

Numerical Heat Transfer (数值传热学)

Chapter 1 Basic concepts of numerical simulation for heat transfer and fluid flow problems



Instructor Tao, Wen-Quan (陶文铨)

Key Laboratory of Thermo-Fluid Science & Engineering
China-Kyrgyzstan Joint Laboratory of Clean Energy and Energy
Storage under the Belt and Road Initiative
Innovative Harbor of West China, Xian

2026-Sept-14

Contents of Chapter 1

1.1 Mathematical formulation (数学描述) of heat transfer and fluid flow (HT & FF) problems

1.2 Condition for unique solution (唯一解) and physical classification (分类) of governing equations

1.3 Mathematical classification of governing equation (方程分类) and its effects on numerical solution

1.4 Fundamental (基本的) contents of numerical heat transfer

1.5 Roles of numerical simulation and stories of Professor Kang FENG and D B Spalding

1.1 Mathematical formulation of heat transfer and fluid flow (HT & FF) problems

1.1.1 Governing equations (控制方程) and their general form

1. Mass conservation (质量守恒)

2. Momentum conservation (动量守恒)

3. Energy conservation (能量守恒)

4. General form (一般形式)

1.1.2 Some remarks

1.1 Mathematical formulation of heat transfer and fluid flow (HT & FF) problems

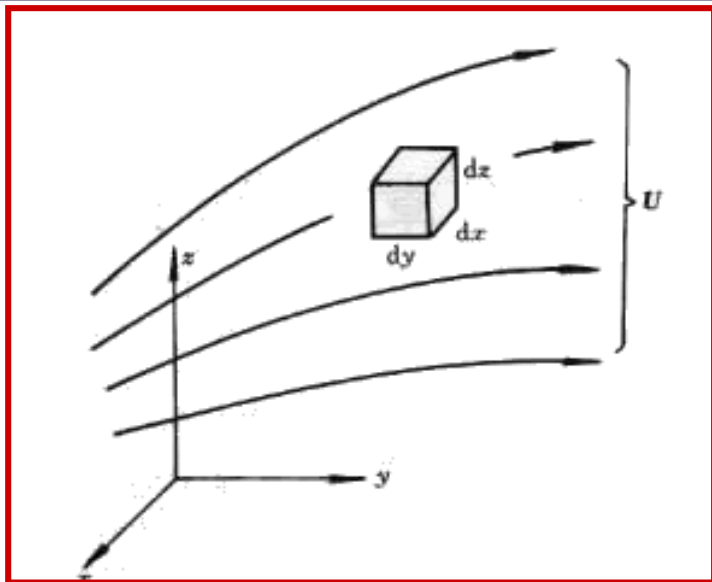
All macro-scale (宏观) HT & FF problems are governed (控制) by three conservation laws: mass, momentum and energy conservation law (守恒定律).

The differences between different problems are in: conditions for the unique solution (唯一解) : (1) initial (初始的) & boundary conditions, (2) physical properties and (3) source terms (源项) .

1-1-1 Governing equations and their general form

1. Mass conservation

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0$$



u, v, w are three components (分量) of $\vec{U}$.

$$\frac{\partial \rho}{\partial t} + \mathbf{div}(\rho \vec{U}) = 0$$

“**div**” (bold type, 粗体) is the mathematical symbol for divergence (散度) :

In Cartesian coordinate
(直角坐标系)

$$\mathbf{div}(\rho \vec{U}) = \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z}$$

For incompressible fluid (不可压缩流体), density is constant,

$$\mathbf{div}(\vec{U}) = 0$$

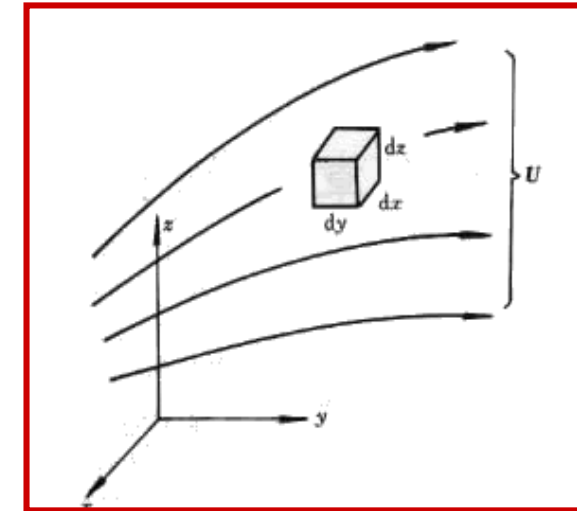
$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

flow without source and sink (没有源与汇的流动). For example, flow of water in a pipe.

2. Momentum conservation

Applying the 2nd law of Newton ($F=ma$) to an elemental control volume (控制容积) in the three-dimensional coordinates:

[Increasing rate of momentum of the CV(控制容积中动量的增加率)] = [Summation of external forces applying on the CV (作用在控制容积中的外力之和)]



Adopting Stokes assumption(采用斯托克斯假设) : stress is linearly proportional to strain (应力与应变成线性关系), we have following governing equation for component u in x-direction:

$$\underbrace{\frac{\partial(\rho u)}{\partial t}}_{\text{Transient term (瞬态项)}} + \underbrace{\frac{\partial(\rho uu)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z}}_{\text{Convection term (对流项)}} = -\frac{\partial p}{\partial x} + \underbrace{\frac{\partial}{\partial x}(\bar{\lambda} \text{div} \vec{U} + 2\eta \frac{\partial u}{\partial x})}_{\text{2nd-order term (部分进入扩散项)}} \quad \text{Source term (源项)}$$

Equation of the variation of fluid momentum in x-direction (ρu) .

$$+ \underbrace{\frac{\partial}{\partial y}[\eta(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y})] + \frac{\partial}{\partial z}[\eta(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x})]}_{\text{2nd-order term (部分进入扩散项)}} + \rho F_x$$

η dynamic viscosity(动力粘度) ,

$\bar{\lambda}$ fluid 2nd molecular viscosity (第2分子粘度) .For gas, $\bar{\lambda} = -\frac{2}{3}\eta$

(For details see the notes of Section 1-1) .

It can be shown (see the notes) that the above equation can be reformulated as (改写为) following general form of Navier-Stokes equation for u component of fluid momentum:

$$\frac{\partial(\rho u)}{\partial t} + \text{div}(\rho u \vec{U}) = \text{div}(\eta \text{grad} u) + S_u$$

Transient term
非稳态项

Convection term
对流项

Diffusion term
扩散项

Source term
源项

u, v, w ----velocity components in x,y,z three directions, respectively, they are the dependent variable (因变量) to be solved;
 $\vec{U}$ ----fluid velocity vector; $\vec{U} = u\vec{i} + v\vec{j} + w\vec{k}$
 S_u ----source term.

For v, w components, similar equations can be derived.

Source term in x-direction:

$$S_u = \frac{\partial}{\partial x} \left(\eta \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\eta \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial z} \left(\eta \frac{\partial w}{\partial x} \right) + \frac{\partial}{\partial x} (\bar{\lambda} \text{div} \vec{U}) + \rho F_x - \frac{\partial p}{\partial x}$$

Similarly:

$$S_v = \frac{\partial}{\partial x} \left(\eta \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial y} \left(\eta \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial z} \left(\eta \frac{\partial w}{\partial y} \right) + \frac{\partial}{\partial y} (\bar{\lambda} \text{div} \vec{U}) + \rho F_y - \frac{\partial p}{\partial y}$$

$$S_w = \frac{\partial}{\partial x} \left(\eta \frac{\partial u}{\partial z} \right) + \frac{\partial}{\partial y} \left(\eta \frac{\partial v}{\partial z} \right) + \frac{\partial}{\partial z} \left(\eta \frac{\partial w}{\partial z} \right) + \frac{\partial}{\partial z} (\bar{\lambda} \text{div} \vec{U}) + \rho F_z - \frac{\partial p}{\partial z}$$

For incompressible fluid (不可压流体) with constant properties the source term does not contain velocity-related part.

3. Energy conservation

[Increasing rate of internal energy in the CV (控制容积内能的增加率)] = [Net heat transfer rate going into the CV] + [Power conducted by body forces and surface forces (进入控制容积的净传热速率 + 体积力与表面力作用在控制容积上的功率)]

Introducing Fourier's law of heat conduction and neglecting the work conducted by forces; Introducing **enthalpy** (焓)

$$h = c_p T$$

We have:

$$\frac{\partial(\rho c_p T)}{\partial t} + \mathbf{div}(\rho c_p T \vec{U}) = \mathbf{div}(\lambda \mathbf{grad}(T)) + S_T$$

$$\mathbf{grad}(T) = \frac{\partial T}{\partial x} \vec{i} + \frac{\partial T}{\partial y} \vec{j} + \frac{\partial T}{\partial z} \vec{k} \quad (\text{温度梯度})$$

4. General form of the governing equations

$$\frac{\partial(\rho^* \phi)}{\partial t} + \text{div}(\rho^* \phi \mathbf{U}) = \text{div}(\Gamma_\phi \mathbf{grad} \phi) + S_\phi$$

Transient

Convection

Diffusion

Source

ϕ is a general dependent variable: u , v , w and T ;

The differences between different problems:

- (1) Different boundary and initial conditions;
- (2) Different nominal source (名义源项) terms;
- (3) Different physical properties (nominal fluid density , 名义流体密度, ρ^*)

Expressions of four general variables for different governing equations

governing equations	ρ^*	ϕ	Γ_ϕ	S_ϕ
mass conservation	ρ	1	0	0
x-momentum eq.	ρ	u	η	$\rho F_x - \partial p / \partial x$
y-momentum eq.	ρ	v	η	$\rho F_y - \partial p / \partial y$
z-momentum eq.	ρ	w	η	$\rho F_z - \partial p / \partial z$
energy conservation	ρc_p	T	λ	S_T

1-1-2 Some remarks (说明)

1. The derived transient 3D **Navier-Stokes** equations can be applied **for both laminar and turbulent flows** (湍流) .
2. When a HT & FF problem is in conjunction with (与...有关) mass transfer process, the component (组份) conservation equation should be included in the governing equations.
3. Radiative heat transfer (辐射换热) is governed by a differential-integral (微分-积分) equation, and its numerical solution will not be dealt with (处理) here. Following book is recommended:

谈和平 余其铮 夏新林, 等. 红外辐射特性与传输的数值计算-计算热 辐射学[M]. 哈尔滨: 哈尔滨工业大学出版社, 2006 .

4. Very recent mathematical research has shown that the N-S equations do not possess regularity (正则性), meaning that their solutions cannot be guaranteed to be smooth and differentiable (光滑可导) throughout the entire domain. However, the excellent agreement between the results of numerous numerical simulations and the experiments makes it seem that we don't need to pay much attention to this mathematical property.

Notes to Section 1.1

In the left hand side

The right hand side :

$$\frac{\partial(\rho uu)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z} = \text{div}(\rho u \vec{U})$$

$$\frac{\partial}{\partial x}(\bar{\lambda} \text{div} \vec{U} + 2\eta \frac{\partial u}{\partial x}) + \frac{\partial}{\partial y}[\eta(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y})] + \frac{\partial}{\partial z}[\eta(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x})] + \rho F_x - \frac{\partial p}{\partial x} =$$

$$\frac{\partial}{\partial x}(\eta \frac{\partial u}{\partial x}) + \frac{\partial}{\partial y}(\eta \frac{\partial u}{\partial y}) + \frac{\partial}{\partial z}(\eta \frac{\partial u}{\partial z}) + \frac{\partial}{\partial x}(\eta \frac{\partial u}{\partial x}) + \frac{\partial}{\partial y}(\eta \frac{\partial v}{\partial x}) + \frac{\partial}{\partial z}(\eta \frac{\partial w}{\partial x}) + \frac{\partial}{\partial x}(\bar{\lambda} \text{div} \vec{U})$$

$\text{div}(\text{grad}(u)) \qquad S_u$

$$\rho F_x - \frac{\partial p}{\partial x} = \text{div}(\eta \text{grad} u) + S_u$$

$$\text{grad}(u) = \frac{\partial u}{\partial x} \mathbf{i} + \frac{\partial u}{\partial y} \mathbf{j} + \frac{\partial u}{\partial z} \mathbf{k}$$

Thus we have:

$$\text{div}(\text{grad}(u)) = \frac{\partial}{\partial x}(\frac{\partial u}{\partial x}) + \frac{\partial}{\partial y}(\frac{\partial u}{\partial y}) + \frac{\partial}{\partial z}(\frac{\partial u}{\partial z})$$

$$\frac{\partial(\rho u)}{\partial t} + \text{div}(\rho u \vec{U}) = \text{div}(\eta \text{grad} u) + S_u$$

Navier-Stokes

Gradient of a scalar (标量的梯度) is a vector:

$$\text{grad}(u) = \frac{\partial u}{\partial x} \vec{i} + \frac{\partial u}{\partial y} \vec{j} + \frac{\partial u}{\partial z} \vec{k}$$

Divergence of a vector (矢量的散度) is a scalar:

$$\text{div}(\text{grad}(u)) = \text{div}\left(\frac{\partial u}{\partial x} \vec{i} + \frac{\partial u}{\partial y} \vec{j} + \frac{\partial u}{\partial z} \vec{k}\right)$$

$$\text{div}(\text{grad}(u)) = \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left(\frac{\partial u}{\partial z} \right)$$

$$\text{div}(\eta \text{grad}(u)) = \frac{\partial}{\partial x} \left(\eta \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\eta \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left(\eta \frac{\partial u}{\partial z} \right)$$

End of Notes to Section 1.1

1.2 Condition for unique solution (唯一解) and physical classification (分类) of governing equations

1-2-1 Conditions for unique solution of HT and FF problems

1. Initial condition (初始条件)

2. Boundary condition (边界条件)

3. Thermo-physical properties and source term (热物性与源项)

1-2-2 Physical classification of governing equations

1. Conservative vs. non-conservative

2. Conservative one can guarantee the conservation within a finite volume.

3. Conservative and non-conservative are referred to a finite space

Example 1-1: Mathematical formulation

1.2 Condition for unique solution and physical classification of governing equations

1-2-1 Conditions for unique solution (定解条件)

Taking a transient heat conduction problem as an example.

1. Initial condition (初始条件) $t = 0, T = f(x, y, z)$

2. Boundary condition (边界条件)

(1) First kind (Dirichlet): $T_B = T_{\text{given}}$

(2) Second kind (Neumann): $q_B = -\lambda \left(\frac{\partial T}{\partial n} \right)_B = q_{\text{given}}$

(3) Third kind (Rubin): Specifying (规定) the relationship between boundary value and its first-order normal derivative (法向导数) :

$$-\lambda \left(\frac{\partial T}{\partial n} \right)_B = h(T_B - T_f)$$

$$q = h(T_w - T_\infty) \quad \text{or} \quad q = h(T_\infty - T_w)$$

wall is cooled

wall is heated

For both cooling and heating

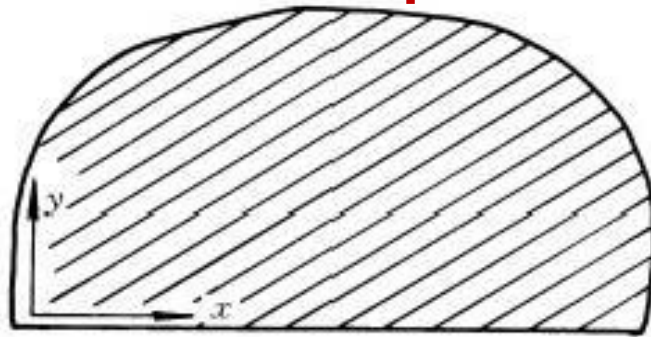
For the 3rd kind boundary condition the only knowns are T_f and h !

3. Fluid thermo-physical properties and source term of the process.

In future discussions, this condition is regarded naturally given.

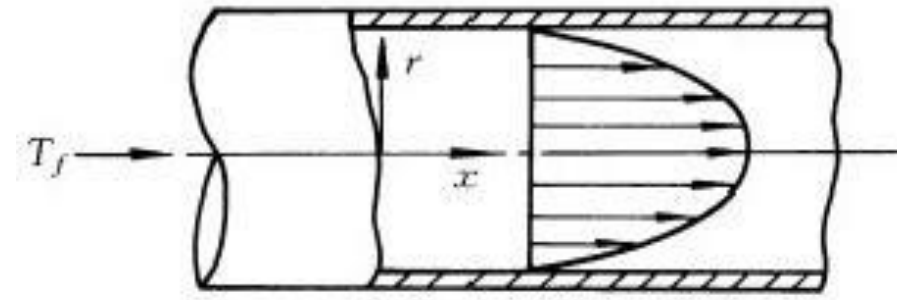
Third kind boundary condition for conduction and convective problem

Conduction problem



Fluid temperature and convective heat transfer coefficient on the solid surface are given to solve the temperature distribution in the solid.

Convective problem



Fluid temperature and convective heat transfer coefficient on the tube outside surface are given to solve the tube inner side fluid temperature distribution.

General expression of the three kinds of boundary conditions

$$AT_b + B\left(\frac{\partial T}{\partial n}\right)_b = C$$

$A=0$, second
kind boundary
condition

$B=0$, 1st kind
boundary
condition

C can be any
value, including
zero

If both A and B are not equal zero, its third kind boundary condition. Such general expression is useful for developing a general code which can deal with 3 kinds of boundary conditions.

1.2.2 Physical classification of governing equations

1. Conservative (守恒型) vs. non-conservative:

Non-conservative: those governing equations whose convective terms are not expressed by divergence form are called **non-conservative governing equation**. For 2D energy eq.:

$$u \frac{\partial(\rho c_p T)}{\partial x} + v \frac{\partial(\rho c_p T)}{\partial y} \text{ is not divergence form}$$

Conservative: those governing equations whose convective terms are expressed by divergence form(散度形式) are called **conservative governing equation**.

$$\frac{\partial(\rho u c_p T)}{\partial x} + \frac{\partial(\rho v c_p T)}{\partial y} \rightarrow \frac{\partial(\rho c_p T u)}{\partial x} + \frac{\partial(\rho c_p T v)}{\partial y} = \mathbf{div}(\rho c_p T \vec{U})$$

These two concepts are only for numerical solution.

2. Conservative GE. can guarantee (保证) the conservation of physical quantity (mass, momentum ,energy , etc.) within a **finite (有限大小) volume**.

$$\frac{\partial(\rho c_p T)}{\partial t} + \mathbf{div}(\rho c_p T \vec{U}) = \mathbf{div}(\lambda \mathbf{grad} T) + S_T c_p$$

$$\frac{\partial}{\partial t} \int_V (\rho c_p T) dV = - \int_V \mathbf{div}(\rho c_p T \vec{U}) dV + \int_V \mathbf{div}(\lambda \mathbf{grad} T) dV + \int_V S_T c_p dV$$

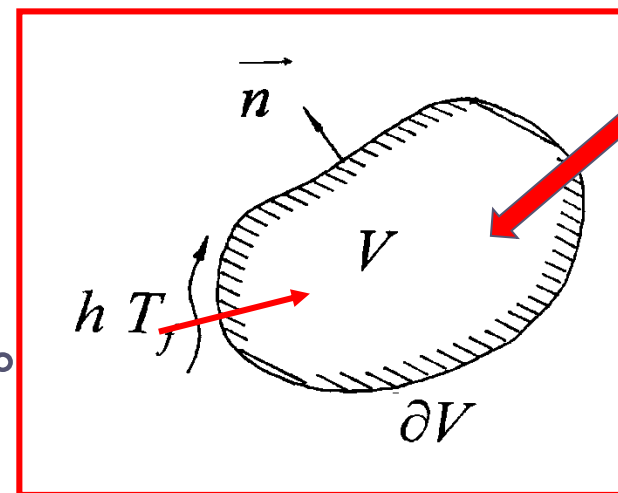
From Gauss theorem(高斯原律)

$$\int_V \mathbf{div}(\rho c_p T \vec{U}) dV = \int_{\partial V} (\rho c_p T \vec{U}) \bullet \vec{n} dA$$

(对散度的体积分等于该矢量与周界法向单位矢量点积的线积分。)

$$\int_V \mathbf{div}(\lambda \mathbf{grad} T) dV = \int_{\partial V} (\lambda \mathbf{grad}(T)) \bullet \vec{n} dA$$

Dot product (矢量的点积)



**Finite volume,
not differential
volume**

(有限大小容积,
不是微分容积)

$$\frac{\partial}{\partial t} \int_V (\rho c_p T) dV = - \int_{\partial V} (\rho c_p T \vec{U}) \cdot \vec{n} dA + \int_{\partial V} (\lambda \text{grad}(T)) \cdot \vec{n} dA + \int_V (S_T c_p) dV$$

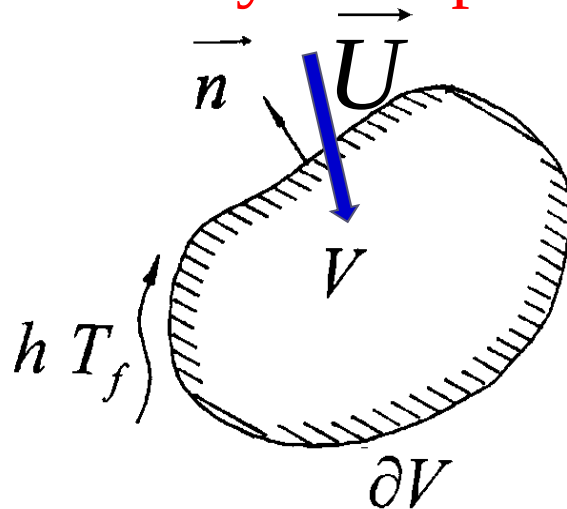
Increment
(增量) of
internal energy

Energy into
the region by
fluid flow

Energy into
the region by
conduction

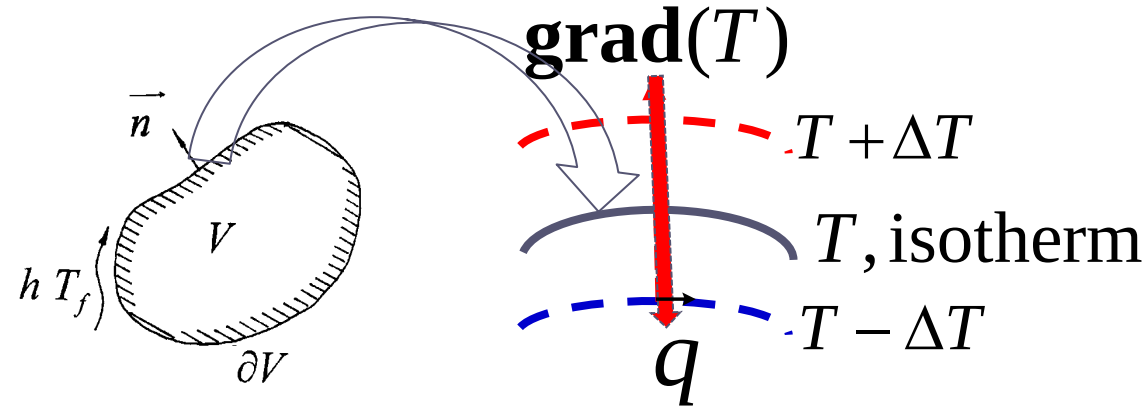
Energy
generated
by source

Exactly an expression of energy conservation!



$$\vec{U} \cdot \vec{n} < 0;$$

$-\vec{U} \cdot \vec{n} > 0$, heat flows in



$$\text{grad}(T) \cdot \vec{n} > 0$$

heat conducts in

Key to have a conservative form of governing equation:
convective term is expressed by divergence. If the convective term is not expressed in divergence form, we can not obtain the above result.

3. Conservative and non-conservative are referred to (指) a finite space (有限空间); For a differential volume (微分容积) they are identical (恒等的). For a differential volume:

$$u \frac{\partial(\rho c_p T)}{\partial x} + v \frac{\partial(\rho c_p T)}{\partial y} + \rho c_p T \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) = \frac{\partial(\rho u c_p T)}{\partial x} + \frac{\partial(\rho v c_p T)}{\partial y}$$

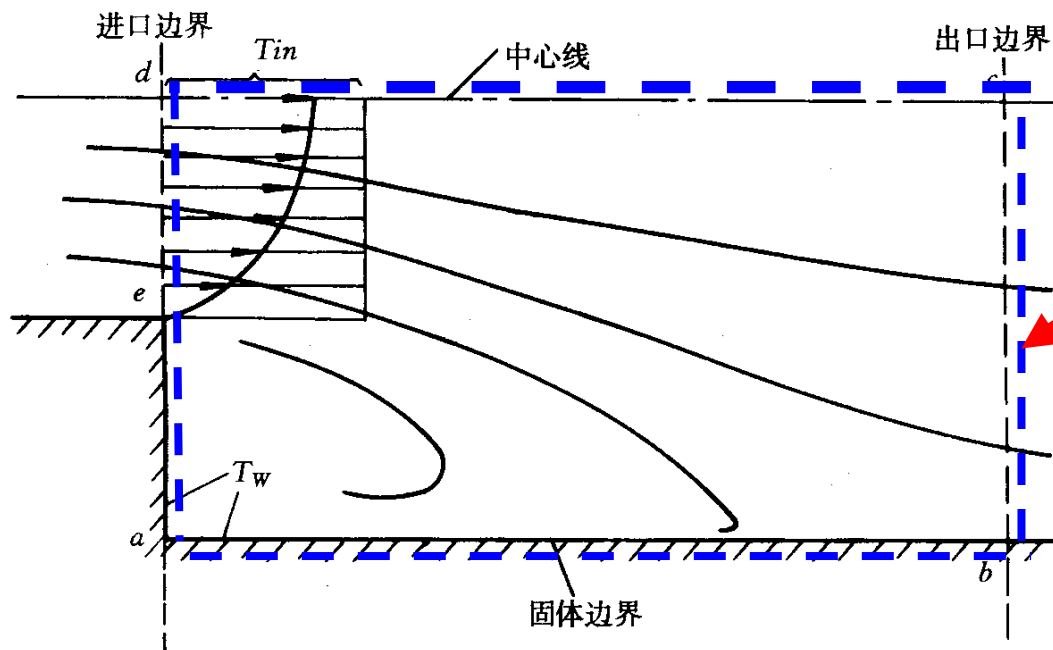
Non-conservative By adding mass conservation eq. Conservative

Generally conservative eq. is expected. Discretization eqs. are suggested to be derived from conservative PDE.

Example 1-1 Mathematical formulation

1. Problem and assumptions

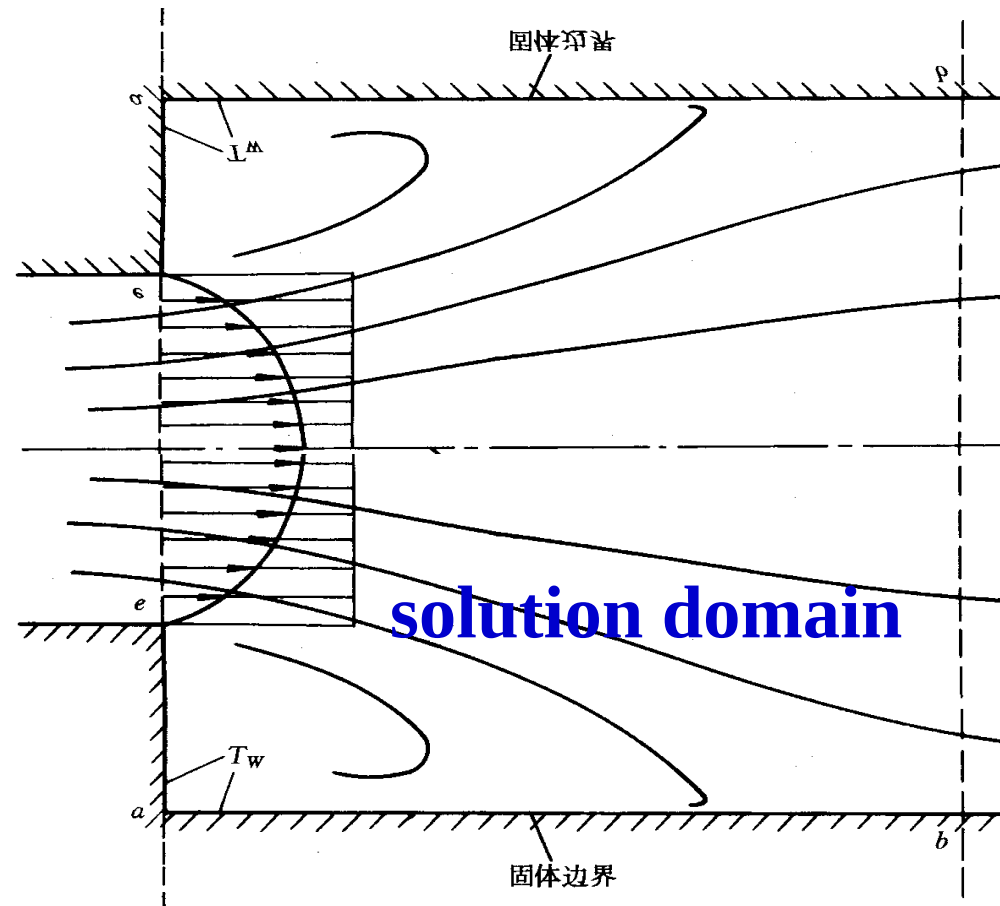
Convective heat transfer in a **sudden expansion region** (突扩区域) : 2D, steady-state, incompressible fluid, constant properties, neglecting gravity and viscous dissipation (粘性耗散) .



Solution domain
(求解区域)

2D Sudden expansion region

By making use of the geometric symmetry (对称) condition, it can be assumed that solution is also symmetry and only half of the region is the solution domain to save computation time.



2. Governing equations

Complete
set of
governing
equations

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

$$\frac{\partial(uu)}{\partial x} + \frac{\partial(uv)}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$

$$\frac{\partial(vu)}{\partial x} + \frac{\partial(vv)}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \nu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right)$$

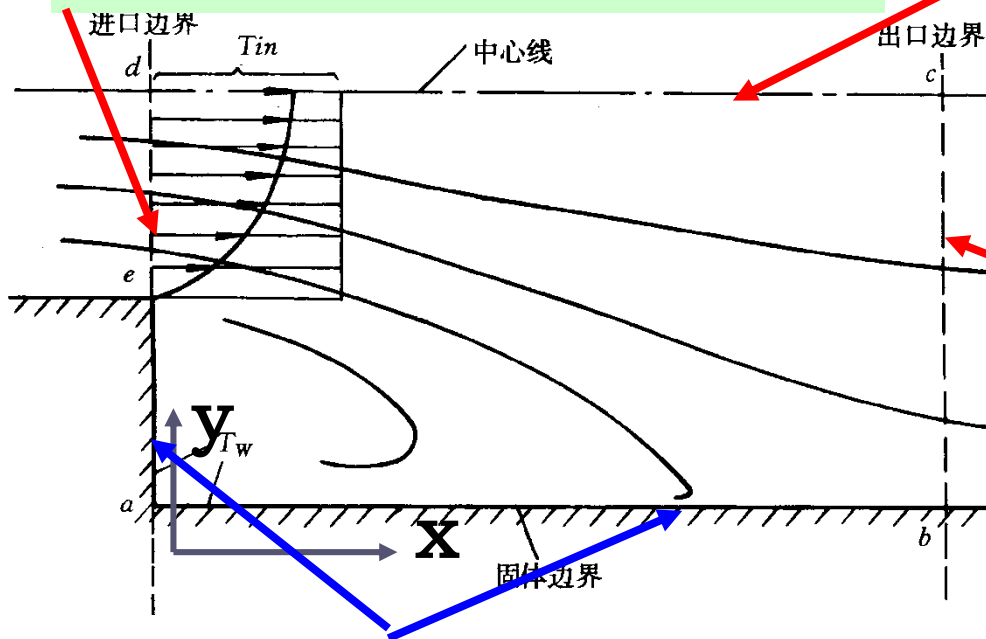
$$\frac{\partial(uT)}{\partial x} + \frac{\partial(vT)}{\partial y} = a \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)$$

$$a = \frac{\lambda}{\rho c_p}$$

**thermal
diffusivity**
(热扩散率)

3. Boundary conditions

(1) **Inlet**: specifying
(说明) variations of u, v, T
with y ;

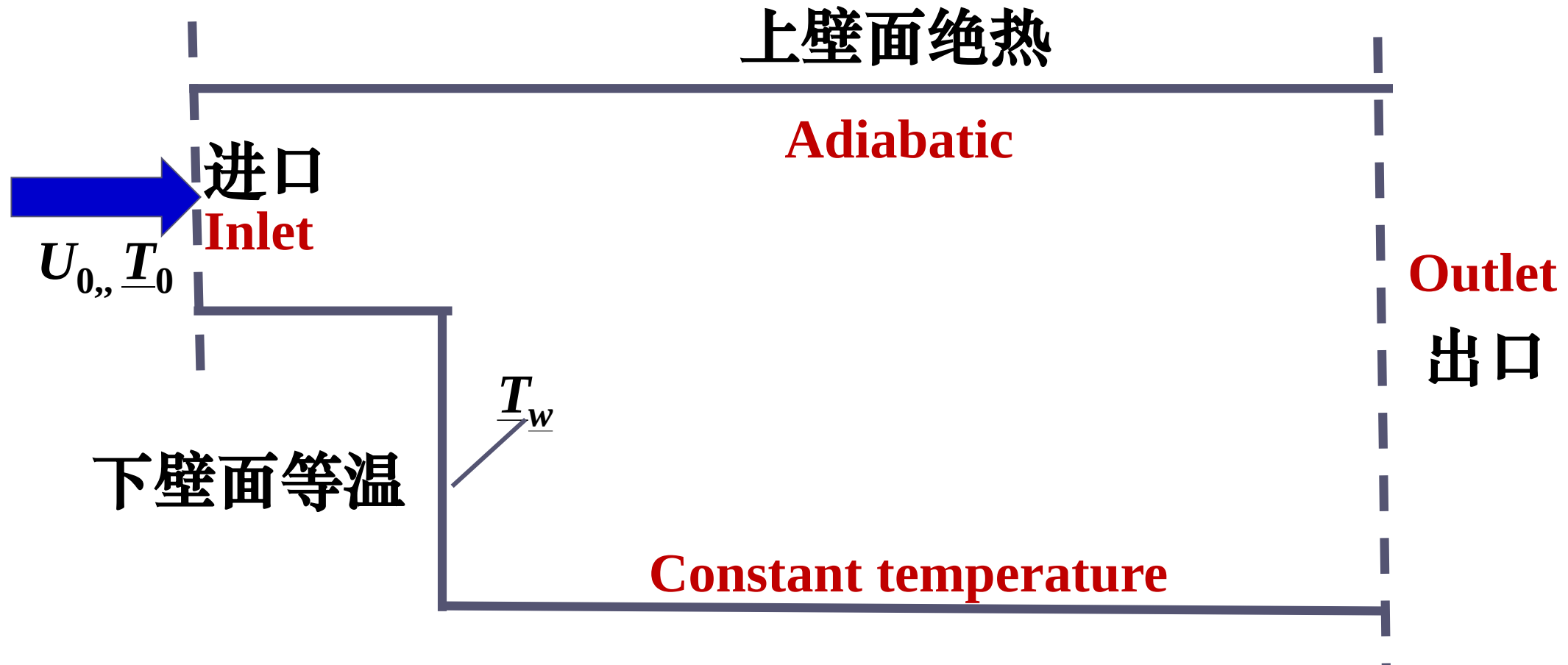


(3) **Center line**:
$$\frac{\partial u}{\partial y} = \frac{\partial T}{\partial y} = 0; \quad v = 0$$

(4) **Outlet**: Mathematically the distributions of u, v, T or their first-order derivatives (一阶导数) are required. Actually, numerical approximations must be made.

(2) **Solid B.C.**: No slip (滑移) in velocity, no jump (跳跃) in temp.

Can we regard this boundary formulation as **heat transfer and fluid flow over a backward step?**



1.3 Mathematical classification of governing eq. and its effect on numerical solution

1-3-1 General form of second –order partial differential eq. (PDE) With two dependent variables

1. General formulation of 2nd order PDEs with two independent variables
2. Basic features of three types of PDEs
3. Effects on numerical solutions

1-3-2 Discussion on the mathematical classification of PDE

Example1-2 Cold start-up of PEMFC---1-D unsteady
heat conduction with source terms

1.3 Mathematical classification of governing eq. and its effect on numerical solution

1-3-1 General form of second –order partial differential eq. (PDE) with two dependent variables

1. General formulation of 2nd order PDEs with two independent variables

$$a\phi_{xx} + b\phi_{xy} + c\phi_{yy} + d\phi_x + e\phi_y + f\phi = g(x, y)$$

ϕ is the dependent variable (因变量) to be solved;

a, b, c, d, e, f can be function of x, y, ϕ

There are three types of PDE depending on the value of $(b^2 - 4ac)$

leading to the difference in domain of dependence (DOD, 依赖区) and domain of influence (DOI, 影响区);

$$b^2 - 4ac \begin{cases} < 0, & \text{Elliptic} & \boxed{\text{椭圆型}} & (\text{回流型}) \\ = 0, & \text{Parabolic} & \boxed{\text{抛物型}} & (\text{边界层}) \\ > 0, & \text{Hyperbolic} & \boxed{\text{双曲型}} & \end{cases}$$

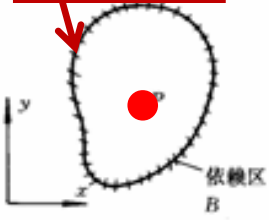
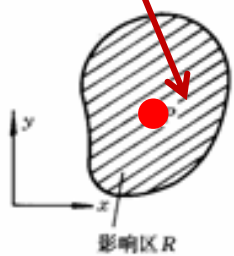
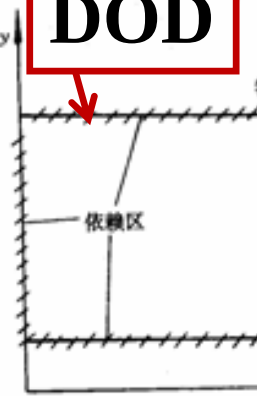
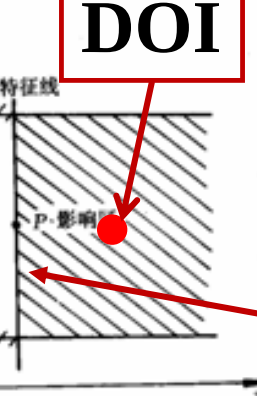
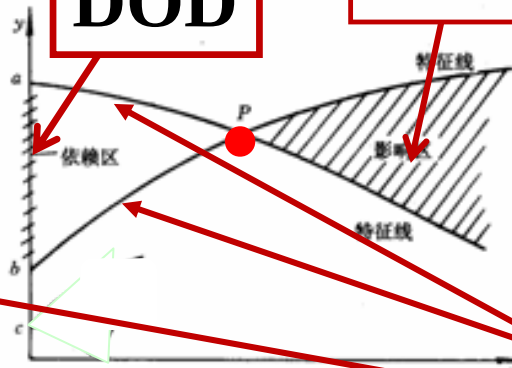
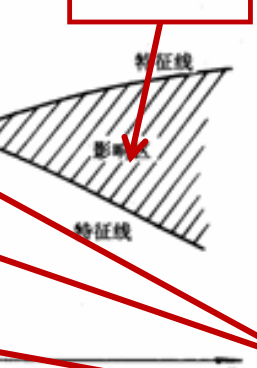
2. Basic features of three types of PDEs

$b^2 - 4ac < 0$, having no real characteristic line (elliptic type);
(没有实的特征线)

$b^2 - 4ac = 0$, having one real characteristic line (parabolic type) ;

$b^2 - 4ac > 0$, having two real characteristic lines (hyperbolic)

For 2-D case, DOD of a node is a line which determines the value of a dependent variable at the node; DOI of a node is an area within which the values of dependent variable are affected by the node.

Elliptic	Parabolic	Hyperbolic
DOD  DOI 	DOD  DOI 	DOD  DOI 
$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$ Steady HC ($a=1, b=0, c=1$) $u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x}$ $+ \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$ 2D N.S. Eq.	$\frac{\partial T}{\partial t} = a \frac{\partial^2 T}{\partial y^2}$ Un-Steady HC ($a=0, b=0, c=a$) $u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x}$ $+ \nu \frac{\partial^2 u}{\partial y^2}$ 2D B. L. Eq.	$\frac{1}{a} \frac{\partial T}{\partial t} + \frac{1}{c^2} \frac{\partial^2 T}{\partial t^2} = \frac{\partial^2 T}{\partial y^2}$ Non-Fourier HC ($a=1/c^2, b=0, c=-1$) $\frac{\partial^2 \phi}{\partial t^2} = C^2 \frac{\partial^2 \phi}{\partial y^2}$ Wave (波动) equation ($a=1, b=0, c=-C^2$)

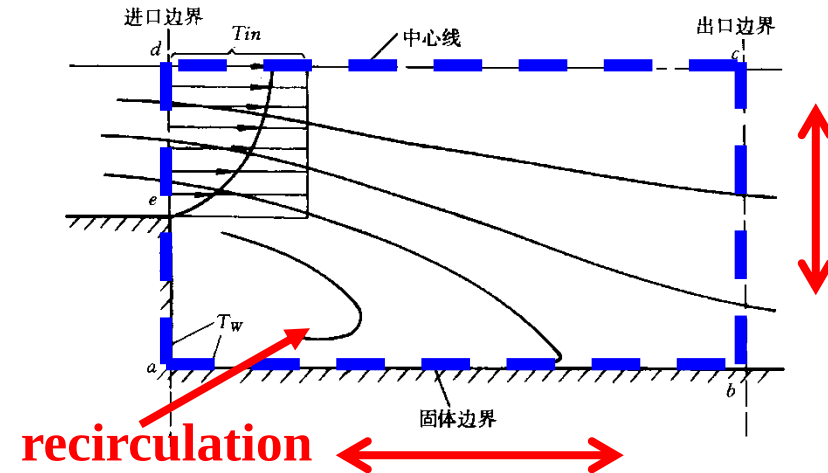
characteristic line

Non-Fourier HC

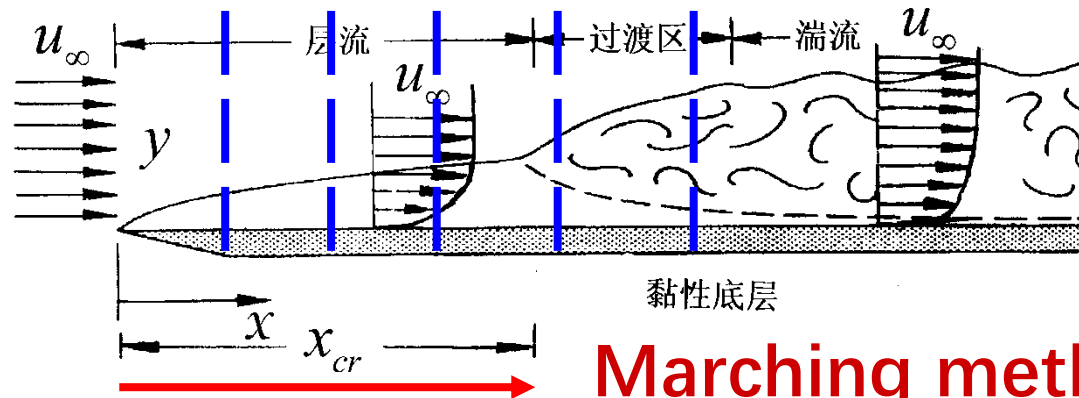
Wave (波动) equation

3. Effects different math type on numerical solution

(1) **Elliptic**: flow **with recirculation** (回流), solution should be done simultaneously (同时) for the whole domain;



(2) **Parabolic**: flow **without recirculation**, solution can be done by **marching method** (步进方法), from step to step, greatly saving computing time!



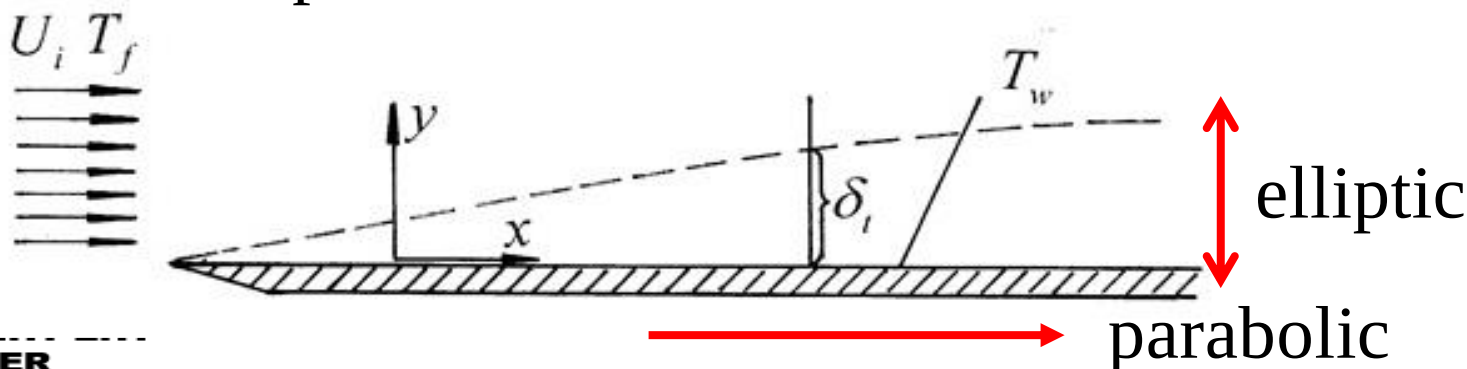
Marching method

1-3-2 Discussion on the mathematical classification of PDE

1. Mathematics only defines different types for 2-D problems. How to deal with for problems with 3-D domain?

Dividing the domain into many 2-D sections. **Each section consisting of two independent variables can be classified according to the above criteria.** Thus for a 3-D domain maybe some sections are elliptic while some others are parabolic.

2. For 1-D unsteady heat conduction, it is parabolic at the time direction, while elliptic in the space direction. The same for boundary layer problem: it is parabolic in the main flow direction, while elliptic in the direction normal to the main flow.



Here elliptic means the grid points on the same vertical line should be solved simultaneously

Example1-2 Cold start-up of PEMFC(燃料电池冷启动)

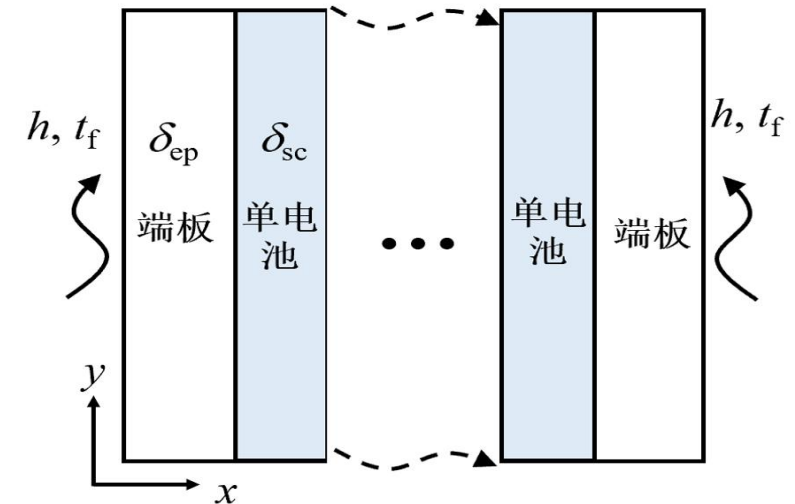
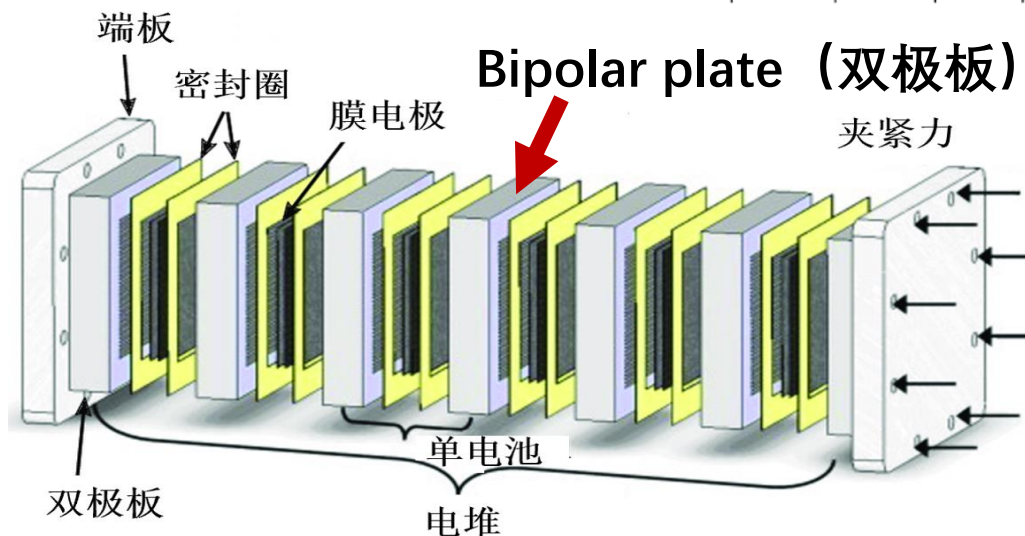
---1-D unsteady heat conduction with source terms.

Write down the mathematical formulation.



Single fuel cell

Fuel cell stack



With many assumptions ,the cold start-up process can be simplified by 1-D transient heat conduction with effective heat capacity and thermal conductivity:

$$(\rho c_p)_{\text{eff}} \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(\lambda_{\text{eff}} \frac{\partial T}{\partial x} \right) + S_T, \quad 0 < x < L$$

Initial condition: $t = -20^\circ \text{C}, 0 \leq x \leq L$

Boundary condition: $-\lambda \frac{\partial t}{\partial n} = h(t_w - t_f) \quad x = 0, x = L$

$$S_T = S_\Omega + S_{\text{act}} + S_{\text{rec}} \quad h = 5 \text{ Wm}^{-2} \text{K}^{-1}$$

$$S_\Omega = I^2 R_{\text{cell}} / \delta_{\text{sc}}, \quad S_{\text{act}} = V_{\text{act}} I / \delta_{\text{sc}}, \quad S_{\text{rec}} = T \Delta s \cdot I / (2F \delta_{\text{sc}})$$

Ohm heat

Activation heat

Reaction heat

1.4 Fundamental (基本的) contents of numerical heat transfer

1-4-1 Basic concepts of numerical solution for HT and FF problems

1-4-2 Brief introduction of existing numerical methods

1. Finite difference method (FDM)

2. Finite volume method (FVM)

3. Finite element method (FEM)

4. Finite analytical method (FAM)

1-4-3 Implementation tools of numerical simulation

1-4-4 Introduction to present course

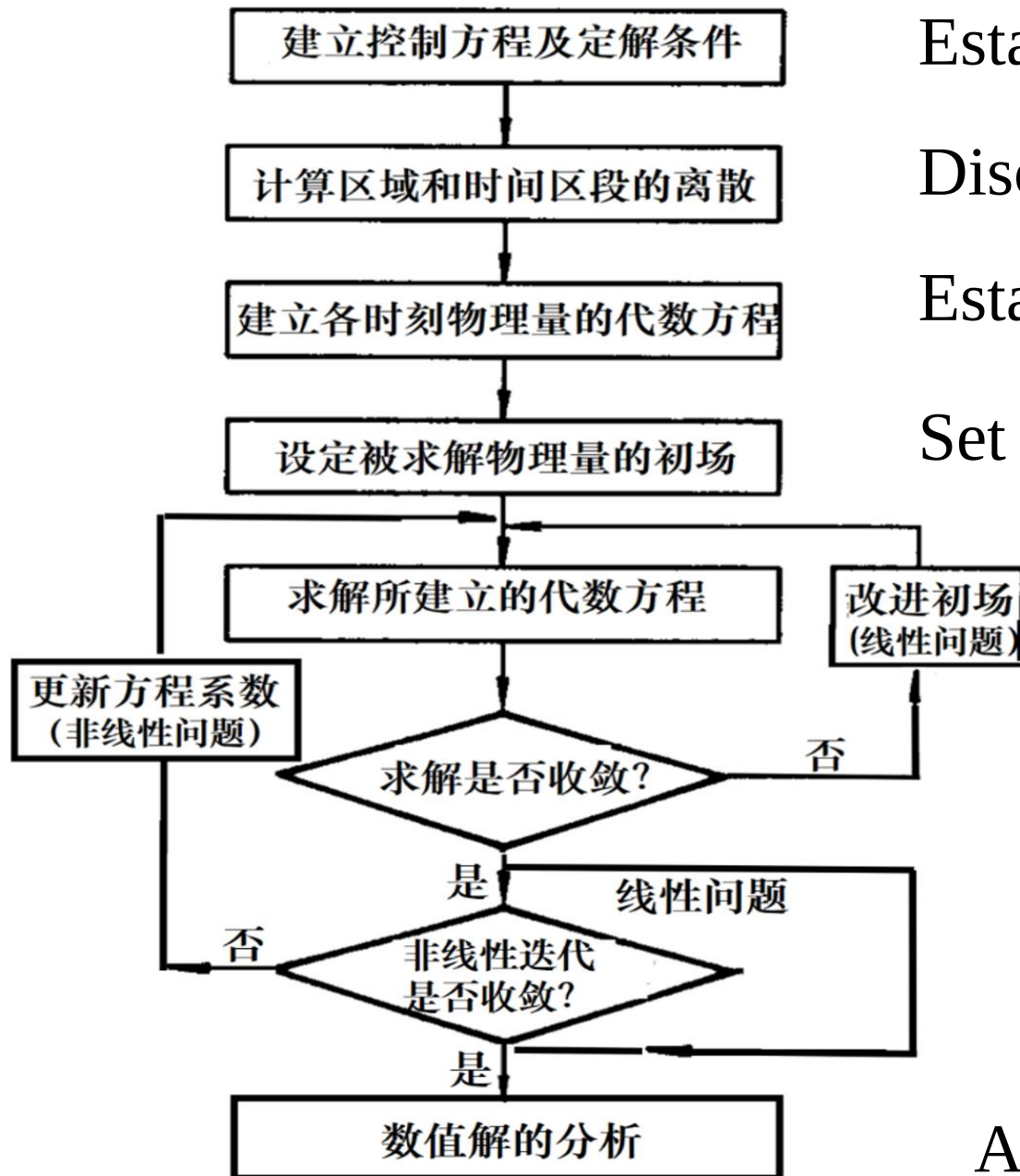
1.4 Fundamental (基本的) contents of numerical heat transfer

1-4-1 Basic concepts of numerical solution for HT and FF problems

Replacing the fields of continuum variables (velocity, temp. etc.) by sets (集合) of values at discrete (离散的) points (nodes, grids 节点) (Discretization of domain, 区域离散);

Establishing algebraic equations for these values at the discrete points by some principles (Discretization of equations, 方程离散);

Solving the algebraic equations by computers to get approximate solutions of the continuum variables (Solution of discretized equation, 方程求解).



Establish governing eqs. and I-B conditions

Discretize (离散) space and time domain

Establish discretized eqs for physical variables

Set initial solutions for iteration

Solve the algebraic equations

Iteration (迭代) process

Analyze the converged solution

1-4-2 Brief introduction of existing numerical methods

1. Finite difference method (**FDM**)

有限差分法: L F Richardson (1910), A Thome (1940s)

2. Finite volume method (**FVM**)

有限容积法: D B Spalding; S V Patankar

3. Finite element method (**FEM**)

有限元法: O C Zienkiewicz; 冯 康 (**Kang Feng**)

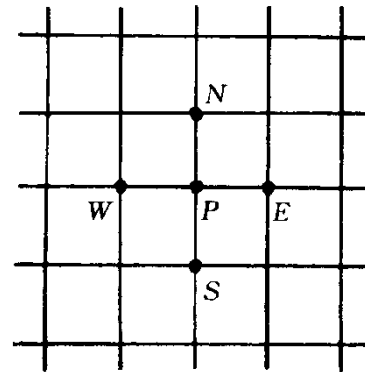
4. Finite analytic method (**FAM**)

有限分析法: 陈景仁(Ching Jen Chen)



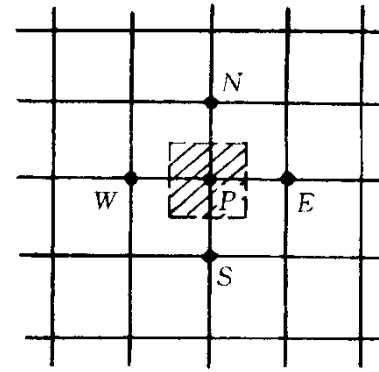
Comparisons of FDM(a),FVM(b),FEM(c),FAM(d)

FDM
有限差分



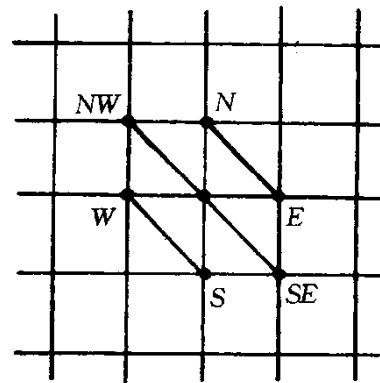
(a)

FVM
有限容积



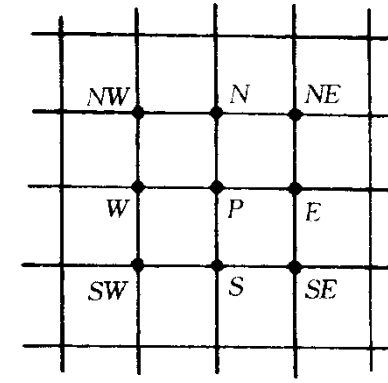
(b)

FEM
有限元



(c)

FAM
有限分析



(d)

All these methods need a grid system (网格系统):
1) Determination of grid positions; 2) Establishing the influence relationships between grids.

1-4-3 Implementation tools of numerical simulation

1. Adopting commercial software

ANSYS FLUENT, ANSYS CFX, COMSOL, STAR-CCM+,
In this course FLUENT will be taught and applied to solve problems.

2. Using open source codes

The most typical one is **OpenFOAM** (Open Field Operation and Manipulation), which was initially developed by some researchers in **Imperial College, London**. An introduction is given in the textbook.

3. Developing proprietary (自主) software is of great significance.

When the world's first commercial software **PHEONICS** was released, it was prohibited (禁止) from selling it to communist party countries like China. Many Chinese researcher have been hardly working on this regard. **Hyperflow, PHengLEI** and **MHT** are some examples developed by Chinese researcher.

国家重大需求和行业关键痛点

能源动力



电子器件



航天航空



船舶



工业软件普遍受制于人



OpenFOAM®

ANSYS
FLUENT®

FloTHERM®

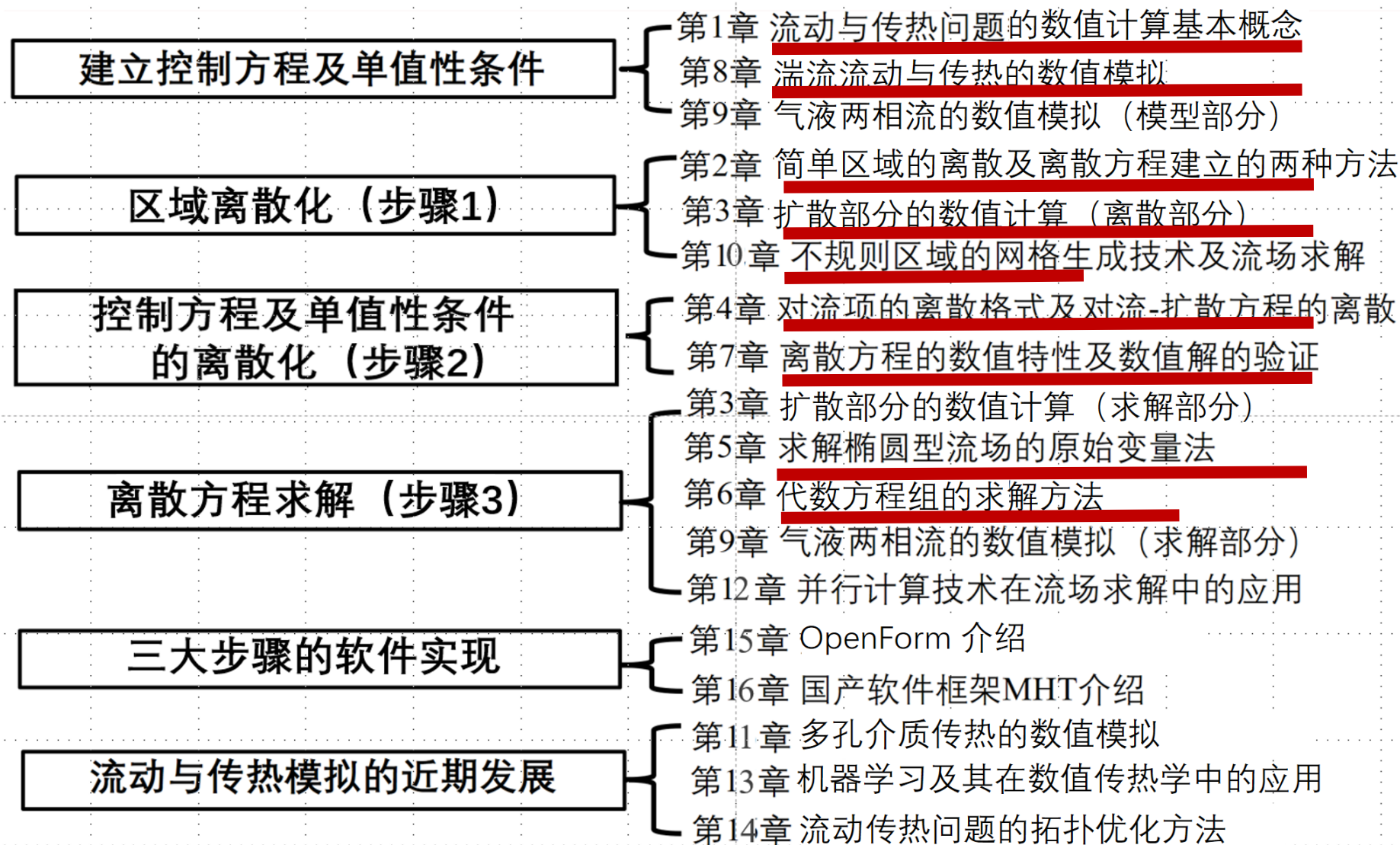
SYNOPSYS®



Numerical heat transfer is the fundamental discipline for developing various industrial software related to thermal phenomena.

数值传热学是开发各类与热现象有关的各类工业软件的基础学科。

1-4-4 Introduction to present course



1.5 Role of numerical simulation and stories of Prof. Kang FENG and D B Spalding

1-5-1 Three fundamental approaches (方法) of scientific research and their relationships

1-5-2 Irreplaceable (不可替代的) application examples

1-5-3 Story of Professor Kang FENG in developing FEM

1-5-4 Story of Professor D B Spalding in developing CFD and commercial software

1-5-5 Some Suggestions for learning the course

1.5 Role of numerical simulation and stories of Prof. Kang FENG and D B Spalding

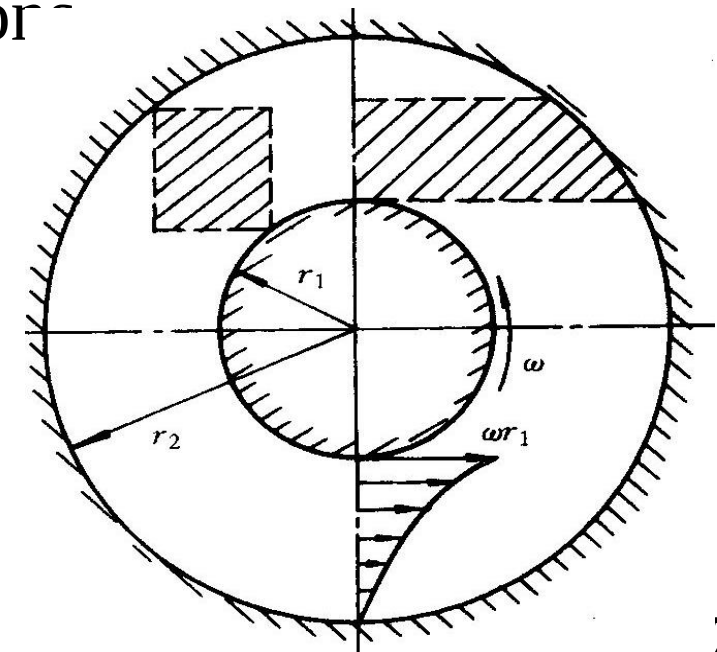
1-5-1 Three fundamental approaches (方法) of scientific research and their relationships

1. Theoretical analysis (Analytical solution)

Its importance should not be underestimated (低估). It provides comparison for verifying (验证) numerical solution -

Examples: The analytic solution (分析解) of velocity from NS eq. for following case

$$\frac{u}{u_1} = \frac{r_1 / r_2}{1 - (r_1 / r_2)^2} \cdot \frac{1 - (r / r_2)^2}{r / r_2}, \quad u_1 = \omega r_1$$



2. Experimental study

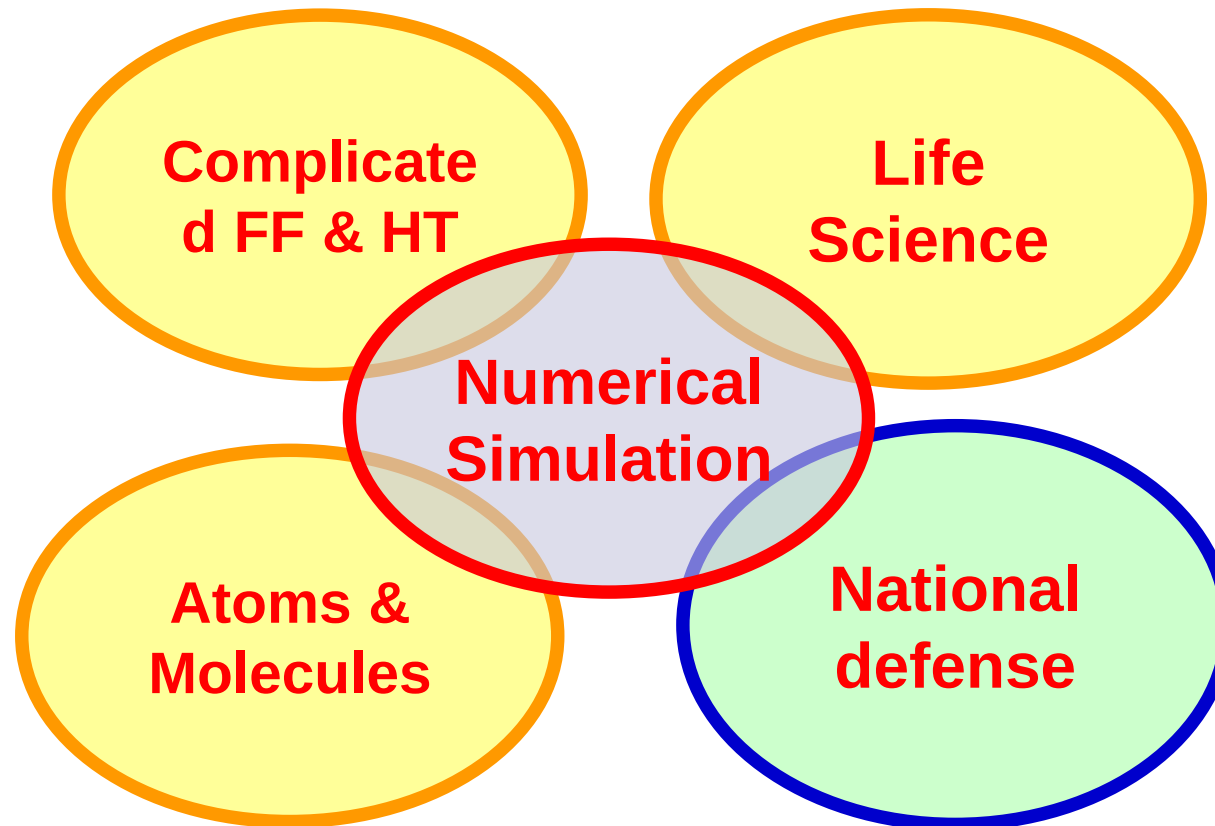
A basic research method: observation(观察); properties measurement; verification (验证) of numerical results

3. Numerical simulation

Numerical simulation is an inter-discipline (交叉学科), and plays an important and un-replaceable role in exploring (探索) unknowns, promoting (促进) the development of science & technology, and for the safety of national defense (国防安全) (探索未知, 促进科技发展, 保证国防安全) .

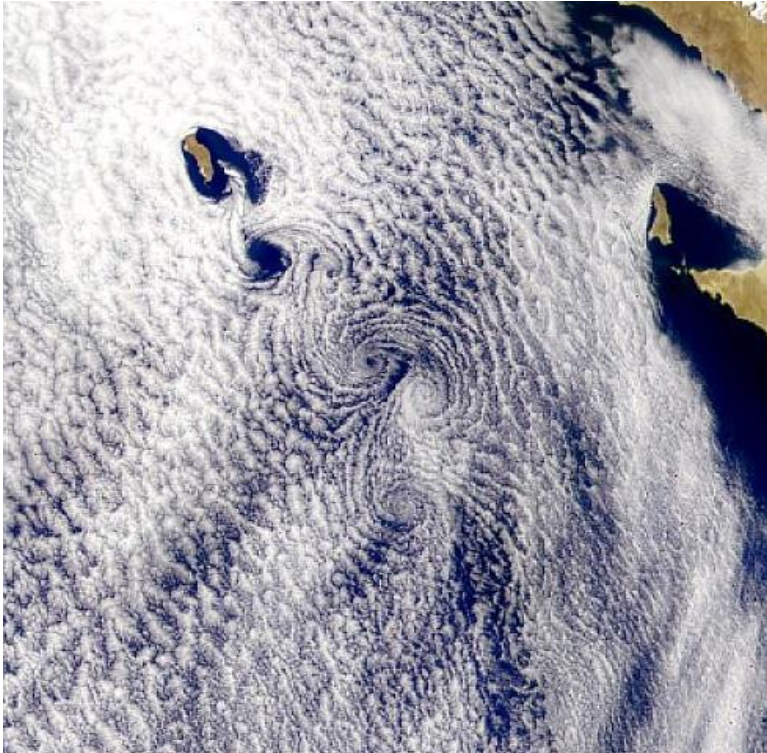
With the rapid development of computer hardware (硬件), the importance and function of the numerical simulation become greater and greater.

Historically, in 1985 the West Europe listed the first commercial software-**PHEONICS** as the one which was not allowed to sell to the communist countries. The prohibition (禁令) was cancelled (取消) in 1990s.



1-5-2 Irreplaceable (不可替代的) application examples

Example 1: Weather forecast— Numerical solution is the only way.



Large scale vortex



Cloud Atlas sent back by a meteorological satellite

Example 2: Fire hazard prediction (住宅火灾危害预测)

NIST



Time: 0.1



Example 3: Fire Prediction in Olympic Stadium Design (奥运场馆设计中的火灾预测)

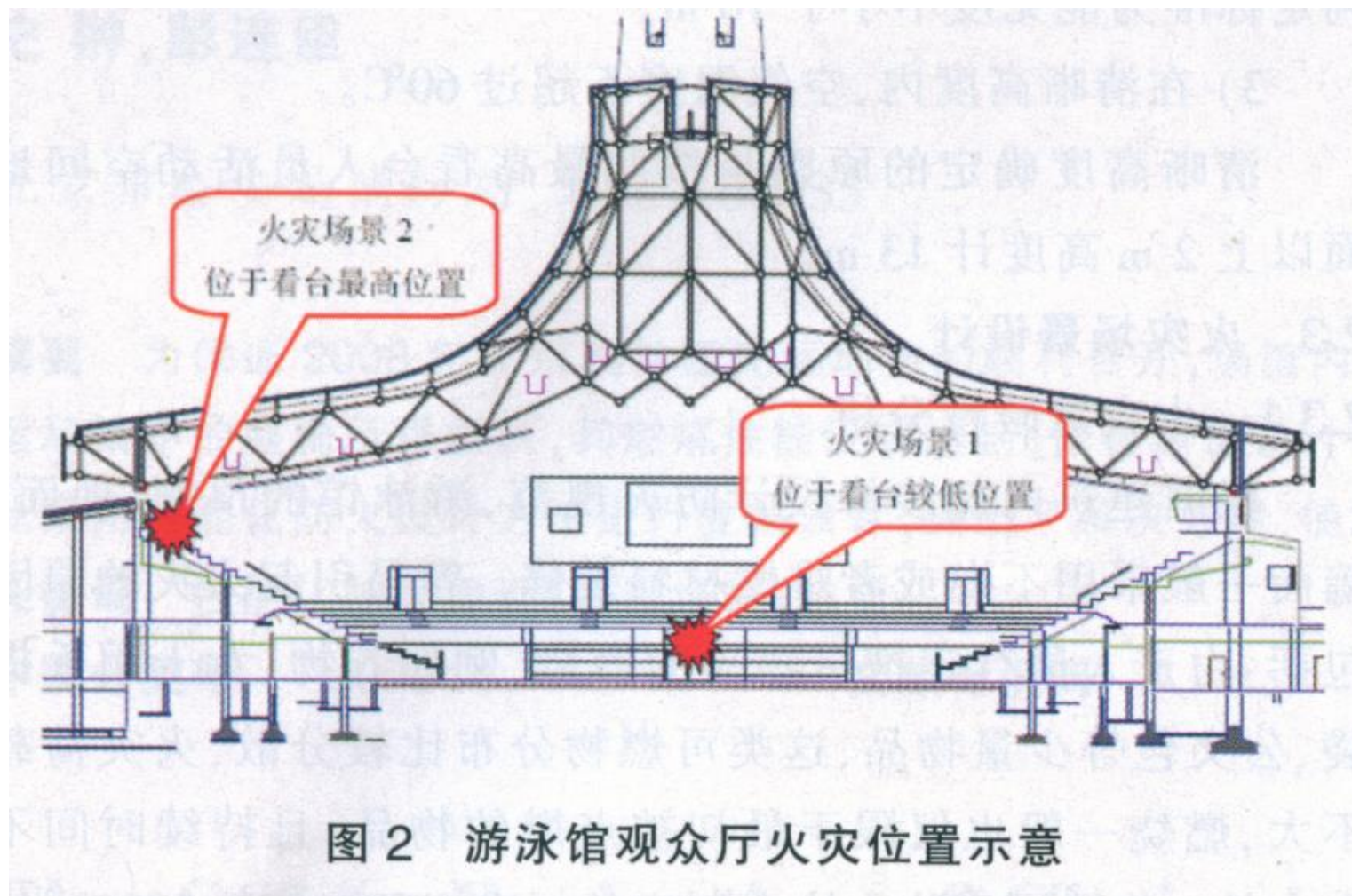




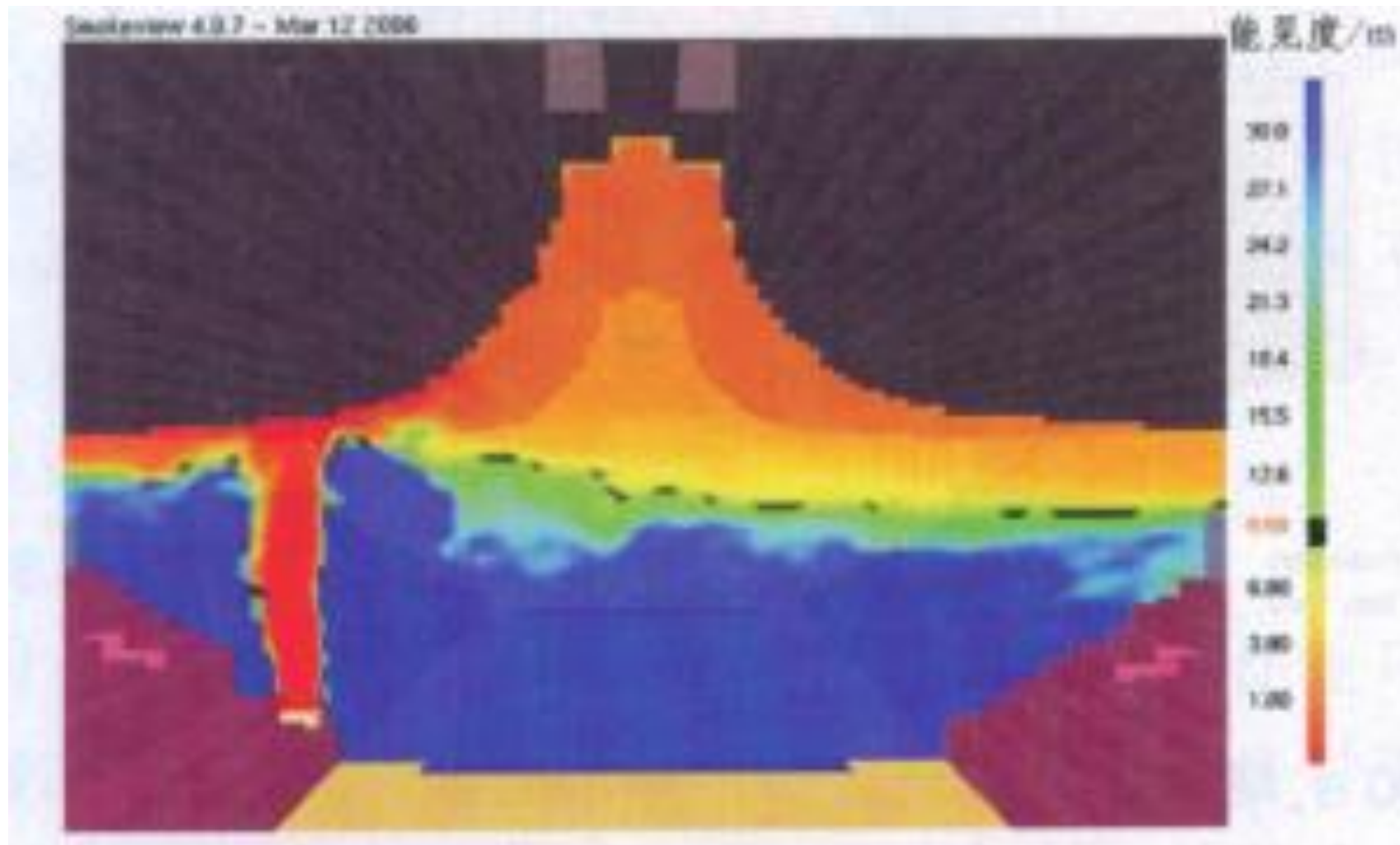
In the design of Olympic indoor swimming pool : the seat material can not meet the high standards of fire safety requirements. **The Olympic sports meeting is about to be held soon, and it's too late to make the change.**

What can we do?

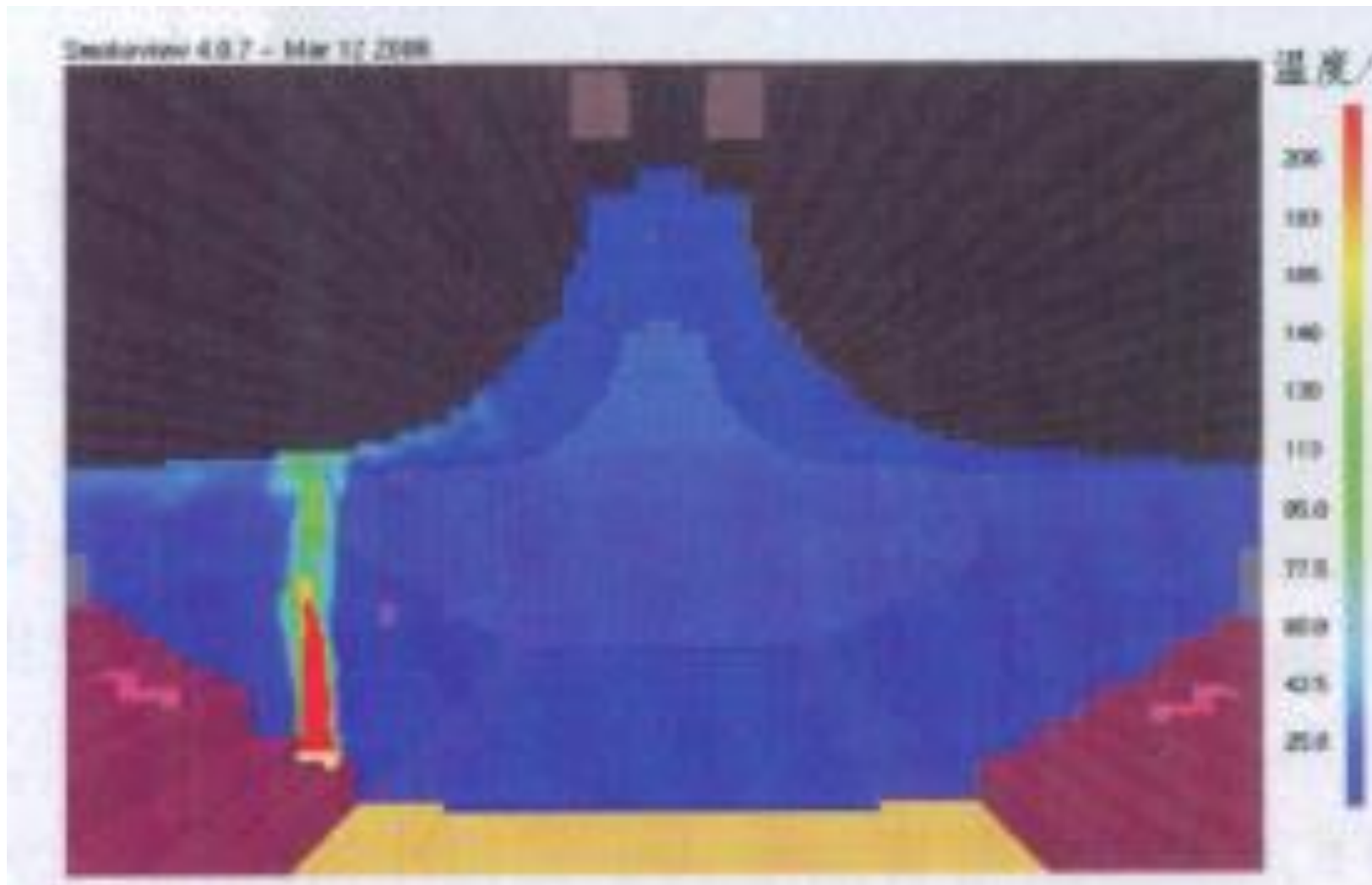
By numerical simulation!



Taking two places as the source of fire . By simulation to reveal after certain time, say 15 minutes, of fire break out whether the audiences can still ran away safely from the natatorium(游泳馆) .

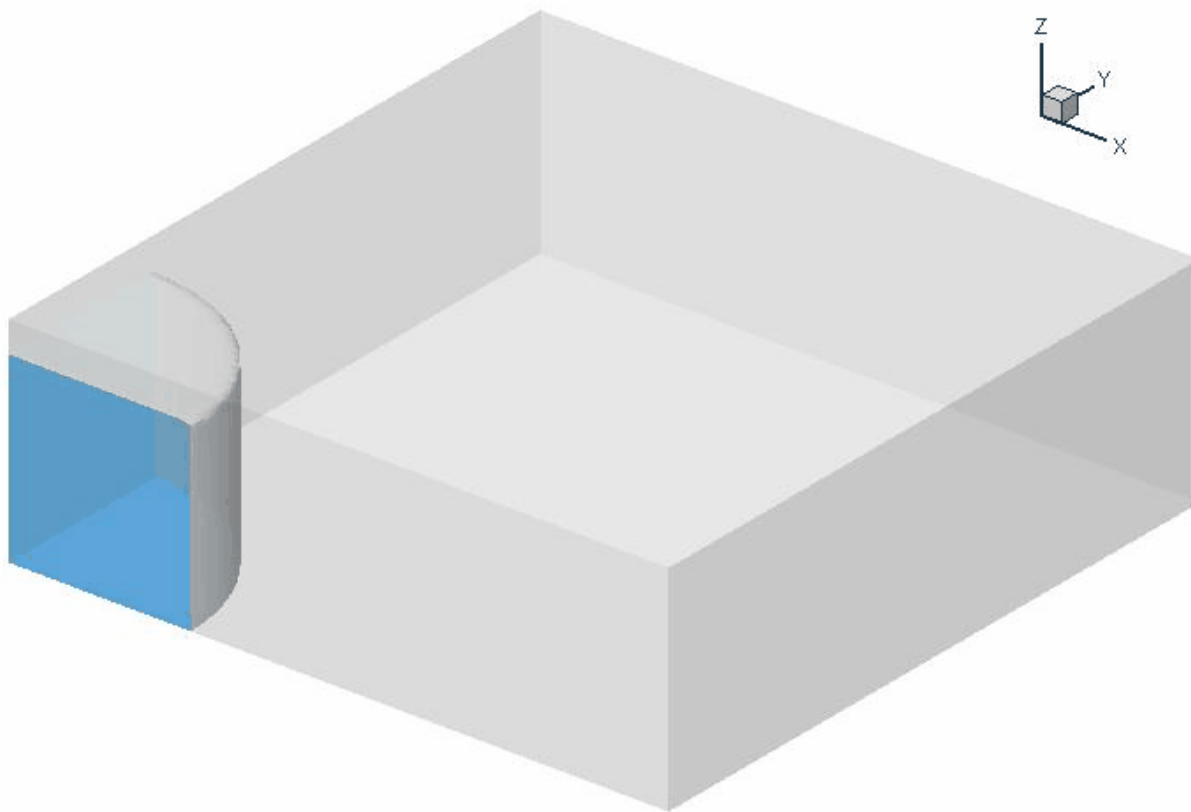


Visibility of the smoke after 900 seconds (900秒后烟气的能见度)

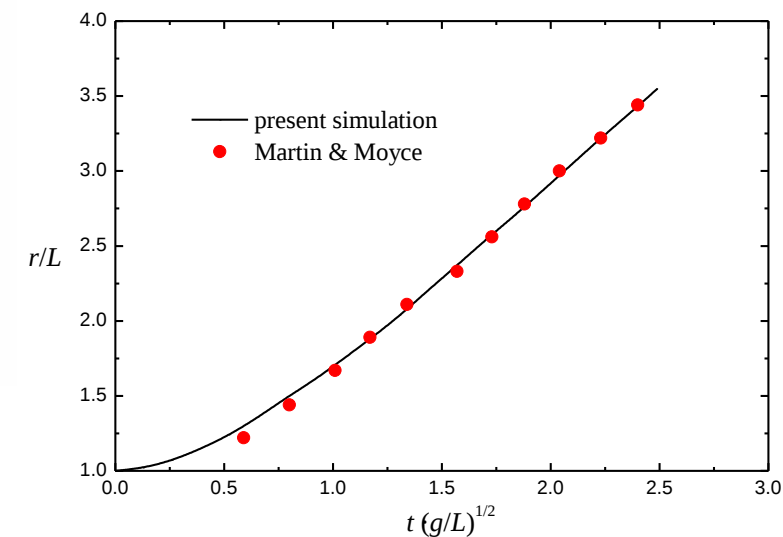


Temperature distribution of smoke in the auditorium after 900 seconds. (900秒后观众厅烟气温度分布)

Example 4: Simulation of breaking dam (溃坝)



Evolution (演变) process of interface

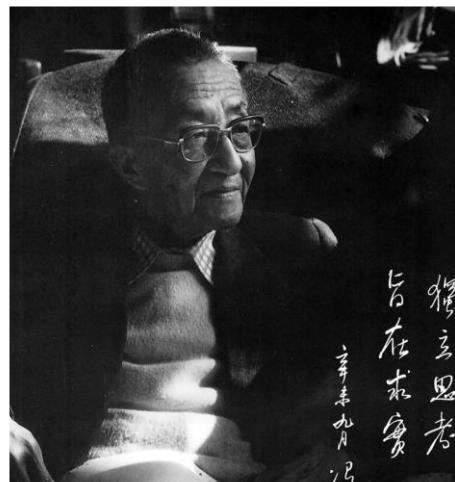


Base radius vs. time

1-5-3 Stories of Professor Kang FENG



叶笃正，气象学家
中科院院士
(Meteorology)



冯康，数学家
中科院院士



冯端，物理学家
中科院院士



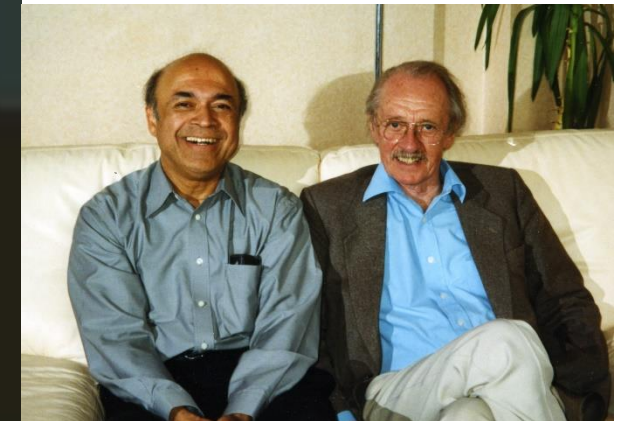
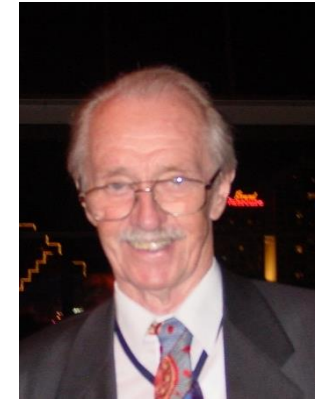
Professor K.FENG
developed very strict and
beautiful mathematical theory
of finite element method(FEM).

**He was not married for
his whole life, and devoted
himself to the innovation
of science & technology in
China .**

The year of 2020 was the 100th birthday of Feng KANG. A solemn (隆重) commemoration (纪念) was held in the Mathematical Institute in Beijing.

冯康. 基于变分原理的差分格式 [J]. 应用数学和计算数学,
1965, 2 (2) : 237-261

1-5-4 Stories of Professor D B Spalding



In 1965, D B Spalding (1923-2016) served as a professor of heat transfer at Imperial College and was in charge of the "Thermal Fluids" department. Later, this department was renamed "Computational Fluid Dynamics Group" (CFDU).

In 1969, Professor Spalding founded CHAM (Concentration, Heat and Momentum), aiming to promote the research results of their team to industrial applications.

In 1974, CHAM moved out of the school and established a company in Wimbledon, London, mainly providing consulting services for the industrial sector.

In 1981, the first commercial version of PHOENICS by CHAM was released. It is an abbreviation of the series of Parabolic Hyperbolic Or Elliptic Numerical Integration Codes, indicating that the PHOENICS program can be used to simulate and calculate for any flow and heat transfer scenarios.

PHOENICS can solve following governing equation

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial}{\partial x_k} \left(\rho U \phi - \Gamma_\phi \frac{\partial \phi}{\partial x_k} \right) = S_\phi$$

Users can independently make choices regarding the discretization methods for the time term, the flow term, the diffusion term, and the source term.

PHOENICS is the pioneer of CFD commercial software. Most commercial CFD software today can trace their origins back to the work done by Spalding and his team.

In 1988, Spalding retired from Imperial College and devoted himself entirely to running the company. Over the following three decades, PHOENICS gradually became widely used in various industrial sectors. At its peak, it had agents in 25 countries and regions such as the United States, and held regular international user conferences and published journals.

In 1985, it was listed by the Western European Community as a product subject to an embargo (禁运品) on Communist countries. Only in 1993 due to the emergence of the heat transfer and flow commercial software market. Subsequently, the PHOENICS version was introduced to China. In 2007, when this group initiated the Asian Computational Heat Transfer Conference, Professor Spalding actively supported it and came to Xi'an to attend the meeting.

Spalding presented the 1st ASCHT (2007, Xi'an, China)

2007 ASIAN SYMPOSIUM ON COMPUTATIONAL HEAT TRANSFER AND FLUID FLOW
2007亚洲计算传热与计算流体会议, XI' AN, CHINA, OCTOBER 17-21, 2007



Prof H

Kawamura

Prof Oteha
USA NSF

Prof D B Spalding

Prof N Hur

ASCHT has been held for 20 years.

In 2007 I initiated The Asian Symposium on Computational Heat Transfer (ASCHT). Professor Spalding was invited to attend the conference. It has become an international conference and is held every two years.



The 2023-ASCHT was held in Saudi. 22 of my group students attended; 2025-ASCHT was held in Wuhan. Next year it will be held in South Korea.

Entering the 21st century, due to the emergence of many flow and heat transfer software, as well as certain deficiencies in the PHOENICS software framework, its share in the software field gradually declined (下降) .

In 2016, Professor Spalding passed away. In 2023, Zhongwang Company purchased 100% of the equity (资产) held by Collen Iona Spalding for 5.55 million pounds from her, thus bringing an end to the CHAM company.

However, the role played by Professor Spalding and his team in the development of computational fluid dynamics and computational heat transfer has been recorded in history.

Some more information about commercial software

In 1983, Jim Swithenbank and his team from the University of Sheffield in the UK developed FLUENT and launched it to the market. In 1988, the New Hampshire-based Creare Company in the US purchased FLUENT and renamed it Fluent. In 2006, Fluent was purchased by ANSYS.

1983年 英国 Sheffield 大学 Jim Swithenbank 和他的团队开发 FLUENT 发放市场。1988年美国 New Hampshire Creare 公司购买了 FLUENT，改名 Fluent。2006年 Fluent 被 ANSYS 收购。



Recently, ANSYS was purchased by Synopsys, which is a major company specializing in electrical component design. Heat dissipation is currently the key to improve the power output of electronic devices.

最近 ANSYS 被 Synopsys 收购，后者是专做电器件设计的大公司，散热是当前电子器件提高功率的关键

From the above brief development history, it can be seen that software for numerical simulation of heat transfer and flow not only has the characteristics of a commodity(商品), but also, due to its significance, serves as a tool in political struggles. As graduate students of a research-led university, one must master the basic knowledge of numerical simulation and cultivate (培养) the ability to develop simulation codes.

从上述发展历史简述可见，类似传热流动数值仿真的软件既具有商品的特性，由于其重要性，也是一种政治斗争的工具；作为研究型大学的研究生必须掌握数值仿真的基本知识，并培养自己开发计算代码的能力。

1-5-5 Some Suggestions for learning the course

1. Understanding numerical methods from basic characteristics of physical process;

2. Mastering (掌握) complete picture and knowing every detail (明其全，析其微) for any numerical method;

3. Practicing simulation method by a computer; Working hard to develop your ability to write code for yourself;

4. Trying hard to analyze simulation results: rationality (合理性) and regularity (规律性);

5. Adopting CSW(商业软件) in conjunction with (与....结合) self-developed code (与自编程序相结合).

The following words are presented in the PPT of this chapter. If you are not familiar with them, please use AI to confirm their meanings and pronunciations (in the order of appearance)

formulation;	adiabatic	discrete	hazard
unique	variable	discretization	stadium
component	elliptic	proprietary	dam
enthalpy	parabolic	significance	evolution
nominal	hyperbolic	irreplaceable	devote
scalar	characteristic line	theoretical	embargo
gradient	domain	Inter-discipline	decline
conservative	recirculation	recirculation	commodity
divergence	marching method	verification	in conjunction with
guarantee	consistent	defense	regularity
increment	fuel cell	explore	theorem

本组网页地址: <http://nht.xjtu.edu.cn> 欢迎访问!

Teaching PPT will be loaded on our website

The pdf file will be posted at our group website and WeChat group.



同舟共济
渡彼岸!

People in the
same boat help
each other to
cross to the other
bank, where....