \frac{\partial E}{\partial Q} = \begin{pmatrix} 0 & 1 & 0 \\ -\frac{3-\rho}{2}u^2 & (3-\gamma)u & \rho-1 \\ (\frac{\rho-1}{2}u^2 - h)u & h - (\rho-1)u^2 & \rho u \end{pmatrix}$$

Property of 1-D Euler equations

Derive eigen value λ

$$A\vec{w} = \lambda\vec{w}$$

$$\begin{vmatrix} -\lambda & 1 & 0 \\ -\frac{3-\rho}{2}u^2 & (3-\gamma)u - \lambda & \rho - 1 \\ (\frac{\rho-1}{2}u^2 - h)u & h - (\rho-1)u^2 & \rho u - \lambda \end{vmatrix} = 0$$

then, $(u - \lambda) \left((u - \lambda)^2 - \gamma \frac{p}{\rho} \right) = 0$

Eigen values are

$$\lambda = u, u + c, u - c$$

Speed of sound:

$$c = \sqrt{\gamma \frac{p}{\rho}}$$

For 2-D, eigen values include another u

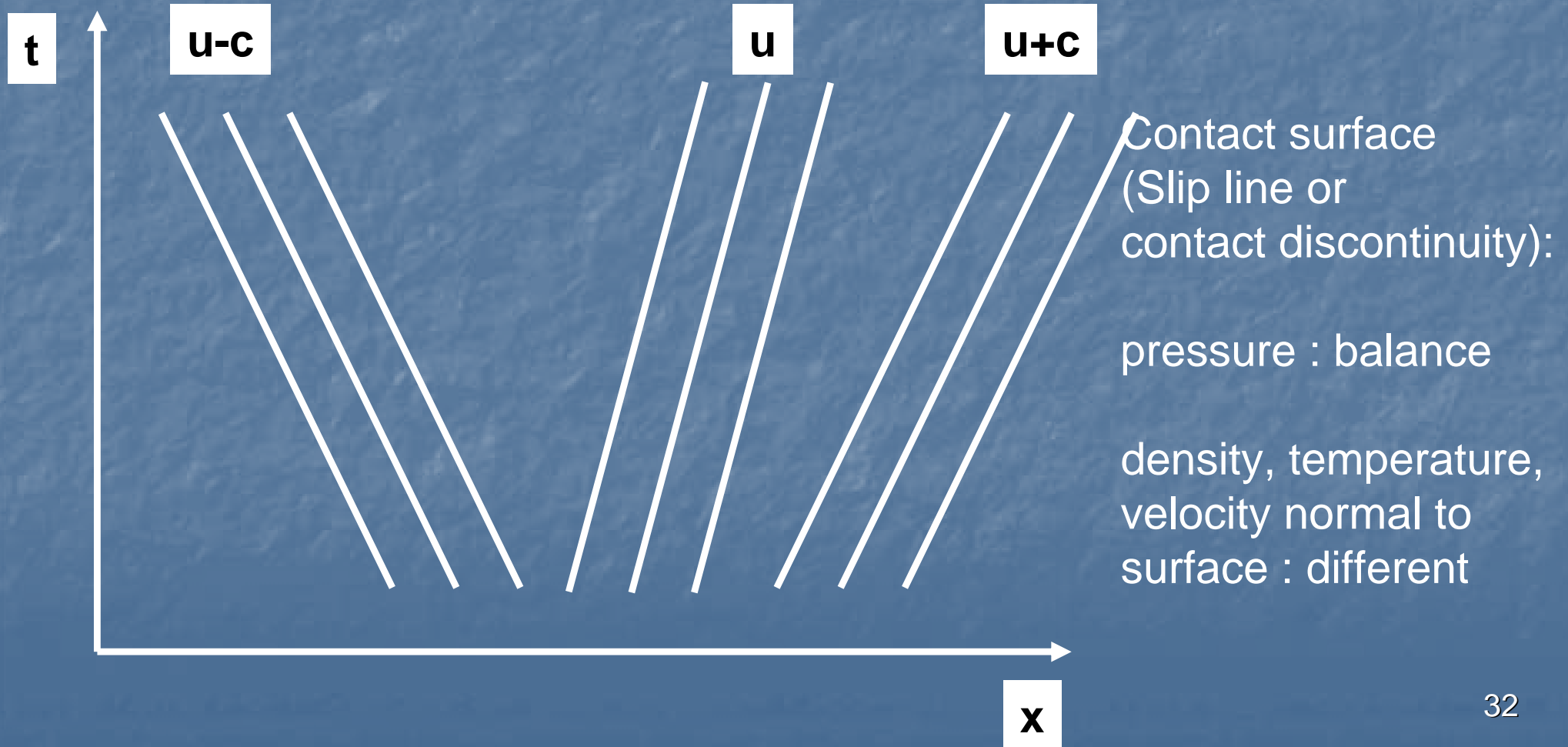
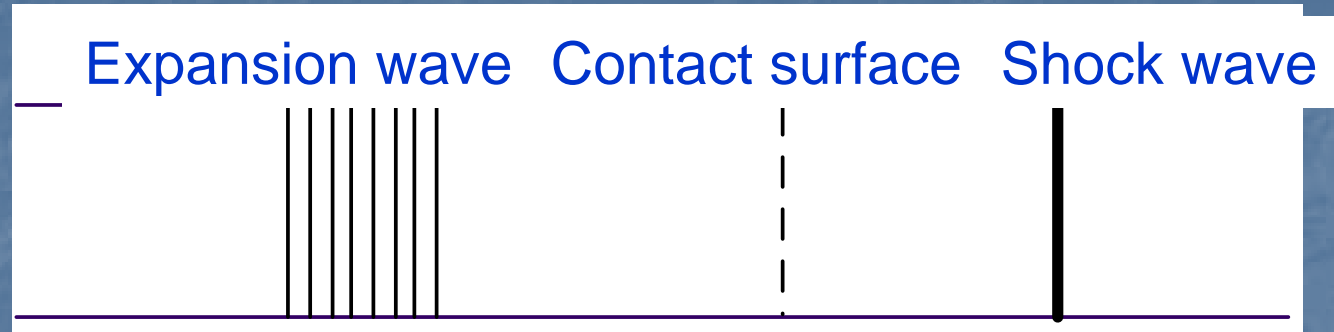
How to derive Jacobian matrix:

$$Q = \begin{pmatrix} \rho \\ m \\ e \end{pmatrix}, E = \begin{pmatrix} m \\ m^2 / \rho + p \\ (e + p) \frac{m}{\rho} \end{pmatrix}$$

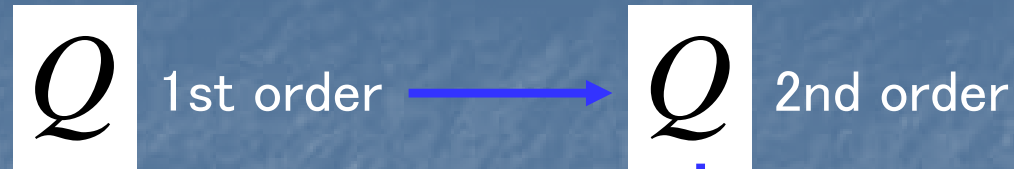
$$p = (\gamma - 1) \left(e - \frac{1}{2} \frac{m^2}{\rho} \right)$$

$$A = \frac{\partial E}{\partial Q} = \begin{pmatrix} \frac{\partial m}{\partial \rho} & \frac{\partial m}{\partial m} & \frac{\partial m}{\partial e} \\ \frac{\partial(m^2 / \rho + p)}{\partial \rho} & \frac{\partial(m^2 / \rho + p)}{\partial m} & \frac{\partial(m^2 / \rho + p)}{\partial e} \\ \frac{\partial((e + p)m / \rho)}{\partial \rho} & \frac{\partial((e + p)m / \rho)}{\partial m} & \frac{\partial((e + p)m / \rho)}{\partial e} \end{pmatrix}$$

Three eigen values corresponds to the propagation velocities in flow



MUSCL+limiter



Flux Difference
Splitting(FDS):
has to solve Riemann
problem

Flux Difference
Splitting(FDS):
has to solve Riemann
problem



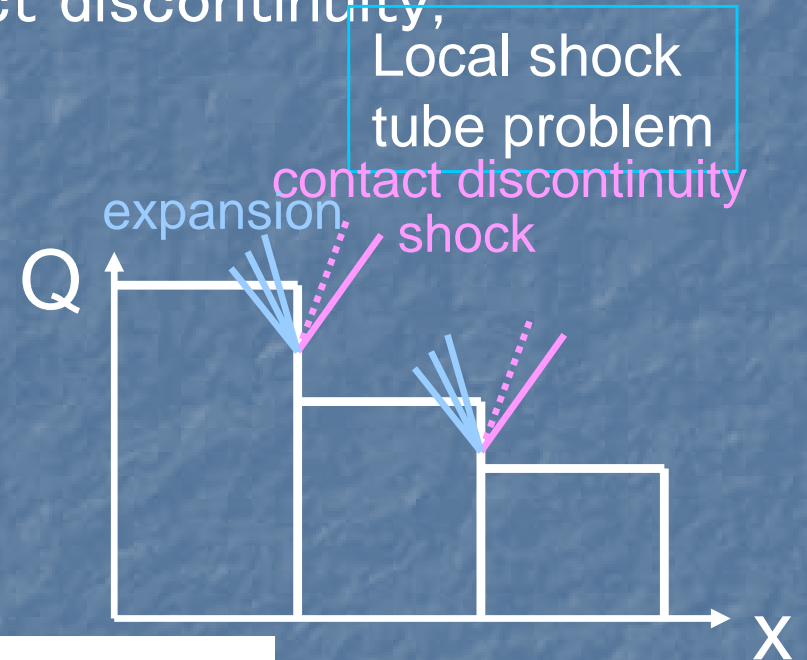
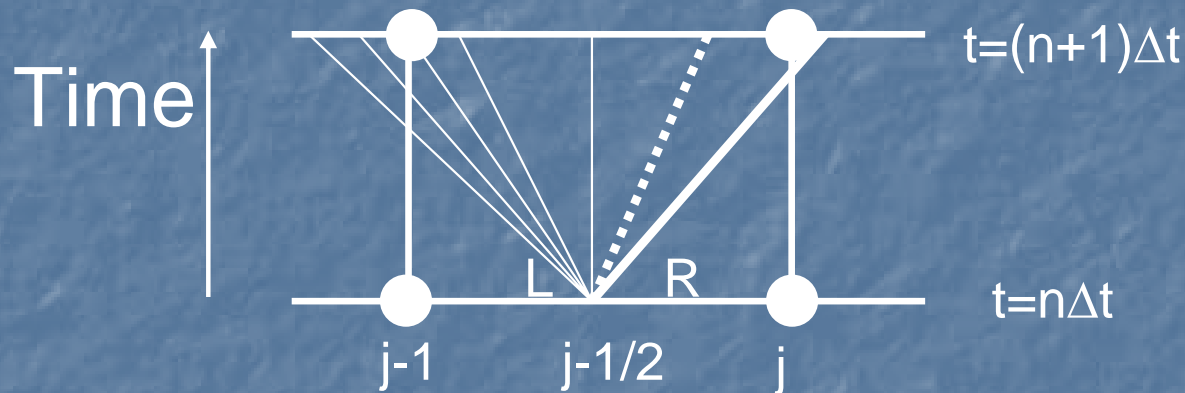
Non-MUSCL+limiter

Another schemes not to belong these procedures:

- Lax method
- Lax-Wendroff method
- 2-step L-W method
- MacCormack method

Approximate Riemann Solver

The shock tube problem is called the Riemann Problem. This problem presents an exact solution of the fully system of one-dimensional Euler equations containing simultaneously a shock wave, a contact discontinuity, and an expansion fan.



$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x} [\tilde{E}_{j+1/2} - \tilde{E}_{j-1/2}]$$

Accurate and physical solution is obtained by solving one-dimensional Euler equations **approximately**.

Relation between Approximate Riemann Solver and Numerical Flux

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x} [\tilde{E}_{j+1/2} - \tilde{E}_{j-1/2}]$$

1) Flux Difference Splitting (FDS)

has to need approximate Riemann solver

2) Flux Vector Splitting (FVS)

does not need approximate Riemann solver.

Finite Difference Splitting Method

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x} [\tilde{E}_{j+1/2} - \tilde{E}_{j-1/2}]$$

$$\tilde{E}_{j+1/2} = \frac{1}{2} [E_{j+1} + E_j - |A|_{j+1/2} (Q_{j+1} - Q_j)]$$

where,

$$|A|_{j+1/2} = R_{j+1/2} |\Lambda|_{j+1/2} R_{j+1/2}^{-1}$$

difference!

Upwind process on eigen values

necessary to calculate this average

Roe Average

Define average states ($j \pm 1/2$) as a non-linear function,
The following conditions have to be satisfied to calculate Roe average:

Shock wave automatically generates.
Characteristic wave speed is correctly calculated.

1.
$$E(Q_R) - E(Q_L) = A(Q_R, Q_L)(Q_R - Q_L)$$
$$= A_{ave}(Q_R - Q_L)$$

2. $A(Q_R, Q_L)$ has real eigen values with linearly independent eigenvectors

3. $A(Q, Q) = A(Q)$ necessary in smooth (differentiable) region

Conservation law is satisfied.

Roe Average

The results are as follows:

$$\rho_{ave} = \sqrt{\rho_L \rho_R}$$

Roe Average

$$u_{ave} = \frac{\sqrt{\rho_L} u_L + \sqrt{\rho_R} u_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}$$

$$H_{ave} = \frac{\sqrt{\rho_L} H_L + \sqrt{\rho_R} H_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}$$

where,
$$c_{ave}^2 = (\gamma - 1)H_{ave} - \frac{1}{2}u_{ave}^2$$

Roe average means a weighted average. However, the integral average form exists (Chakaravathy & Osher).

Higher Order FDS

Previous discussion is based on 1st order in space.
Then how to increase accuracy in space?

1. Approach by using MUSCL

Monotone-Upstream centered Schemes for Conservation Laws

2. Approach by using non-MUSCL

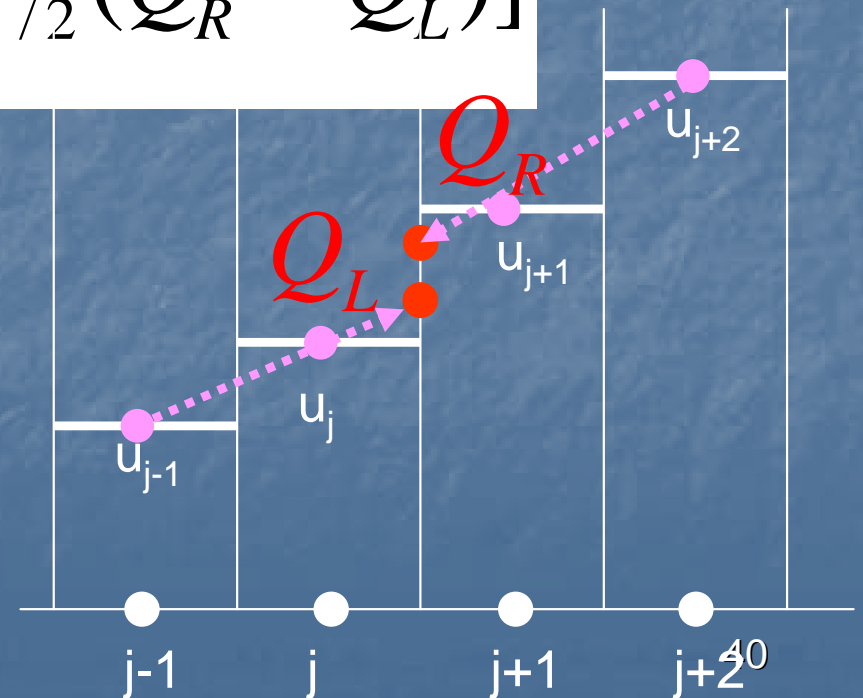
Higher Order FDS by MUSCL

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x} [\tilde{E}_{j+1/2} - \tilde{E}_{j-1/2}]$$

where $\tilde{E}_{j+1/2}$ is calculated by left and right side quantities Q_L, Q_R which are interpolated

$$\tilde{E}_{j+1/2} = \frac{1}{2} [E_R + E_L - |A|_{j+1/2} (Q_R - Q_L)]$$

piecewise linear



Higher Order FDS by MUSCL

For example,
slope limiter(Van Albada limiter):

$$\text{slope } s = \frac{2\Delta_+\Delta_- + \varepsilon}{(\Delta_+)^2 + (\Delta_-)^2 + \varepsilon}$$

$$Q_{j+1/2L} = Q_j + \frac{s}{4} \left[(1 - \kappa s) \bar{\Delta}_- Q_j + (1 + \kappa s) \bar{\Delta}_+ Q_j \right]$$

$$Q_{j+1/2R} = Q_{j+1} - \frac{s}{4} \left[(1 - \kappa s) \bar{\Delta}_+ Q_{j+1} + (1 + \kappa s) \bar{\Delta}_- Q_{j+1} \right]$$

Interpolated variables in MUSCL are:

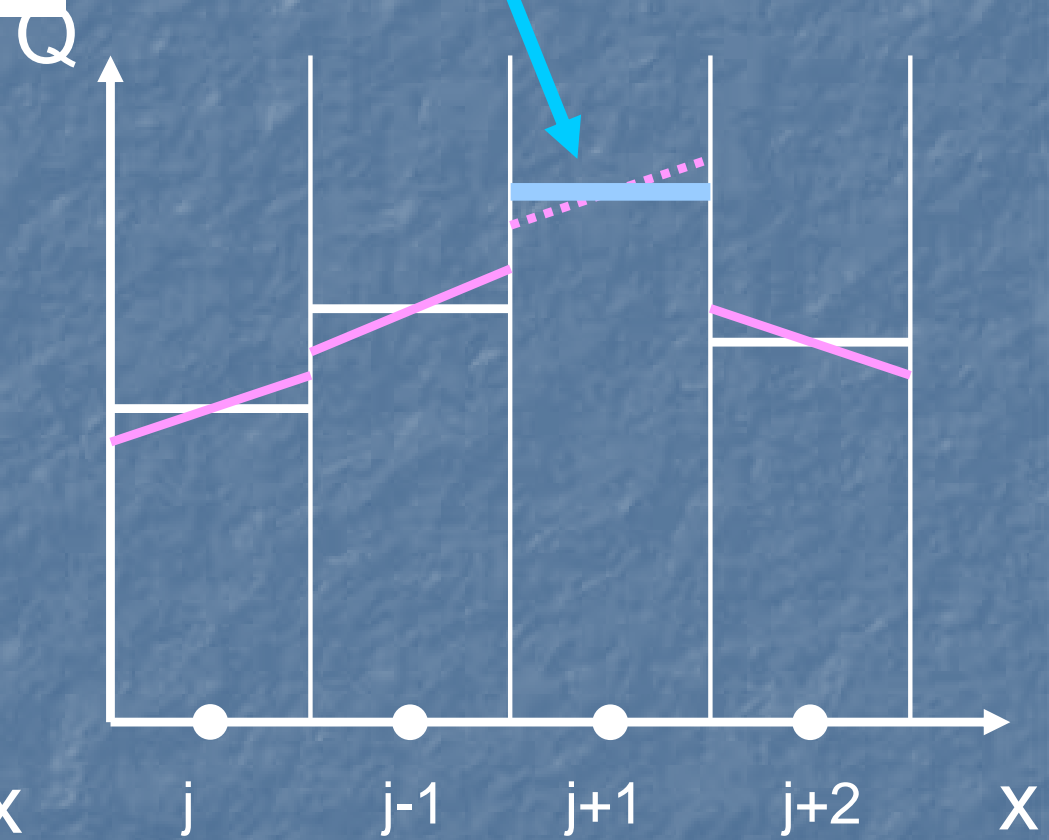
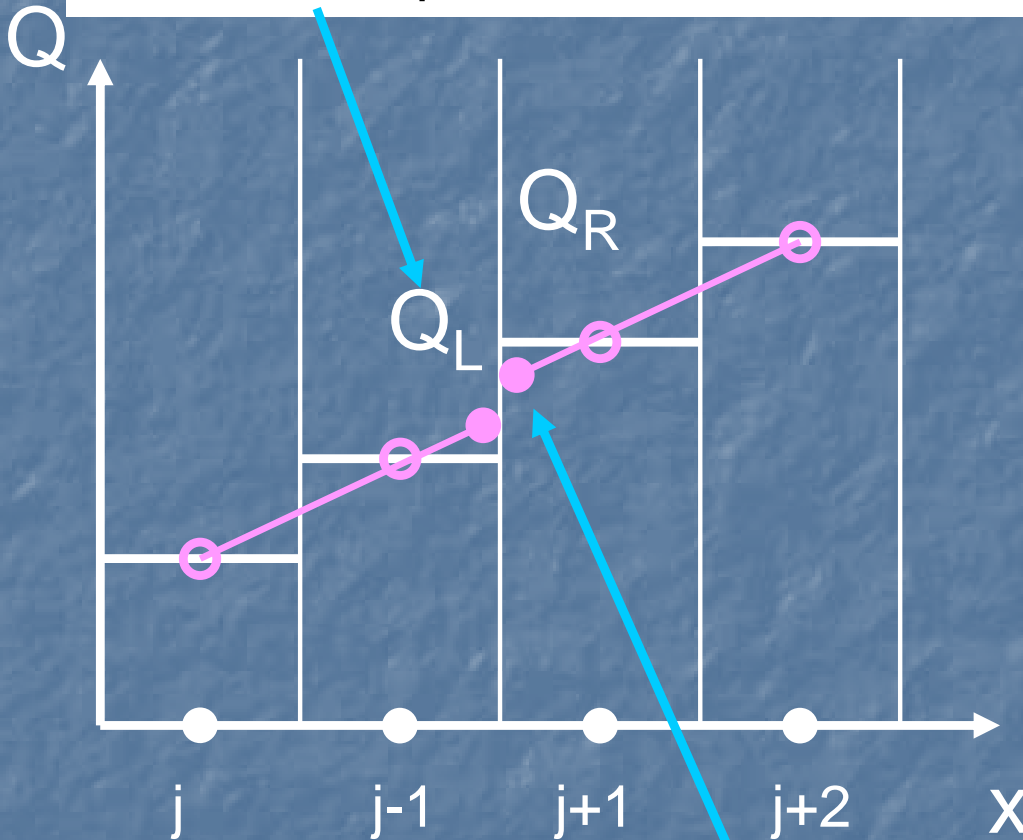
- Conservative variables : density, momentum, energy
- Primitive variables : density, velocity, pressure
- Characteristic variables : variables transported by waves such as entropy

Higher Order FDS by MUSCL

MUSCL and role of limiter

$$Q_{j+1/2L} = Q_j + \frac{1}{4} \left[(1-\kappa) \bar{\Delta}_- Q_j + (1+\kappa) \bar{\Delta}_+ Q_j \right]$$

Because a extreme causes numerical instability, spatial order decrease 1st order. (monotone)



$$Q_{j+1/2R} = Q_{j+1} - \frac{1}{4} \left[(1-\kappa) \bar{\Delta}_+ Q_{j+1} + (1+\kappa) \bar{\Delta}_- Q_{j+1} \right]$$

Non-MUSCL TVD Method

$$\tilde{E}_{j+1/2} = \frac{1}{2} [(E_{j+1} + E_j) + R_{j+1/2} \Phi_{j+1/2}]$$

* Yee's Upwind-TVD

$$\phi_{j+1/2}^l = \underbrace{\sigma(c_{j+1/2}^l)}_{\text{limiter}} (g_j^l + g_{j+1}^l) - \underbrace{\psi(c_{j+1/2}^l + \gamma_{j+1/2}^l)}_{\text{Modified flux}} \alpha_{j+1/2}^l$$

limiter

Modified flux

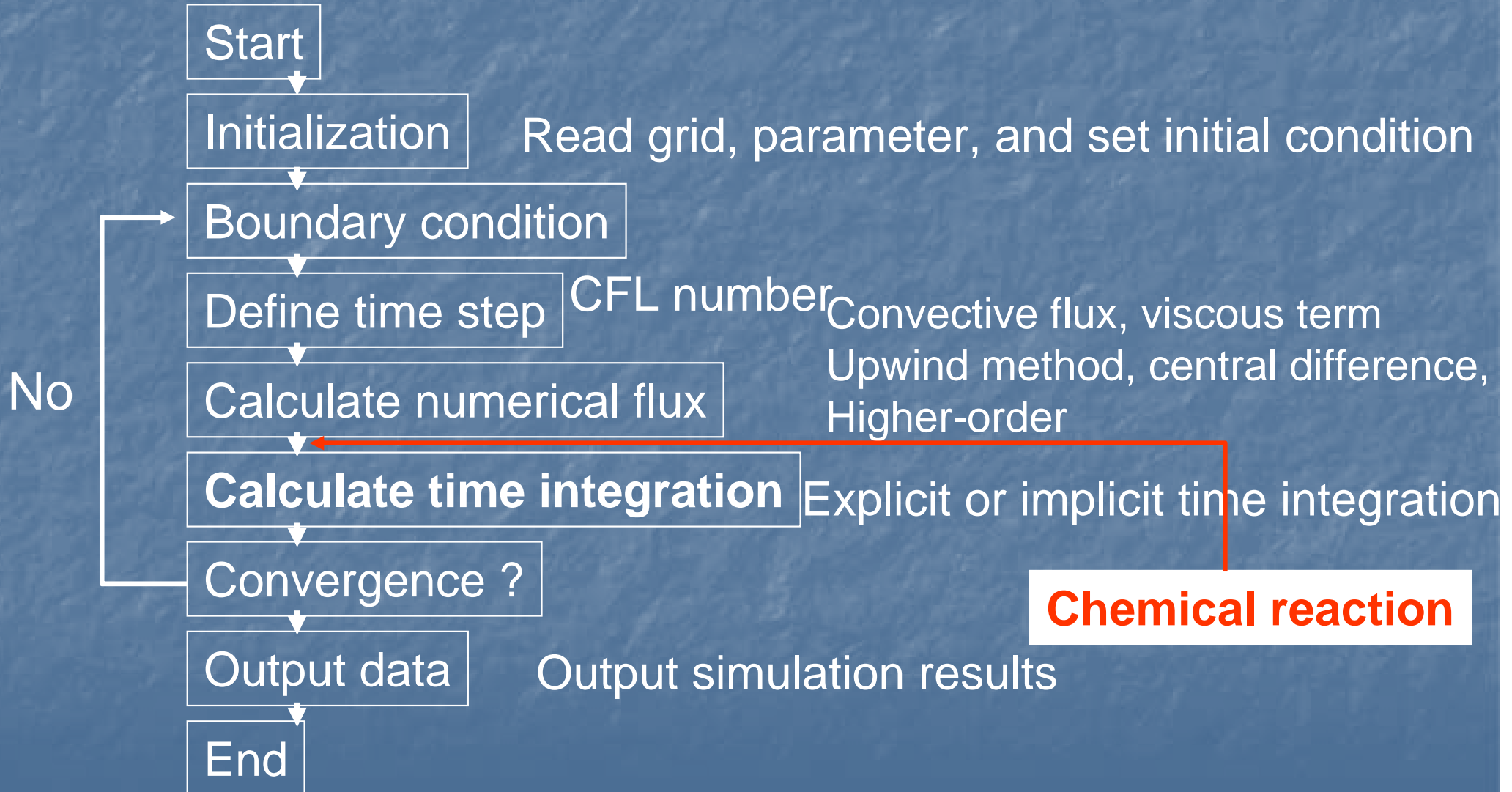
References

- Hirsch, C., Numerical Computation of Internal and External Flows Vol.2, John Wiley & Sons, 1990
- Yee, H., Upwind and Symmetric Shock-Capturing Scheme, NASA TM 89464, 1987.

System Equation with Chemical Reactions

Numerical Analysis for Fluid: Finite Different Method

Define flowchart of program after discretization and grid are decided



About Simulation of Combustion

Problems for simulation of combustion

- Computational code with combustion is few because:
 - reaction mechanism is complex
 - hard task to construct computational code (especially point implicit on reaction source term)
 - computational time is large
 - stiffness problem for detailed reaction model: restrict time step
- Detailed reaction model is at most proposed for hydrogen system,



Low-order simulation may done when vaporization, condensation, and heterogeneous combustion are include.

Normalized Parameter for Combustion Phenomena

- Specific heat ratio
- Mach number
- Reynolds number

-First Damköhler number

$$D_I = \frac{\tau_a}{\tau_c} = \frac{\text{Characteristic time of fluid}}{\text{Characteristic time for chemical reaction}}$$

$$\tau_a \gg \tau_c$$

Reaction locally (combustion)

$$\tau_a \approx \tau_c$$

Reaction near mixing zone
(Catalysis near accelerator, photochemical smog)

$$\tau_a \ll \tau_c$$

Uniform reaction in field
(in a small scale experimental device)

Combustion: $10^{-3} \sim 10^{-2}$ sec

Similarity law for combustion phenomena is not discovered! 48

Modified Points for Fluid Calculation Code (Compressible Equations)

From non-reactive code (constant specific heat ratio)
to gas-phase reactive code:

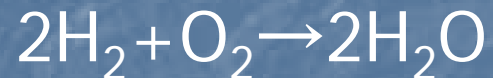
1. Specific heat ratio depends on temperature
2. Mass equations for chemical species (H_2, O_2, \dots) are added
3. Source term including reaction is added
4. viscous coefficients, heat conduction coefficients, and diffusive coefficients depend on temperature

5. Reaction model has to select

Chemical Reaction Model

1. Detailed reaction model vs. global reaction model

For example, reaction of hydrogen:



is global reaction. Most Hydrogen reaction systems have about 8 species and 20 elemental reactions.

2. Detailed reaction model

Elemental reactions should be included as much as possible after sensitivity analysis for elemental reactions are done.

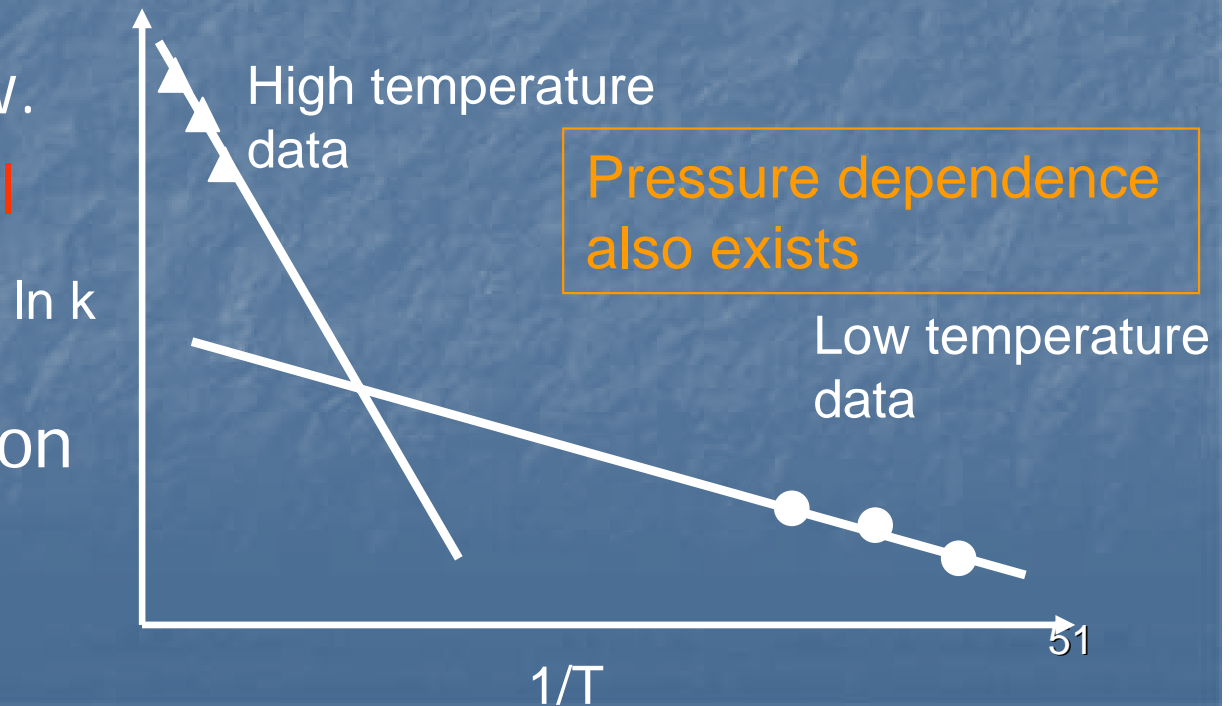
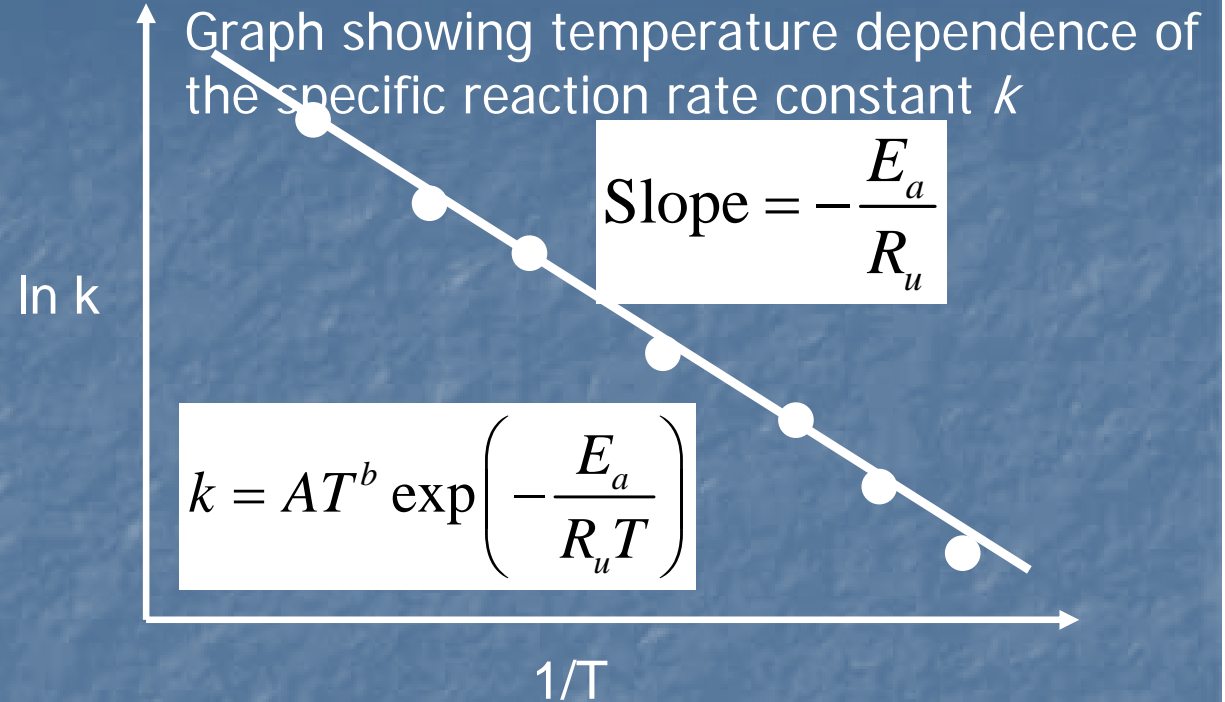
Chemical Reaction Model

k is decided by experimental data

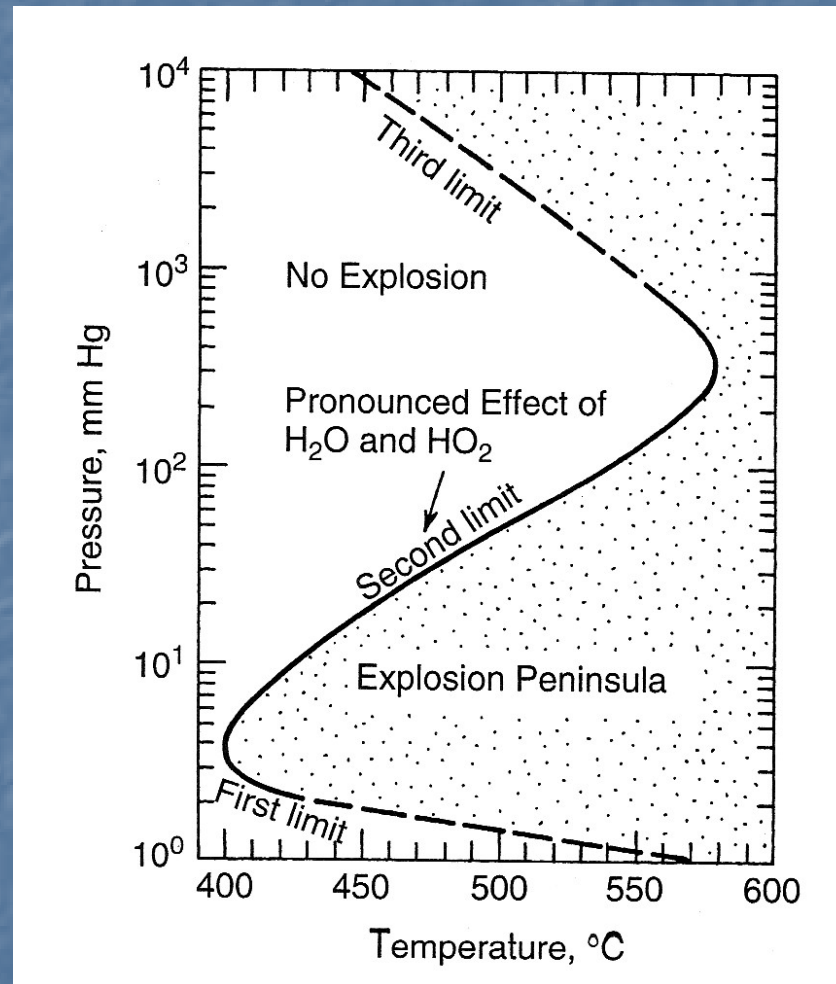
$$\ln k = \ln(AT^b) - \frac{E_a}{R_u T}$$

However, k depends on both temperature and temperature range although many reactions follows the Arrhenius law.

Detailed reaction model does not constructed for all cases. Therefore you should select valid reaction model to reproduce phenomena.



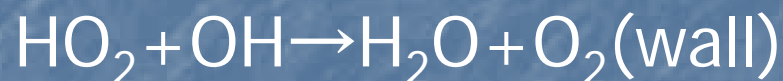
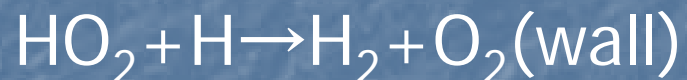
Explosion Limit of H₂O₂ System



Pressure-temperature explosion diagram of a stoichiometric H₂/O₂ mixture in a spherical vessel. (explosion peninsula)

Explosion Limit of H₂O₂ System

First limit : The destruction of HO₂ on the wall causes. This is dependent on the size of vessel.

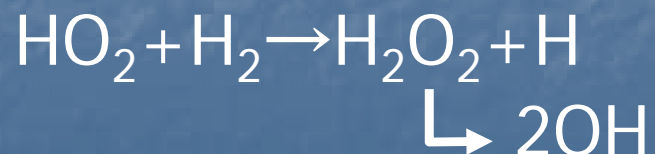


Second limit : The following reactions dominate.

HO₂ is relatively unreactive.



Third limit : HO₂ can collide and react with H₂ molecules to form H₂O₂ and H atm. H₂O₂ can dissociate to effectively generate OH.

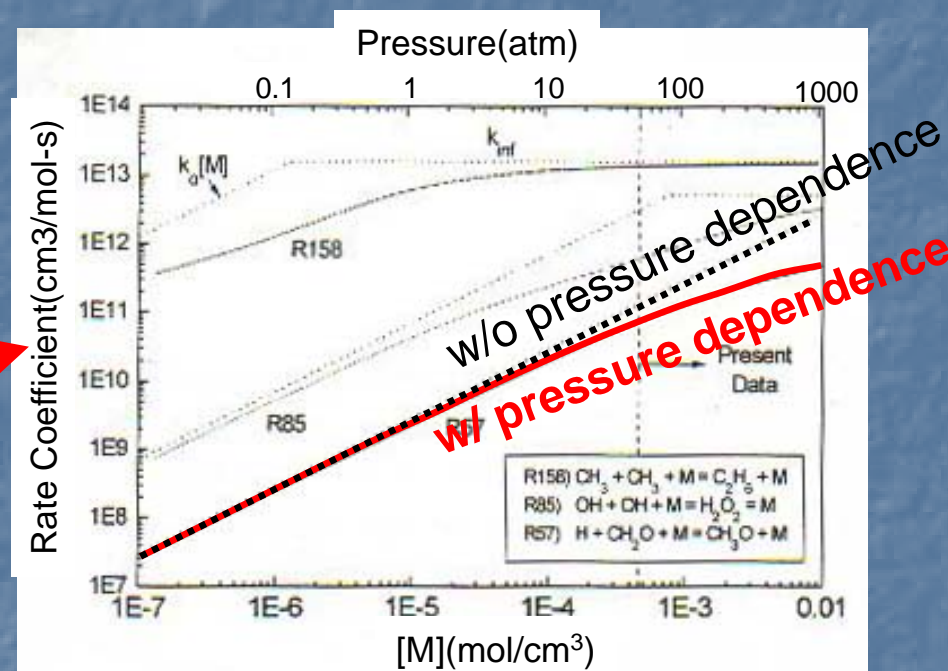


Example of Detailed Reaction Model

Petersen and Hanson model

Reaction	A_k	n_k	E_{a_k}	comments
(1) $O + H_2 \rightleftharpoons H + OH$	5.00×10^4	2.70	6290	
(2) $H + O_2 + M \rightleftharpoons HO_2 + M$	2.80×10^{18}	-0.90	0	<i>i</i>
(3) $H + O_2 + O_2 \rightleftharpoons HO_2 + O_2$	3.00×10^{20}	-1.70	0	
(4) $H + O_2 + H_2O \rightleftharpoons HO_2 + H_2O$	9.38×10^{18}	-0.80	0	
(5) $H + O_2 + N_2 \rightleftharpoons HO_2 + N_2x$	2.60×10^{19}	-1.20	0	
(6) $H + O_2 \rightleftharpoons O + OH$	8.30×10^{13}	0.00	14413	
(7) $H + HO_2 \rightleftharpoons O_2 + H_2$	2.80×10^{13}	0.00	1068	
(8) $H + HO_2 \rightleftharpoons OH + OH$	1.34×10^{14}	0.00	635	
(9) $H + H_2O_2 \rightleftharpoons HO_2 + H_2$	1.21×10^7	2.00	5200	
(10) $OH + H_2 \rightleftharpoons H_2O + H$	2.16×10^8	1.50	3430	
(11) $OH + OH + M \rightleftharpoons H_2O_2 + M$	7.40×10^{13}	-0.40	0	$k_{inf}^{a,b}$
	2.30×10^{18}	-0.90	-1700	k_0
(12) $OH + HO_2 \rightleftharpoons O_2 + H_2O$	2.90×10^{13}	0.00	-500	
(13) $OH + H_2O_2 \rightleftharpoons HO_2 + H_2O$	1.75×10^{12}	0.00	320	k_a^c
	5.80×10^{14}	0.00	9560	k_b^c
(14) $HO_2 + HO_2 \rightleftharpoons O_2 + H_2O_2$	1.30×10^{11}	0.00	-1630	k_c^d
	4.20×10^{14}	0.00	12000	k_d^d
(15) $O + O + M \rightleftharpoons O_2 + M$	1.20×10^{17}	-1.00	0	<i>e</i>
(16) $O + H + M \rightleftharpoons OH + M$	5.00×10^{17}	-1.00	0	<i>f</i>
(17) $H + OH + M \rightleftharpoons H_2O + M$	2.20×10^{22}	-2.00	0	<i>g</i>
(18) $H + H + M \rightleftharpoons H_2 + M$	1.00×10^{18}	-1.00	0	<i>h</i>

Reaction (11): pressure dependence defined by Troe's formula



[M] : Mole fraction rate of 3rd body

Governing Equations for Combustion System

Compressible Navier-Stokes Equations

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} = \frac{\partial E_v}{\partial x} + \frac{\partial F_v}{\partial y} + \frac{\partial G_v}{\partial z} + S$$

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ e \\ \rho_i \end{bmatrix}, E = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ (e + p)u \\ \rho_i u \end{bmatrix}, F = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vw \\ (e + p)v \\ \rho_i v \end{bmatrix}, G = \begin{bmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ (e + p)w \\ \rho_i w \end{bmatrix}$$

Species conservation equations are included

$$E_v = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ \tau_{xz} \\ u\tau_{xx} + v\tau_{xy} + w\tau_{xz} - q_x \\ \rho D_i \frac{\partial Y_i}{\partial x} \end{bmatrix}, F_v = \begin{bmatrix} 0 \\ \tau_{yx} \\ \tau_{yy} \\ \tau_{yz} \\ u\tau_{yx} + v\tau_{yy} + w\tau_{yz} - q_y \\ \rho D_i \frac{\partial Y_i}{\partial y} \end{bmatrix}, G_v = \begin{bmatrix} 0 \\ \tau_{zx} \\ \tau_{zy} \\ \tau_{zz} \\ u\tau_{zx} + v\tau_{zy} + w\tau_{zz} - q_z \\ \rho D_i \frac{\partial Y_i}{\partial z} \end{bmatrix}, S = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \dot{\omega}_i \end{bmatrix}$$

Governing Equations for Combustion System

Equation of State

$$p = \sum_{i=1}^N \rho_i R_i T = \sum_{i=1}^N \rho_i \frac{R}{W_i} T$$

R : universal gas constant

Energy

$$e = \sum_{i=1}^N \rho_i h_i - p + \frac{\rho}{2} (u^2 + v^2 + w^2)$$

If γ is constant,

$$e = \frac{1}{\gamma - 1} \frac{p}{\rho} + \frac{1}{2} \rho u^2$$

Specific heat of constant pressure

$$\frac{C_{pi}}{R_i} = a_{1i} + a_{2i} T + a_{3i} T^2 + a_{4i} T^3 + a_{5i} T^4$$

Enthalpy

$$\frac{h_i}{R_i T} = a_{1i} + \frac{a_{2i}}{2} T + \frac{a_{3i}}{3} T^2 + \frac{a_{4i}}{4} T^3 + \frac{a_{5i}}{5} T^4 + \frac{a_{6i}}{T}$$

Entropy

$$\frac{s_i^0}{R_i} = a_{1i} \ln T + a_{2i} T + \frac{a_{3i}}{2} T^2 + \frac{a_{4i}}{3} T^3 + \frac{a_{5i}}{4} T^4 + a_{7i}$$

Temperature dependence!

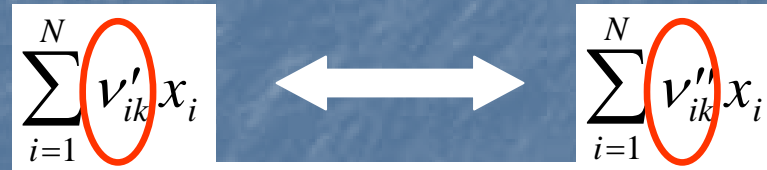
$$C_p = \text{const}$$

$$h = C_p T$$

Coefficients in C_p , h , and s are calculated from JANAF Table by least square method. Coefficients for low-temperature ($T < 1000\text{K}$) and high-temperature ($T > 1000\text{K}$) exist.

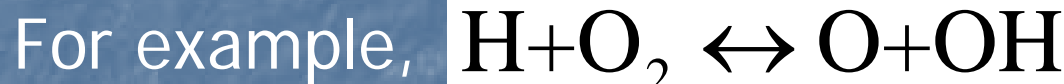
Governing Equations for Combustion System

The most general opposing chemical reactions,



Stoichiometric coefficients of i-species, k-th reaction

: The number of elemental reactions is k.



then, $v'_{H,1} = 1, v'_{O_2,1} = 1, v''_{O,1} = 1, v''_{OH,1} = 1$

The number of elemental reaction is k. -> Table is created.

i-species' production rate
[kg/m³/s]

$$\dot{\omega}_i = W_i \sum_{k=1}^K (v''_{ik} - v'_{ik}) RP_k$$

i-th species' mole concentration

Reaction rate [mol/m³/s]
(Two-body reaction)

$$RP_k = k_{f,k} \prod_{i=1}^N (c_{\chi i})^{v'_{ik}} - k_{b,k} \prod_{i=1}^N (c_{\chi i})^{v''_{ik}}$$

Forward rate constant

Backward rate constant

Governing Equations for Combustion System

Forward rate constant (Modified Arrhenius)

$$k_{f,k} = A_k T^{n_k} \exp\left(-\frac{Ea_k}{RT}\right)$$

Collision frequency

Activation Energy

Backward rate constant

They are calculated using experimental data

$$k_{b,k} = \frac{k_{f,k}}{Kc_k}$$

Equilibrium constant of concentration

$$Kc_k = Kp_k \left(\frac{p_{atm}}{RT}\right)^{\sum_{i=1}^N (v''_{ik} - v'_{ik})} \quad (p_{atm} = 1 \text{ atm})$$

$$Kp_k = \exp\left[\sum_{i=1}^N \left\{ (v''_{ik} - v'_{ik}) \frac{s_i^0}{R_i} \right\} - \sum_{i=1}^N \left\{ (v''_{ik} - v'_{ik}) \frac{h_i}{R_i T} \right\}\right]$$

Equilibrium constant of pressure :
function of entropy s and enthalpy h

Governing Equations for Combustion System

Jacobian matrix:

$$A = \frac{\partial \hat{E}}{\partial \hat{Q}}, \frac{\partial \hat{F}}{\partial \hat{Q}}, \frac{\partial \hat{G}}{\partial \hat{Q}} =$$

0	k_x	k_y	k_z	0	0	...	0
$k_x p_p - \theta_u$	$\theta + k_x(u + p_M)$	$k_y u + k_x p_N$	$k_z u + k_x p_L$	$k_x p_e$	$k_x p_{\rho 1}$...	$k_x p_{\rho N}$
$k_y p_p - \theta_v$	$k_x v + k_y p_M$	$\theta + k_y(v + p_N)$	$k_z v + k_y p_L$	$k_y p_e$	$k_y p_{\rho 1}$...	$k_y p_{\rho N}$
$k_z p_p - \theta_w$	$k_x w + k_z p_M$	$k_y w + p_N$	$\theta + k_z(w + p_L)$	$k_z p_e$	$k_z p_{\rho 1}$...	$k_z p_{\rho N}$
$(p_p - H)\theta$	$k_x H + p_M \theta$	$k_y H + p_N \theta$	$k_z H + p_L \theta$	$(1 + p_e)\theta$	$p_{\rho 1} \theta$...	$p_{\rho N} \theta$
$-Y_1 \theta$	$k_x Y_1$	$k_y Y_1$	$k_z Y_1$	0	θ	...	0
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\ddots	\vdots
$-Y_N \theta$	$k_x Y_N$	$k_y Y_N$	$k_z Y_N$	0	0	...	θ

Increase with species

$$H = \frac{e + p}{\rho}, \quad \theta = k_x u + k_y v + k_z w$$

Pressure differential by i-species' density

$$p_{\rho i} = \frac{1}{1 - \sum_{j=1}^N \rho_j C_{pj} / \sum_{j=1}^N \rho_j R_j} \left\{ h_i - \frac{\sum_{j=1}^N \rho_j C_{pj}}{\sum_{j=1}^N \rho_j R_j} R_i T \right\}$$

Eigenvalue

$$\theta, \theta, \theta + ak, \theta - ak, \underbrace{\theta, \dots, \theta}_{N \text{個}}$$

Frozen speed of sound

$$a^2 = p_p + \sum_{j=1}^N Y_j p_{\rho j} + p_e (H - u^2 - v^2 - w^2)$$

Governing Equations for Combustion System: Source Term

Calculation for source term:

Equations have a stiffness problem for reactive flow

-> Point implicit method is applied.

Though the point implicit affects on time accuracy for DNS simulation, an explicit integration is used with significantly small time step.

Governing Equations for Combustion System: Source Term

$$\Delta Q^n + \Delta t \frac{\partial}{\partial x} \left[E_j^n + \left(\frac{\partial E}{\partial Q} \right)_j^n \Delta Q^n + \dots \right] = \Delta t S_j^{n+1}$$

Unknown

Crank-Nicholson type
implicit method

$$\left[I - \frac{\Delta t}{2} \frac{\partial S}{\partial Q} \right] \Delta Q_j^n = -\Delta t \left(\frac{\partial E}{\partial x} \right)_j^n + \Delta t S_j^n$$

Known

Governing Equations for Combustion System: Source Term

Jacobian matrix for source term is necessary for point implicit.

Increase with species

$$\hat{S} = J^{-1}S = J^{-1} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \dot{\omega}_i \end{bmatrix}$$

$$\frac{\partial \hat{S}}{\partial \hat{Q}} =$$

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 \\ \frac{\partial \dot{\omega}_1}{\partial \rho} & \frac{\partial \dot{\omega}_1}{\partial(\rho u)} & \frac{\partial \dot{\omega}_1}{\partial(\rho v)} & \frac{\partial \dot{\omega}_1}{\partial(\rho w)} & \frac{\partial \dot{\omega}_1}{\partial e} & \frac{\partial \dot{\omega}_1}{\partial \rho_1} & \dots & \frac{\partial \dot{\omega}_1}{\partial \rho_j} & \dots & \frac{\partial \dot{\omega}_1}{\partial \rho_N} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial \dot{\omega}_i}{\partial \rho} & \frac{\partial \dot{\omega}_i}{\partial(\rho u)} & \frac{\partial \dot{\omega}_i}{\partial(\rho v)} & \frac{\partial \dot{\omega}_i}{\partial(\rho w)} & \frac{\partial \dot{\omega}_i}{\partial e} & \frac{\partial \dot{\omega}_i}{\partial \rho_1} & \dots & \frac{\partial \dot{\omega}_i}{\partial \rho_j} & \dots & \frac{\partial \dot{\omega}_i}{\partial \rho_N} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial \dot{\omega}_N}{\partial \rho} & \frac{\partial \dot{\omega}_N}{\partial(\rho u)} & \frac{\partial \dot{\omega}_N}{\partial(\rho v)} & \frac{\partial \dot{\omega}_N}{\partial(\rho w)} & \frac{\partial \dot{\omega}_N}{\partial e} & \frac{\partial \dot{\omega}_N}{\partial \rho_1} & \dots & \frac{\partial \dot{\omega}_N}{\partial \rho_j} & \dots & \frac{\partial \dot{\omega}_N}{\partial \rho_N} \end{bmatrix}$$

Governing Equations for Combustion System: Source Term

Example of each component in Jacobian matrix for source term

$$\frac{\partial \dot{\omega}_i}{\partial \rho} = \frac{\partial T}{\partial \rho} \frac{\partial \dot{\omega}_i}{\partial T} = \frac{\partial T}{\partial \rho} \cdot W_i \sum_{k=1}^K \left[(v''_{ik} - v'_{ik}) \left\{ \frac{dk_{f,k}}{dT} \prod_{l=1}^N (c_{\chi l})^{v'_{ik}} - \frac{dk_{b,k}}{dT} \prod_{l=1}^N (c_{\chi l})^{v''_{ik}} \right\} \right]$$

$$\frac{\partial T}{\partial \rho} = \frac{1}{\sum_{j=1}^N \rho_j R_j} \left[\frac{1}{1 - \frac{\sum_{j=1}^N \rho_j C_{pj}}{\sum_{j=1}^N \rho_j R_j}} \left\{ -\frac{1}{2} (u^2 + v^2 + w^2) \right\} \right]$$

Differential of forward rate constant

$$\frac{dk_{f,k}}{dT} = \frac{k_{f,k}}{T} \left(n_k + \frac{Ea_k}{RT} \right)$$

Differential of backward rate constant

$$\frac{dk_{b,k}}{dT} = \frac{1}{Kc_k} \left[\frac{dk_{f,k}}{dT} - \frac{k_{f,k}}{T} \left[\sum_{i=1}^N \left\{ (v''_{ik} - v'_{ik}) \frac{h_i}{R_i T} \right\} - \sum_{i=1}^N (v''_{ik} - v'_{ik}) \right] \right]$$

Governing Equations for Combustion System: Source Term

Inversion of Jacobian matrix for source term:

Inverse matrix is calculated by Gauss Jordan method.

Matrix is divided into four.

In the case of 9 species, 14x14 matrix becomes 9x9 matrix (3D).

$$M = \left(I - \frac{\Delta t}{2} \frac{\partial \hat{S}}{\partial \hat{Q}} \right)^n = \begin{pmatrix} I & \vdots & O \\ \dots & \dots & \dots \\ A_{21} & \vdots & A_{22} \\ \vdots & \vdots & \vdots \end{pmatrix}$$

Inverse matrix

$$M^{-1} = \begin{pmatrix} I & \vdots & O \\ \dots & \dots & \dots \\ A_{21} & \vdots & A_{22} \\ \vdots & \vdots & \vdots \end{pmatrix}^{-1} = \begin{pmatrix} I & \vdots & O \\ \dots & \dots & \dots \\ -A_{22}^{-1} A_{21} & \vdots & -A_{22}^{-1} \\ \vdots & \vdots & \vdots \end{pmatrix}$$

Governing Equations for Combustion System: Determination of Temperature

Definition of temperature : energy is a polynomial of temperature. Therefore it is impossible to calculate temperature directly.

$$e = \sum_{j=1}^N \rho_j h_j - \sum_{j=1}^N \rho_j R_j T + \frac{\rho}{2} (u^2 + v^2 + w^2)$$

$$\frac{h_i}{R_i T} = a_{1i} + \frac{a_{2i}}{2} T + \frac{a_{3i}}{3} T^2 + \frac{a_{4i}}{4} T^3 + \frac{a_{5i}}{5} T^4 + \frac{a_{6i}}{T}$$

Newton method is applied to obtain temperature iteratively.

$$F(T) = \sum_{j=1}^N \rho_j h_j - \sum_{j=1}^N \rho_j R_j T + \frac{\rho}{2} (u^2 + v^2 + w^2) - e$$

Two or three iterations are enough.

Summary

- Numerical simulation on detonation has to use compressible governing equations.
- But viscous effects are quite limited except DDT.
- Chemical reaction model including high pressure effects is better but should be more research.
- Numerical simulation on detonation using a detailed reaction model requires high hardware performance and high numerical techniques yet.

References

- K.K. Kuo, Principle of Combustions
- M. Hishida, Ph.D Thesis in Nagoya University, 1993

Thanks

- To Prof. Vladimir Molkov for the invitation
- To Morley Robert for assist of visiting Belfast
- To Prof A.Koichi Hayashi for his special advices