

# Numerical Heat Transfer

## (数值传热学)

### Chapter 1 Introduction



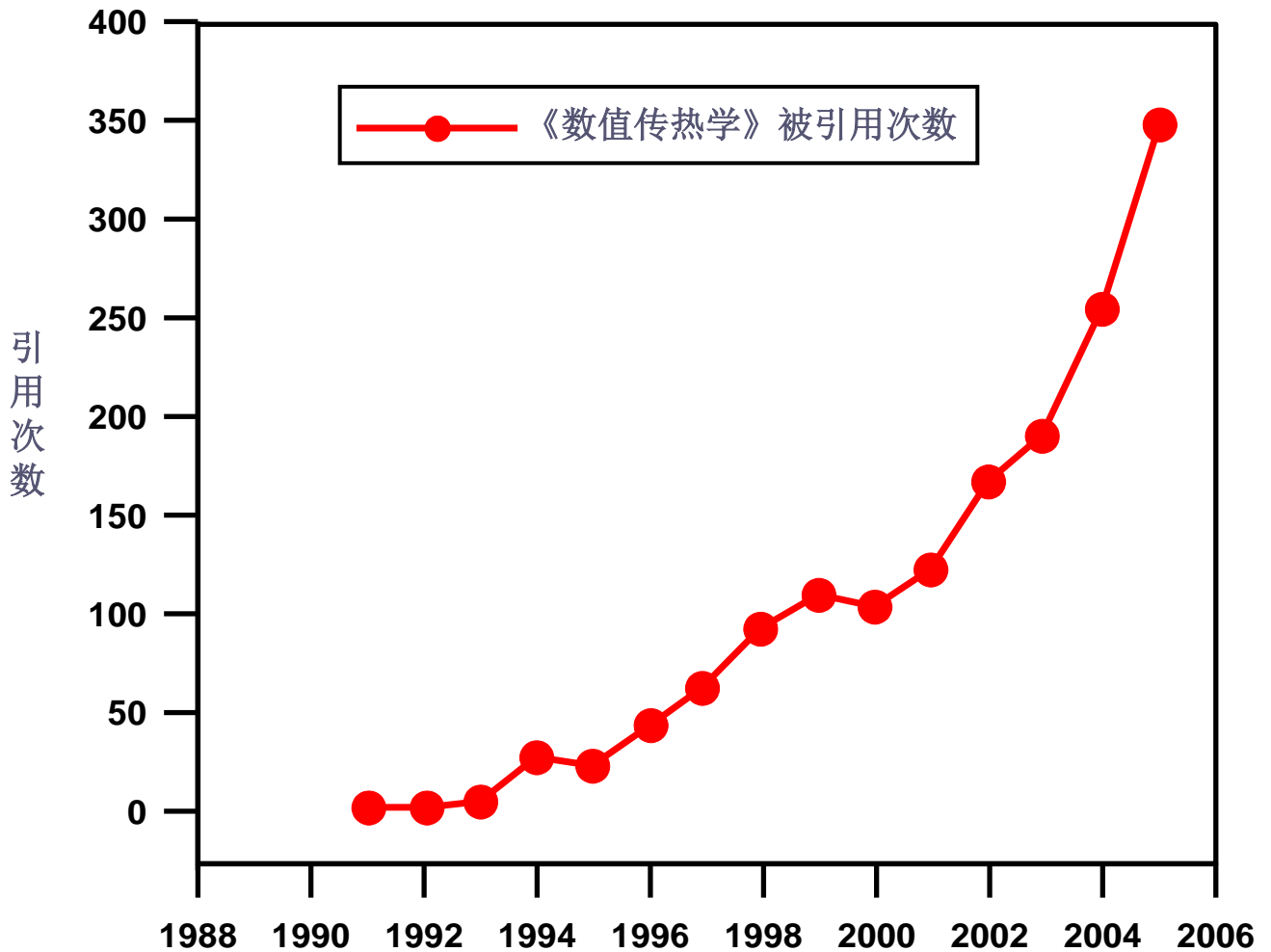
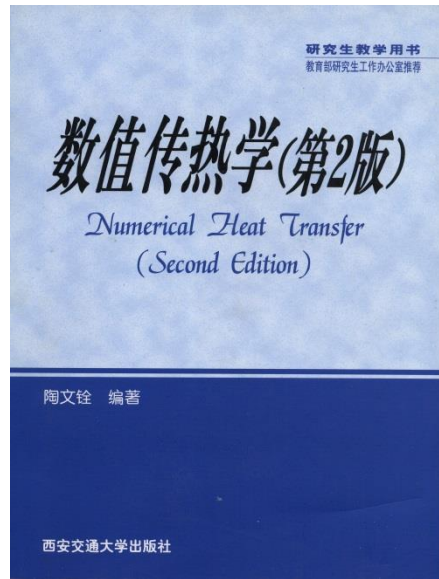
**Instructor Tao, Wen-Quan**

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**Key Laboratory of Thermo-Fluid Science & Engineering of MOE**  
**Xi'an Jiaotong University**  
**Xi'an, 2016-Sept-12**

## Brief Introduction to Course

1. Textbook— 《数值传热学》, 2<sup>nd</sup> ed., 2001
2. Teaching hours— 50 hrs-basic principles;  
about 10 hrs-code
3. Course score(课程成绩)— Home work/Computer-  
aided project: —50/50
4. Methodology— **Open, Participation and  
Application** (开放, 参与, 应用)
5. Teaching assistants— Pu KE(何璞), Le LEI (雷  
乐), Xing-Jie RENG (任兴杰), Peng HE (和鹏)

For convenience of discussion , a **qq-group** has been set up:  
**573633261**



《数值传热学》 Citations of the textbook

Total citation number home and abroad > 8000

## Relative International Journal 有关的主要国外期刊

1. Numerical Heat Transfer, Part A- Applications; Part B- Fundamentals
2. International Journal of Numerical Methods in Fluids.
3. Computer & Fluids
4. Journal of Computational Physics
5. International Journal of Numerical Methods in Engineering
6. International Journal of Numerical Methods in Heat and Fluid Flow
7. Computer Methods of Applied Mechanics and Engineering
8. Engineering Computations
9. Progress in Computational Fluid Dynamics
10. Computer Modeling in Engineering & Sciences (CMES)
11. ASME Journal of Heat Transfer
12. International Journal of Heat and Mass Transfer
13. ASME Journal of Fluids Engineering
14. International Journal of Heat and Fluid Flow
15. AIAA Journal

# Methods for improving teaching and studying

1. **Speaking simple but clear English** with Chinese note (注释) of new terminology (术语) and some words;
2. **Enhancing (加强) communications** between students and teachers: a QQ-group has been set up, and my four assistants will help me in this regard;
3. **Understanding (理解) the importance** of numerical simulation method: not just for a credit(学分), but it's an important technique for job-looking (谋职);
4. **Previewing (预习) PPT** of 2015 loaded in our group; website: <http://nht.xjtu.edu.cn>

## 5. Teaching theory and code alternatively (交替地):

From 1983 to 2015, theory and code were separately taught with theory first and code second;

From this year following change will be made;

Chapter 1-Chapter 7----Basic theory for NHT

Chapter 8- Introduction to teaching code

Chapter 9- Seven examples for conduction and laminar flow and heat transfer

Chapter 10- Stream function-vorticity method

Chapter 11- Turbulence model **with code implementation (example 8)**

Chapter 12- Grid generation techniques

# Contents of Chapter 1

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

**1.2 Basic concepts of NHT and its application examples**

**1.3 Mathematical and physical classification of HT & FF problems and its effects on numerical solution**

**1.4 Recent advances (进展) in numerical simulation of HT & FF problems**

# 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**

**2. Momentum conservation**

**3. Energy conservation**

**4. General form**

## 1.1.2 Conditions for unique solution (唯一解)

## 1.1.3 Example of mathematical formulation



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

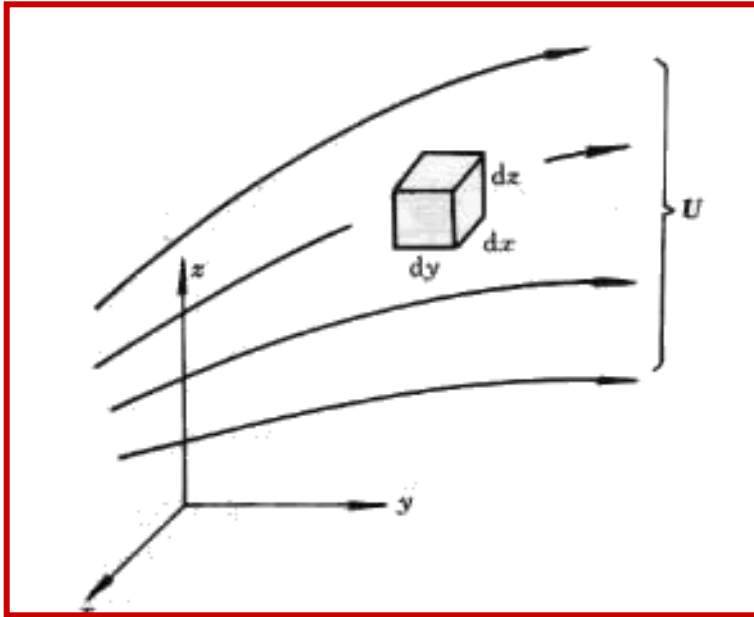
All macro-scale (宏观) HT & FF problems are governed by three conservation laws: mass, momentum and energy **conservation law**.

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

## 1.1.1 Governing equations and their general form

### 1. Mass conservation

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



“div” is the mathematical symbol for divergence (散度) .

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho \vec{U}) = 0 \quad \text{div}(\rho \vec{U}) = \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z}$$

For incompressible fluid (不可压缩流体) :

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

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

called flow without divergence (流动无散条件)。

## 2. Momentum conservation

Applying the 2<sup>nd</sup> law of Newton ( $F=ma$ ) to the elemental control volume (控制容积) shown above in the three-dimensional coordinates:

[Increasing rate of momentum of the CV] = [Summation of external (外部) forces applying on the CV]

Adopting Stokes assumption: stress is linearly proportional to strain (应力与应变成线性关系), We have:

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho uu)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z} = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} (\underbrace{\bar{\lambda} \text{div} \vec{U}}_{\text{molecular}} + \underbrace{2\eta \frac{\partial u}{\partial x}}_{\text{dynamic}})$$

$$+ \frac{\partial}{\partial y} [\underbrace{\eta (\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y})}_{\text{dynamic}}] + \frac{\partial}{\partial z} [\underbrace{\eta (\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x})}_{\text{dynamic}}] + \rho F_x$$

$\eta$  dynamic viscosity,  $\bar{\lambda}$  fluid 2<sup>nd</sup> molecular viscosity.

It can be shown that the above equation can be reformulated as **(改写为)** following general form of Navier-Stokes equation:

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

**Transient term**

**Convection term**

**Diffusion term**

**Source term**

$u$  ----dependent variable **(因变量)** to be solved;

$\vec{U}$  ----fluid velocity vector;

$S_u$  ----source term.

## Source term in x-direction:

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

## Similarly:

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

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

**For incompressible fluid with constant properties the source term does not contain velocity-related part.**

### 3. Energy conservation

[Increasing rate of internal energy in the CV]= [Net heat going into the CV]+[Work conducted by body forces and surface forces]

Introducing **Fourier's law of heat conduction** and neglecting the work conducted by forces; Introducing enthalpy (焓)  $h = c_p T$ , assuming  $c_p = \text{Constant}$ :

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

$$\frac{\lambda}{c_p} \rightarrow \frac{\lambda \eta}{c_p \eta} \rightarrow \left(\frac{\lambda}{c_p \eta}\right) \eta \rightarrow \frac{\eta}{\text{Pr}}$$

## 4. General form of the governing equations

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

Transient

Convection

Diffusion

Source

The differences between different variables:

- (1) Different boundary and initial conditions;
- (2) Different nominal source (名义源项) terms;
- (3) Different physical properties (nominal diffusion coefficients)

## 5. Some remarks (说明)

1. The derived transient 3D **Navier-Stokes** equations can be applied **for both laminar and turbulent flows**.
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. Although  $c_p$  is assumed constant, the above governing equation can also be applied to cases with weakly changed  $c_p$ .
4. Radiative (辐射) heat transfer is governed by a differential-integral (微分-积分) equation, and its numerical solution will not be dealt with here.



## 1.1.2 Conditions for unique solution

### 1. Initial condition

$$t = 0, \quad T = f(x, y, z)$$

### 2. Boundary condition

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

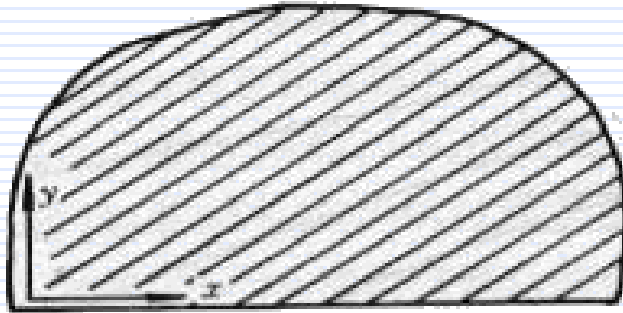
(2) **Second kind (Neumann)**:  $q_B = -\lambda \left( \frac{\partial T}{\partial n} \right)_B = q_{\text{given}}$

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

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

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

# 3<sup>rd</sup> kind boundary conditions for solid heat conduction and convective heat transfer problems



(a)

**Heat conduction with 3rd kind B.C. at surface**

*$h, T_\infty$  are known*



(b)

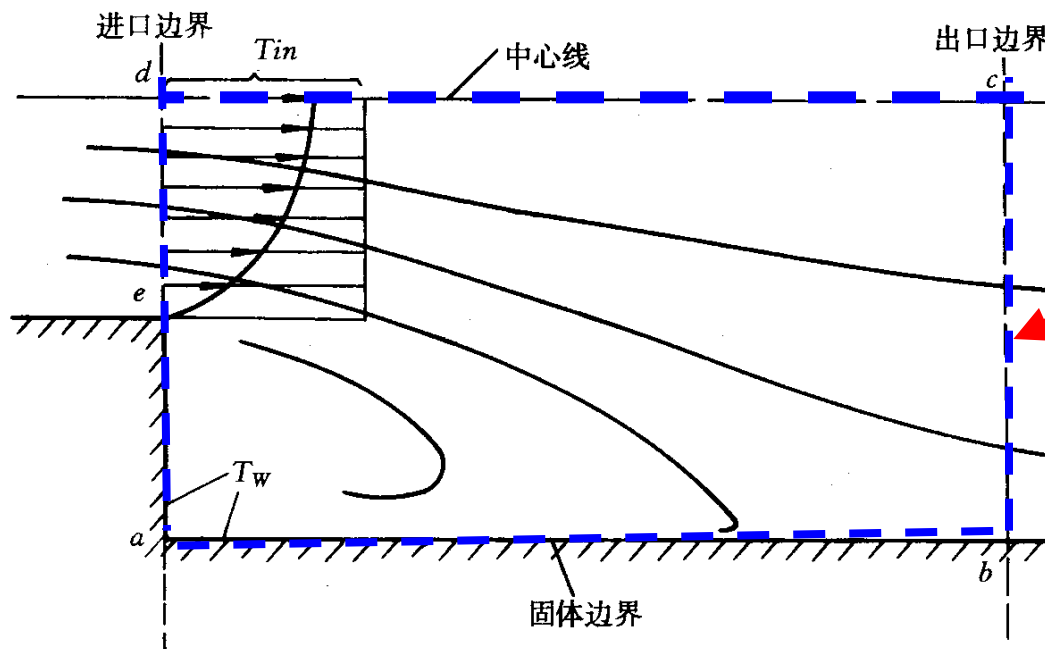
**Inner convective heat transfer with 3rd kind condition at wall outside**

*$h_e, T_\infty$  are known*

# 1.1.3 Example of mathematical formulation

## 1. Problem and assumptions

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



**Solution domain**

## 2. Governing equations

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

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

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

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

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

### 3. Boundary conditions

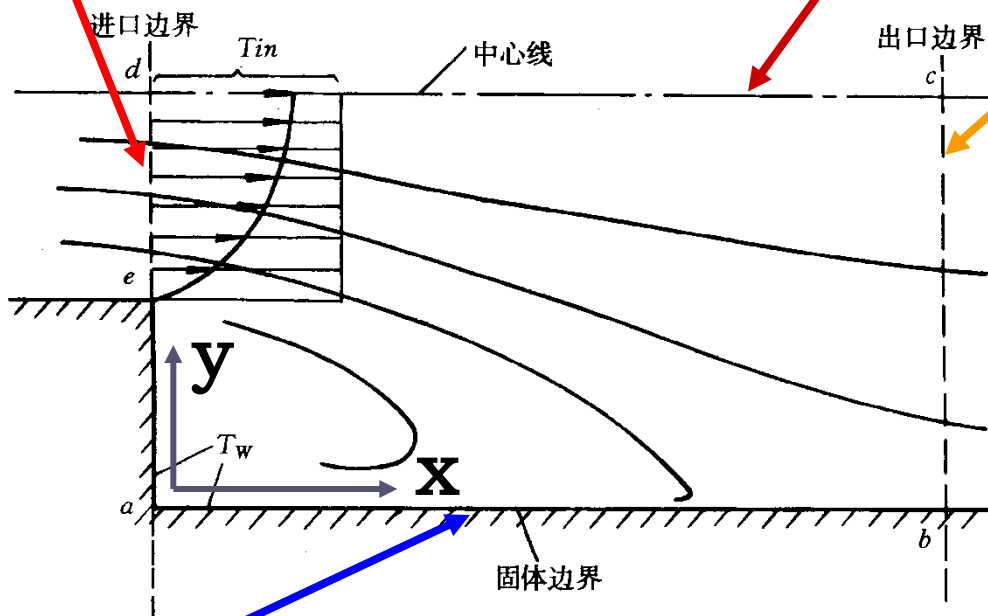
(1) **Inlet:** specifying variations of  $u, v, T$  with  $y$  ;

(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 are required.

**Approximations must be made.**



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

# Notes to Section 1.1

In the left hand side

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

The right hand side :

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

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

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

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

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

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:**

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

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

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

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

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

**End of Notes to Section 1.1**

# 1.2 Basic concepts of NHT and its application examples

## 1.2.1 Basic concepts of numerical solutions based on continuum assumption

## 1.2.2 Classification of numerical solution methods based on continuum assumption

## 1.2.3 Three fundamental approaches of scientific research and their relationships

## 1.2.4 Application examples

## 1.2.5 Some suggestions



## 1.2 Basic concepts of NHT and its application examples

### 1.2.1 Basic concepts of numerical solutions based on continuum assumption (连续性假设)

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

Establishing algebraic equations for these values at the discrete points by some principles (---Discretization of equations);

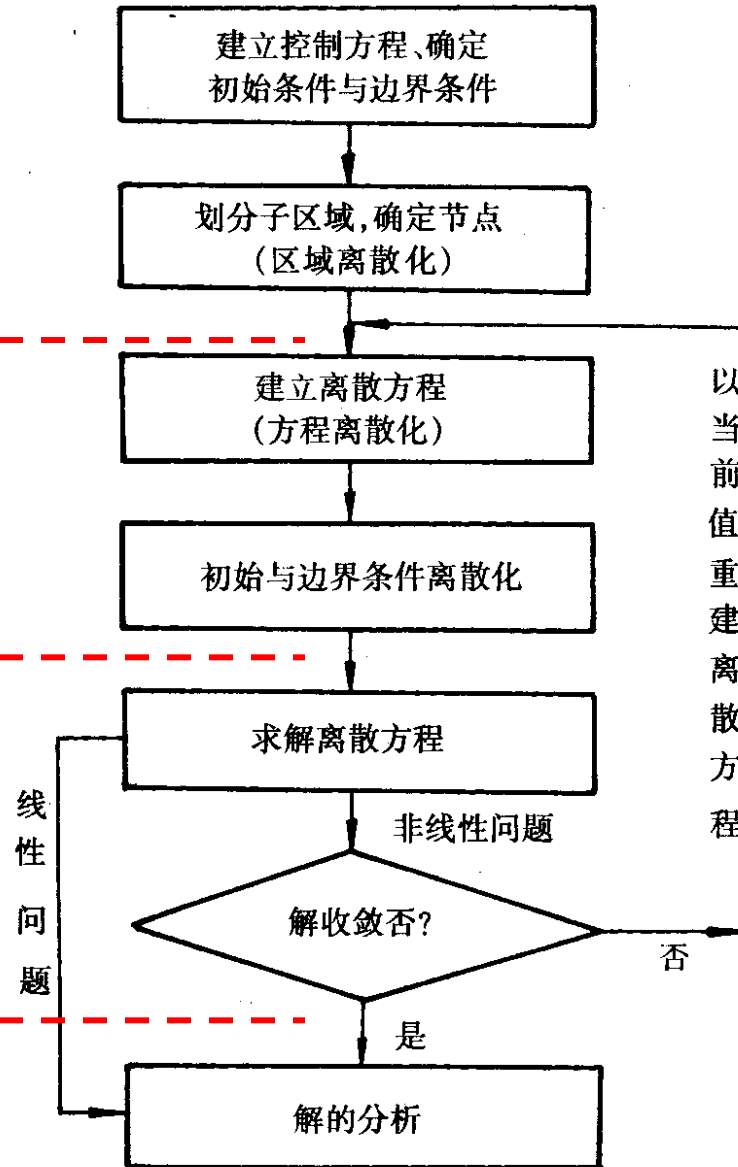
Solving the algebraic equations by computers to get approximate solutions of the continuum variables (---Solution of equation).

**Discretizing domain**

**Discretizing equations**

**Solving algebraic equations**

**Analyzing numerical results**



**Flow chart (流程图)**

## 1.2.2 Classification of numerical solution methods based on continuum assumption

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

L F Richardson(1910), A Thom

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

D B Spalding; S V Patankar

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

O C Zienkiewicz; 冯 康(Kang Feng)

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

陈景仁(Ching Jen Chen)

5. Boundary element method (**BEM**)

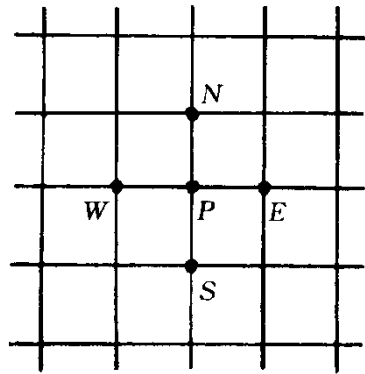
D B Brebbia

6. Spectral analysis method (**SAM**)

(谱分析法)

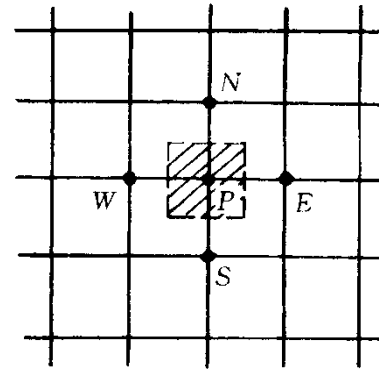
# Comparisons of FDM(a), FVM(b), FEM(c), FAM(d)

**FDM**  
有限差分



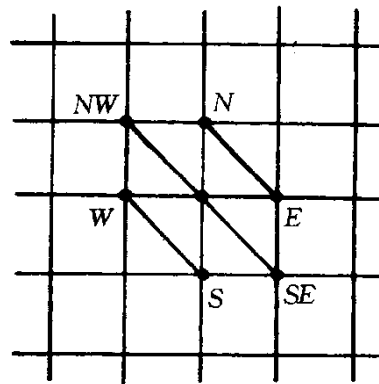
(a)

**FVM**  
有限容积



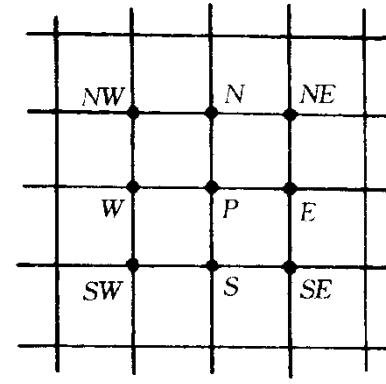
(b)

**FEM**  
有限元



(c)

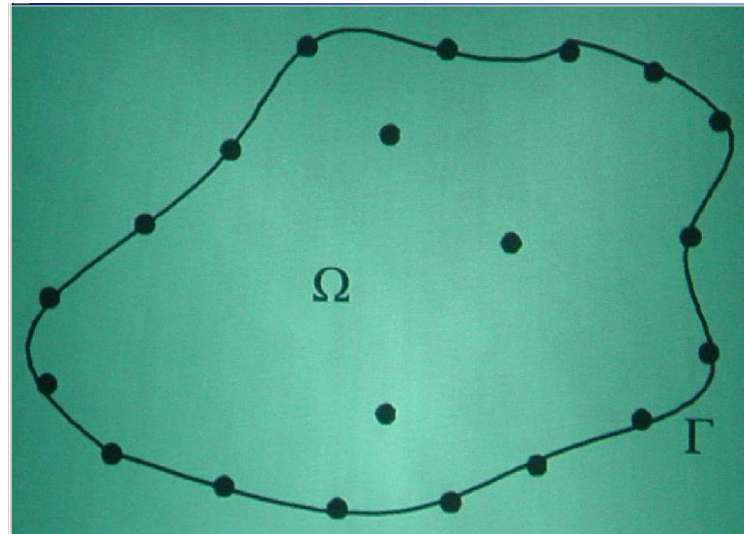
**FAM**  
有限分析



(d)

All these methods need a grid system(网格系统):

- 1) Determination of grid positions;
- 2) Establishing the influence relationships between grids.

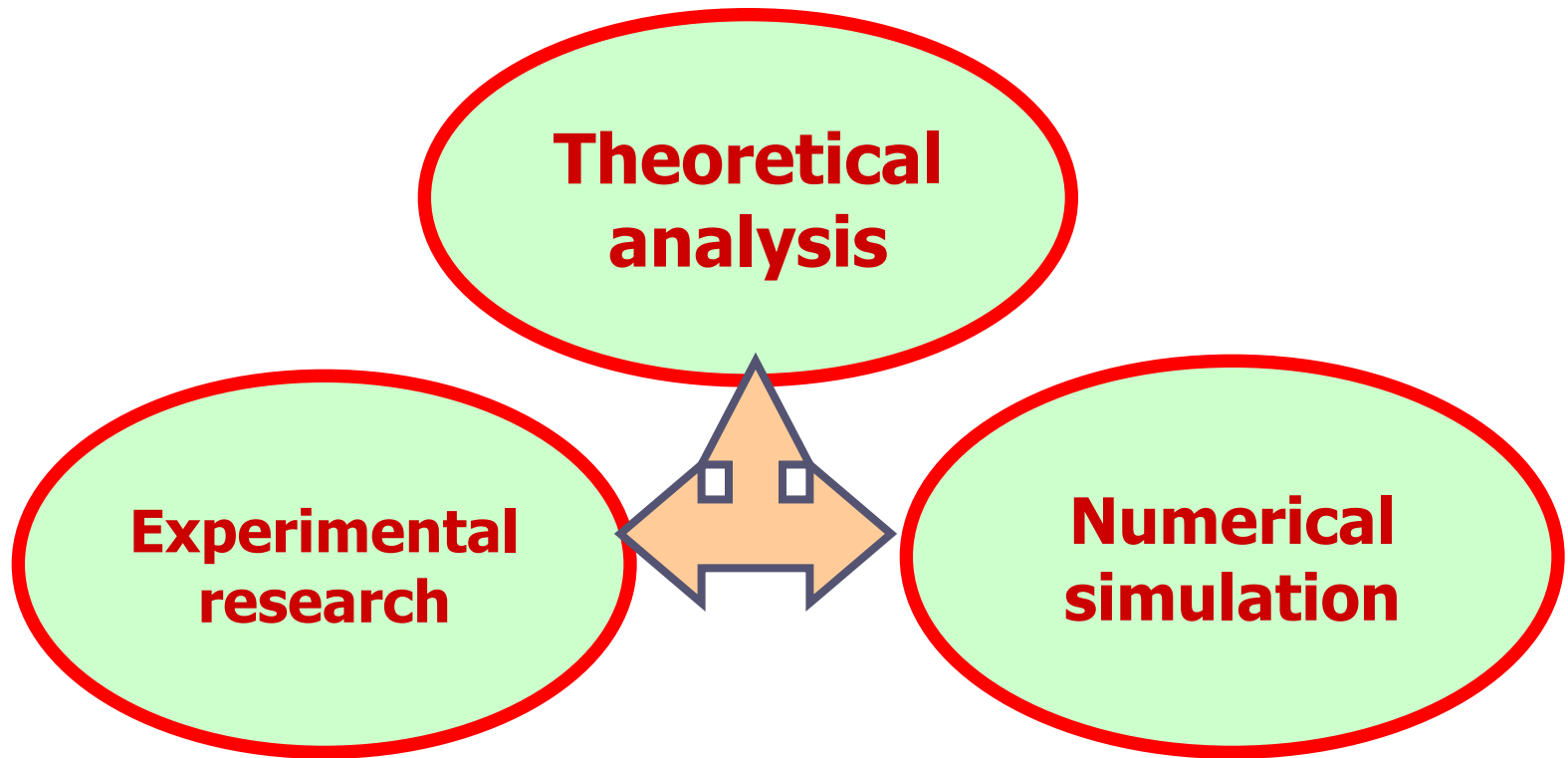


**BEM (边界元)** requires a basic solution, which greatly limits its applications in convective problems.

**SAM** can only be applied to geometrically simple cases.

**Manole、Lage 1990–1992 statistics (统计)** : FVM --47%; adopted by most commercial softwares; Our statistics of NHT in 2007 even much higher.

## 1.2.3 Three fundamental approaches (方法) of scientific research and their relationships



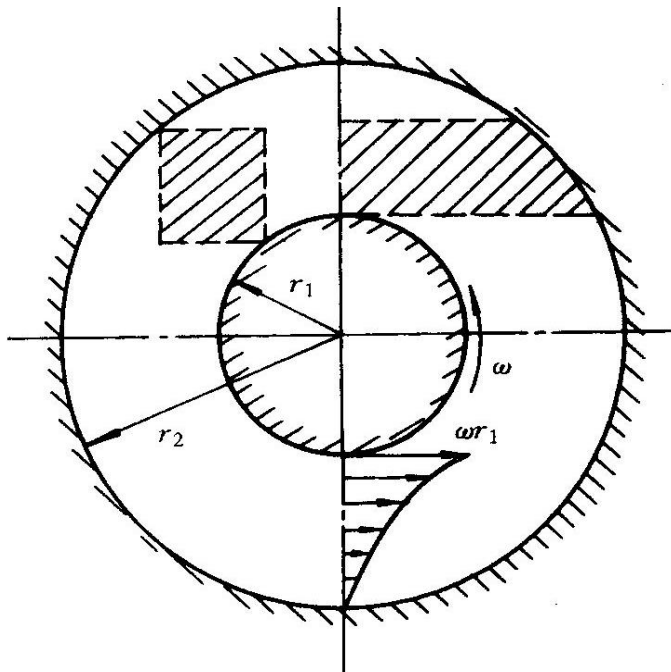
The starting point of numerical simulation for physical problems is Fluid Dynamics. Thus it is often called **Computational Fluid Dynamics---CFD.**

# 1. Theoretical analysis

Its importance should not be underestimated (低估) .

It provides comparison basis for the verification (验证) of numerical solutions.

**Examples:** The analytic solution of velocity from NS equation for following case :



$$\frac{u}{u_1} = \frac{r_1 / r_2}{1 - (r_1 / r_2)^2} \bullet \frac{1 - (r / r_2)^2}{r / r_2}$$

$$u_1 = \omega r_1$$

## 2. Experimental study

A basic research method: observation; properties measurement; verification of numerical results

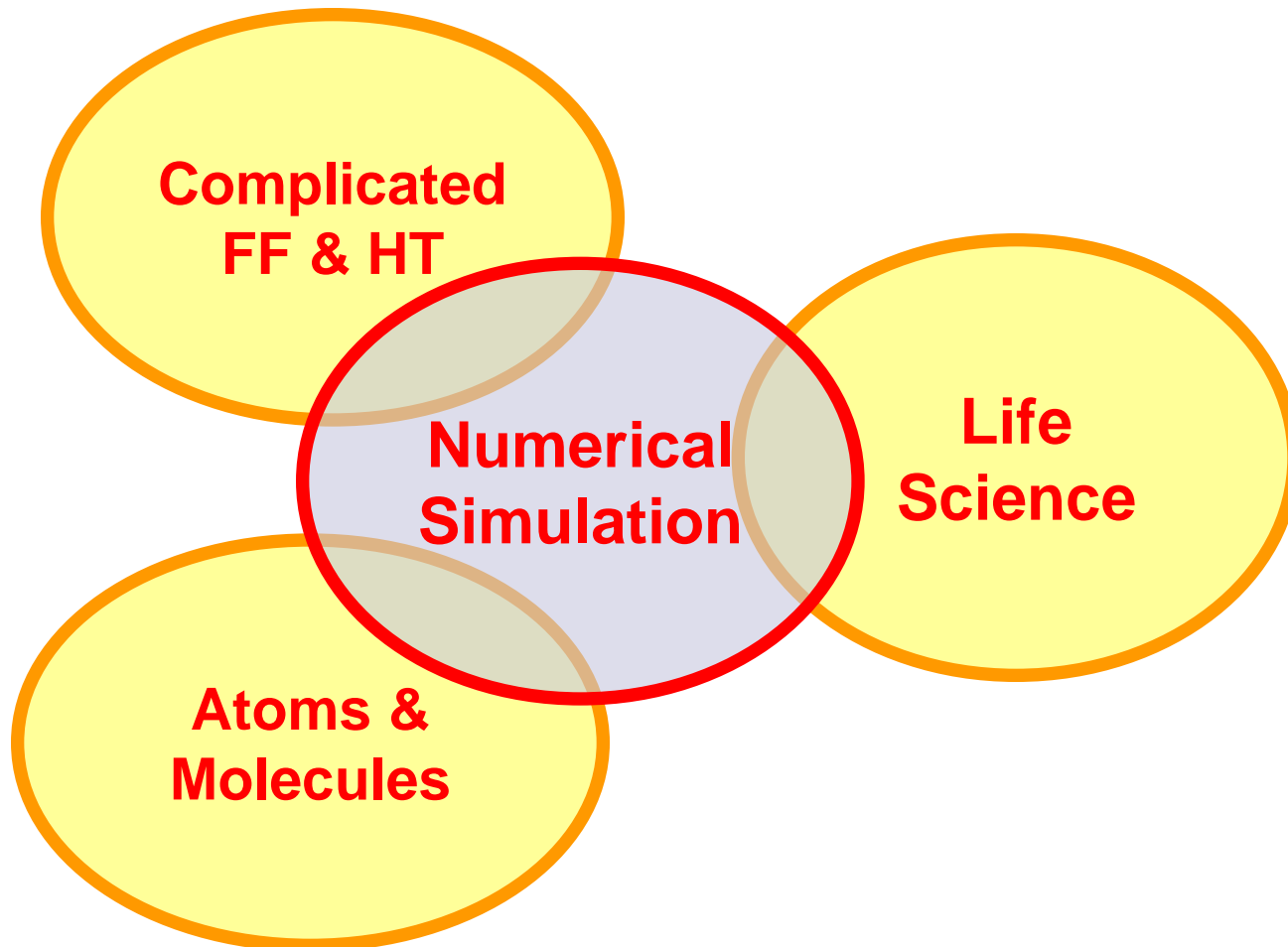
## 3. Numerical simulation

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) .

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

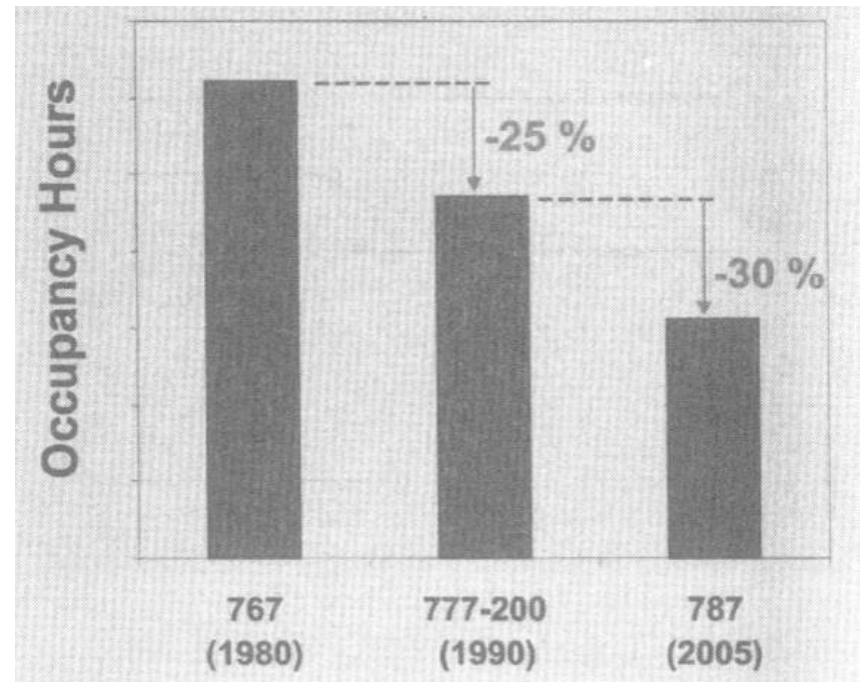


Historically, in 1985 the West Europe listed the first commercial software-**PHEONICS** as the one which was not allowed to sell to the communist countries.



**In 2005 the USA President Advisory Board put forward a suggestion to the president that in order to keep competitive power (竞争力) of USA in the world it should develop scientific computation.**

**In the year of 2006 the director of design department of Boeing, M. Grarett, reported to the US Congress (国会) indicating that the high performance computers have completely changed the way of designing Boeing airplane.**

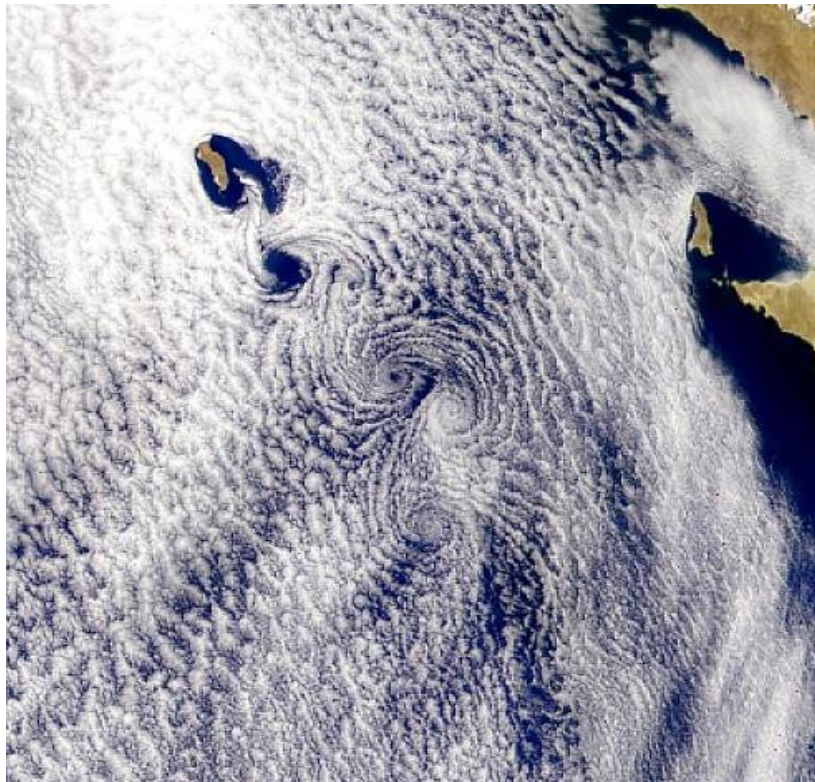


**Numerical simulation plays an important role in the design of Boeing airplane**

# 1.2.4 Application examples

Example 1: Weather forecast—

**Num. solution is the only way.**

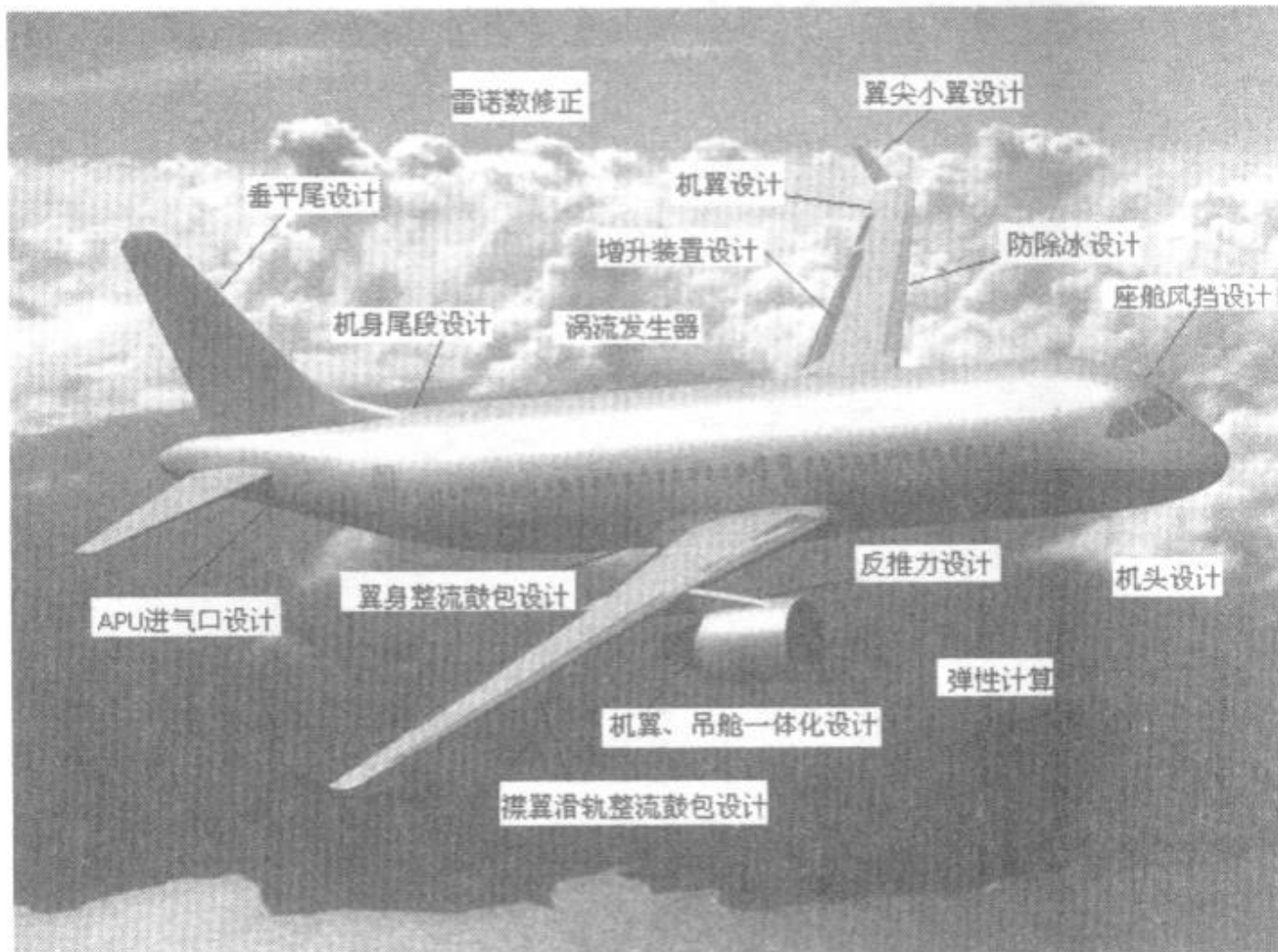


**Large scale vortex**



**Cloud Atlas sent back by a meteorological satellite**

# Example 2: Aeronautical & aerospace (航空航天) engineering



## Example 3: Hydraulic construction (水利建设)

The mud (泥) and sand (沙) content of our Yellow River is about  $35 \text{ kg/m}^3$ , ranking No. 1 in the world, leading to following unpleasant situation: the ground floor of some cities is lower than the riverbed (河床) of Yellow River: **Kai Feng-13m lower, Xin Xiang- 20m lower**

In 2002 the idea of three yellow rivers was proposed:

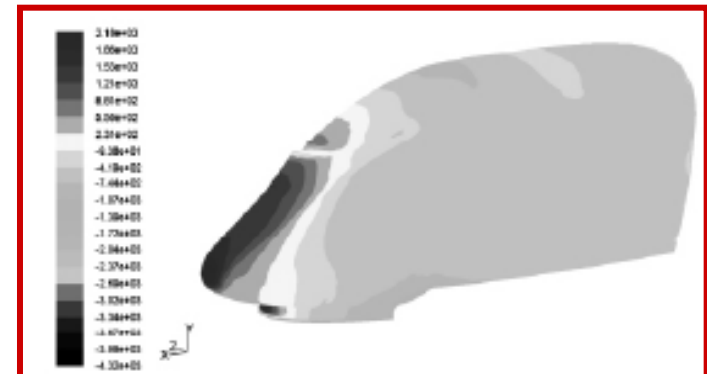
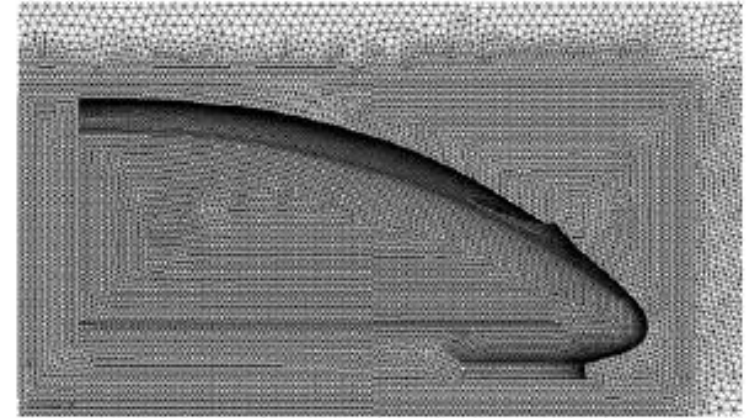
- (1) Original YR;
- (2) Numerical YR;
- (3) Modele YR.

**Through 8 times of modeling and simulation the height of the riverbed was averagely decreased by 1.5 m.**



# Example 4: Design of head shape of high-speed train

The front head shape of the high speed train is of great importance for its aerodynamic performance (空气动力学特性). Numerical wind tunnel is widely used to optimize the front head shape.



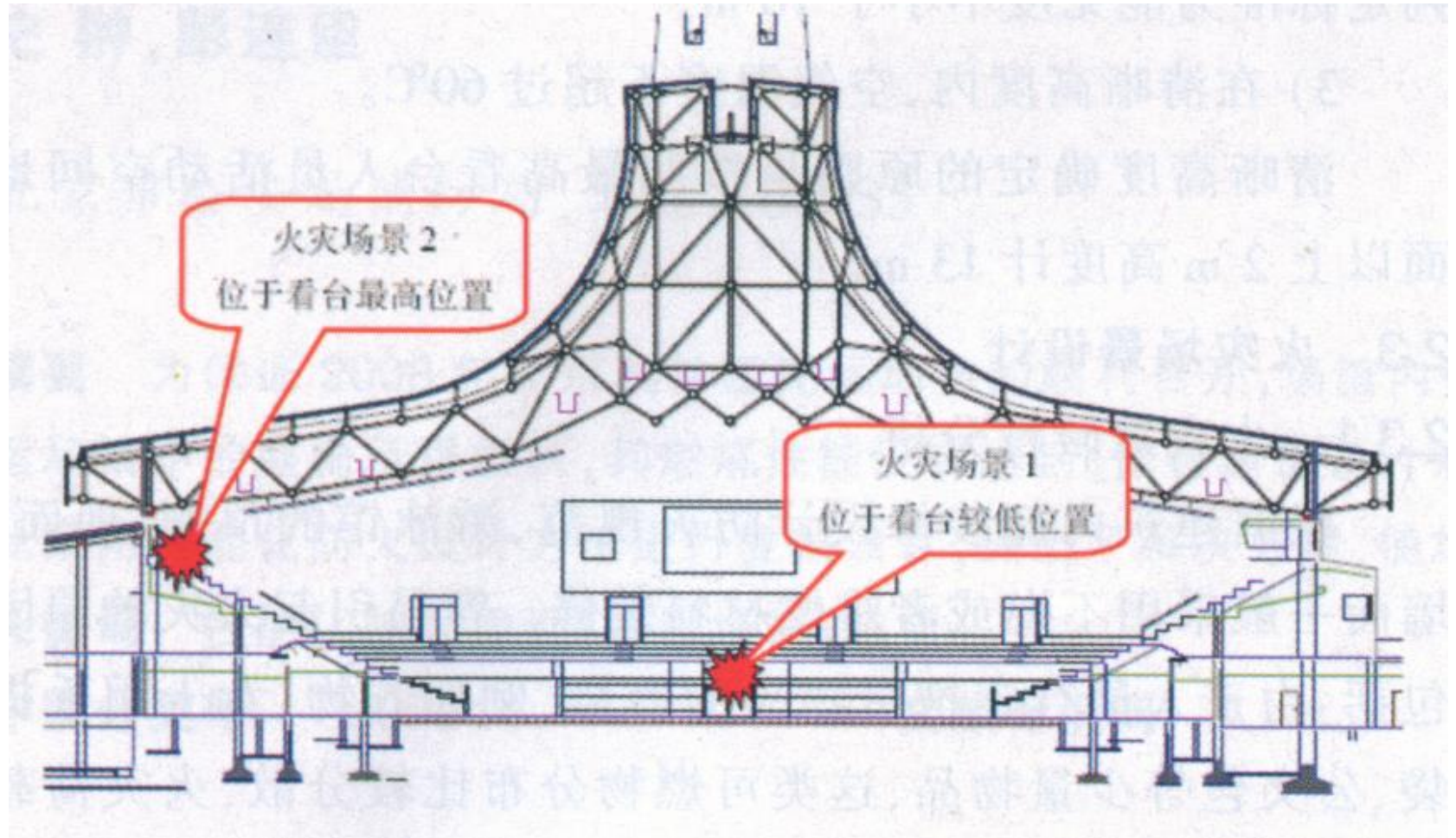
# Example 5: Prediction of fire disaster (火灾) for Olympic Gymnasium (体育馆)



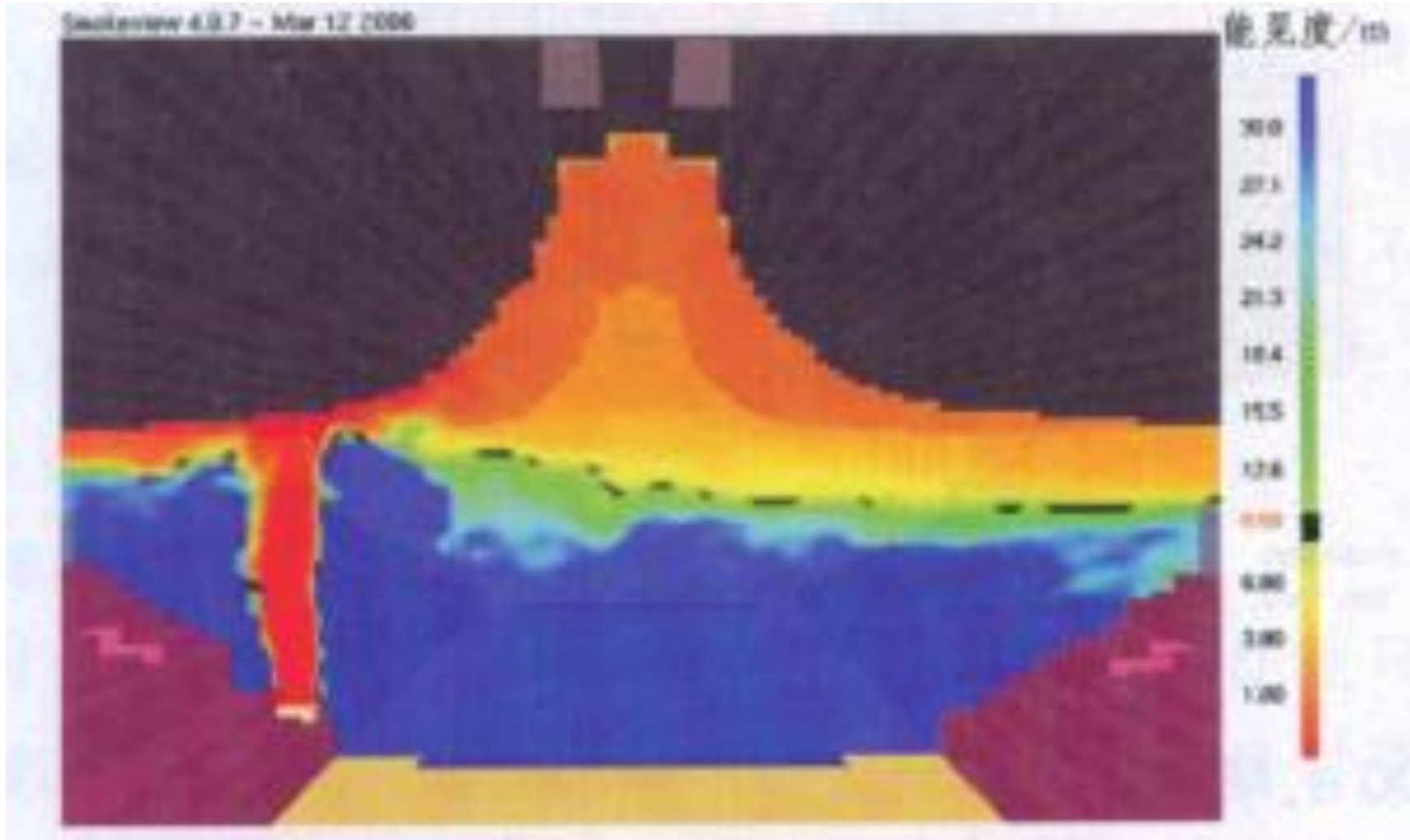


**In the construction of gym :the chair material cannot meet the requirement of fireproof (防火) . A decision should be made asap on whether such material can be used. Numerical simulation was adopted.**

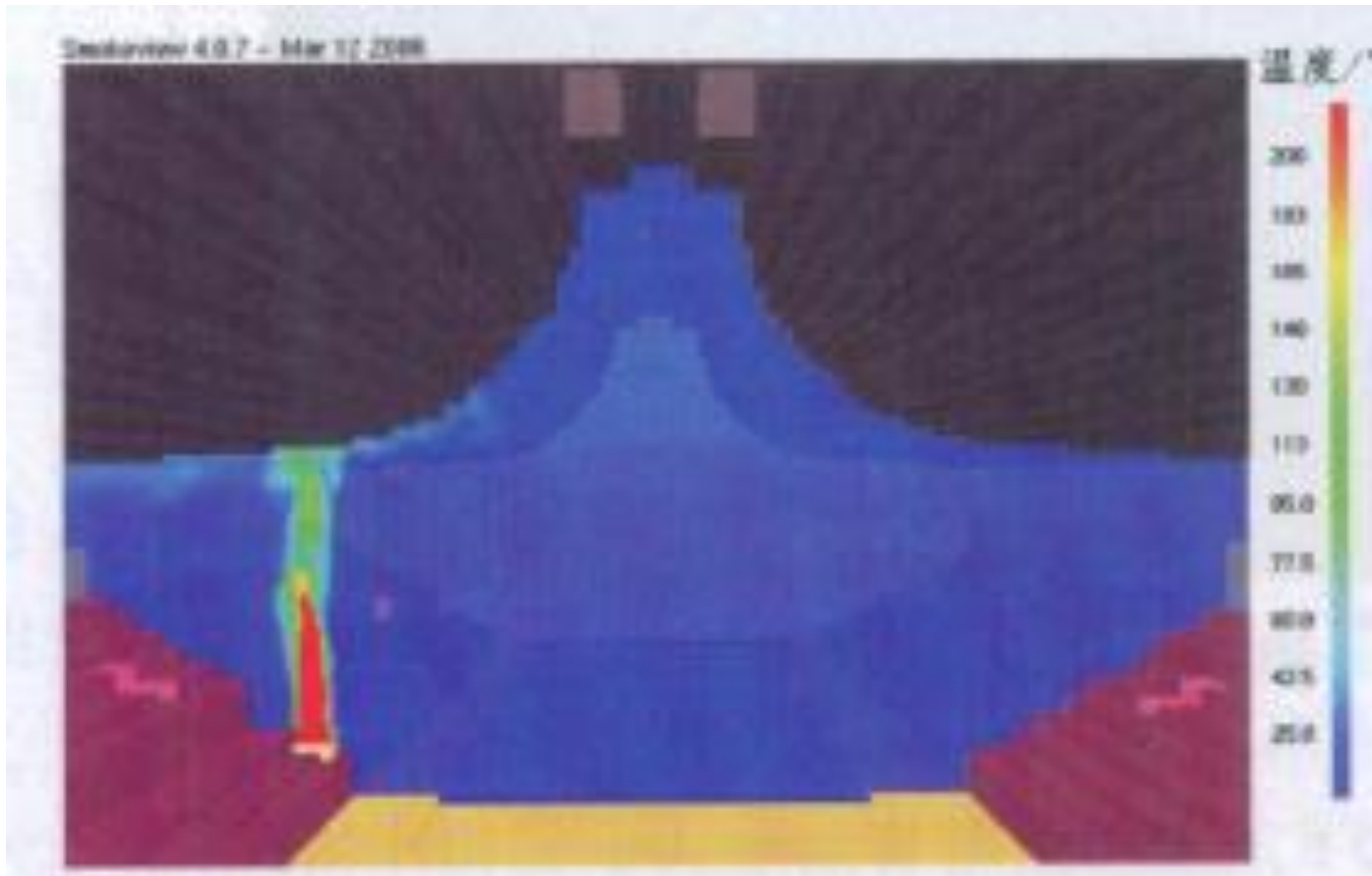




## Fire prediction for indoor swimming pool



**Predicted visibility (能见度) after 900 seconds of fire outbreak**



**Predicted gas temperature distribution  
after 900 seconds of fire outbreak**

# Example 6: House safety – Fire prediction

NIST

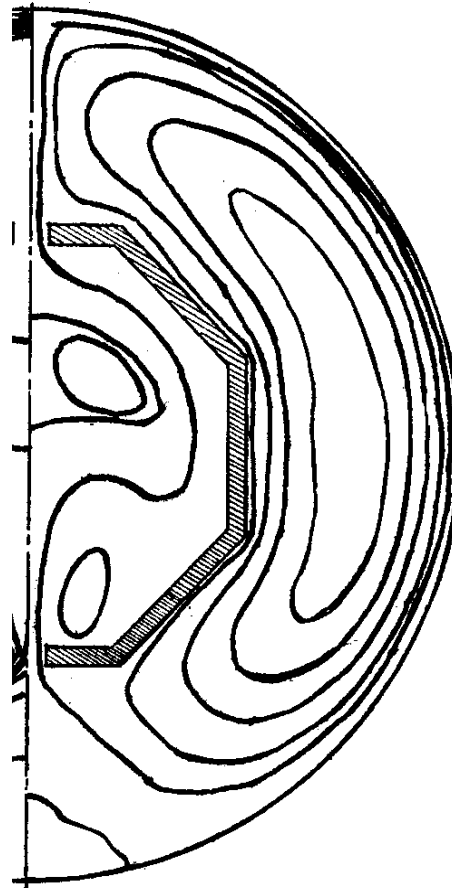
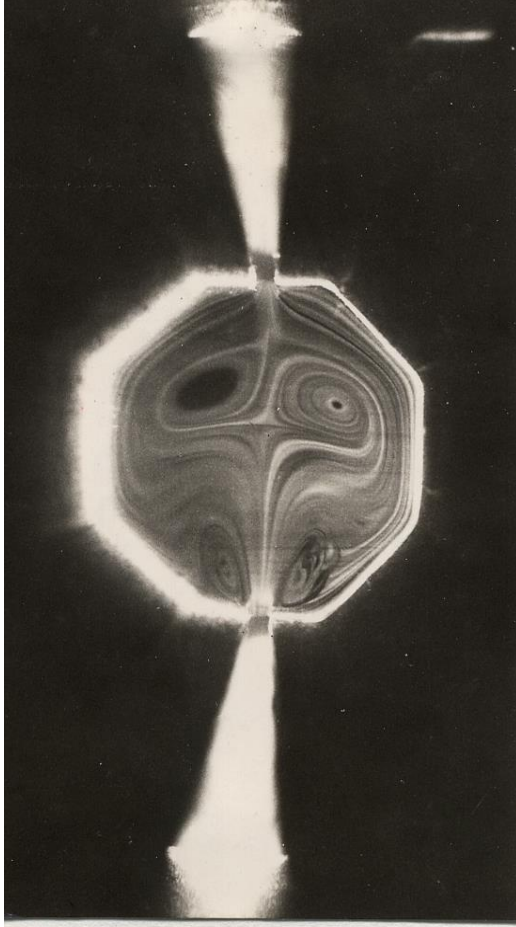


Time: 0.1



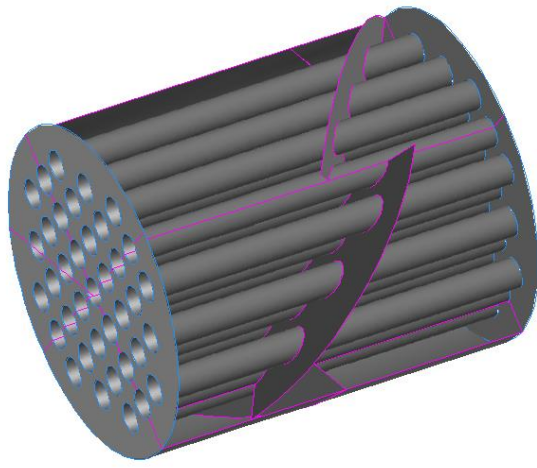
The major purpose is to guarantee (保证) that once fire outbreak (火灾) occurs, the persons living in the house can safely leave for outside within a certain amount of time.

# Example 7: Heat transfer characteristics of large electric current bar (电流母线)



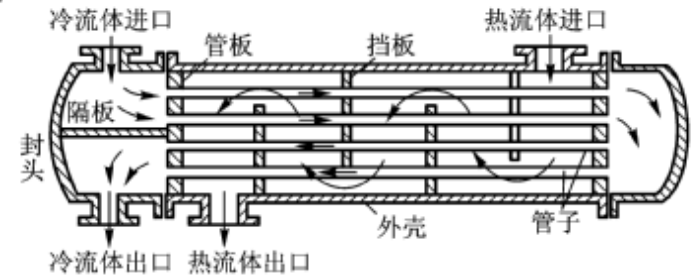
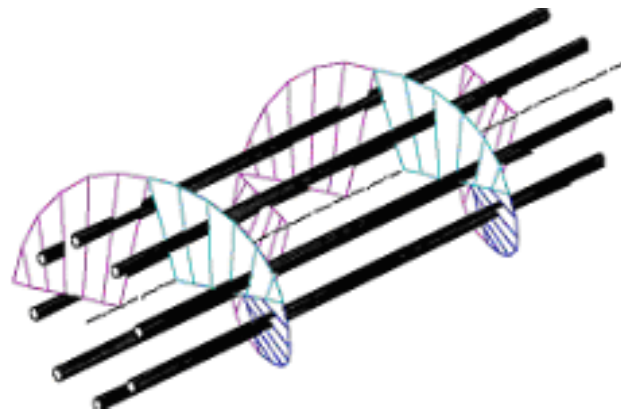
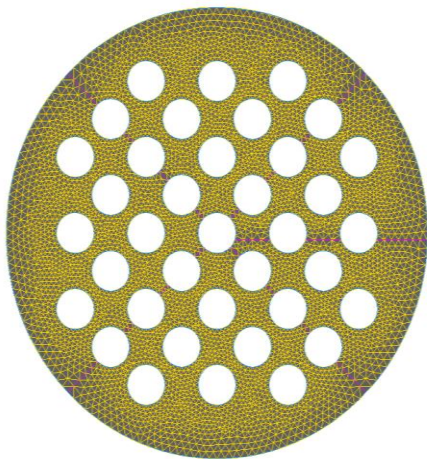
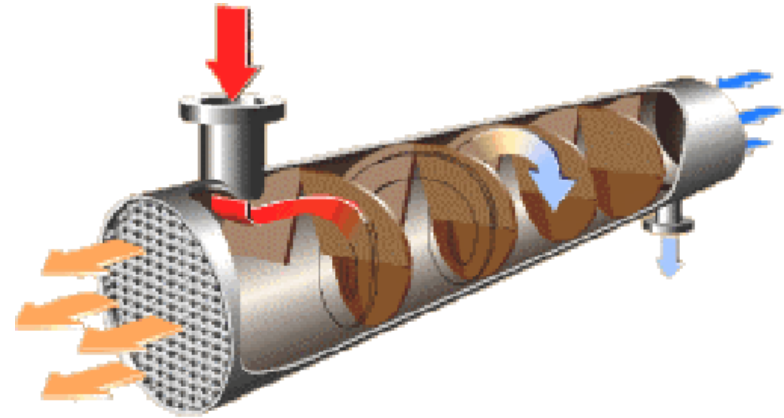
Comparisons of predicted and simulated flow fields

# Example 8: Shell-side simulation of helical baffle (螺旋折流板) heat exchanger



$$1.34 \times 10^6$$

$$2.73 \times 10^6$$



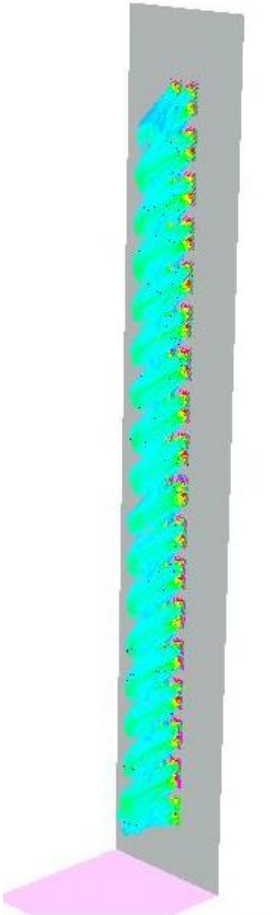
## Example 9: Velocity and temperature distribution simulation to improve design of air-conditioning system

淮南市茂业时代广场项目空调系统CFD气流温度场分析

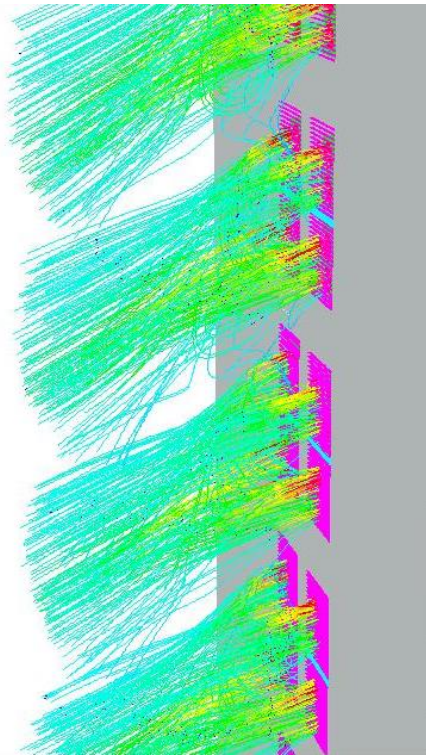
佛山金科大厦项目空调系统CFD气流温度场分析；

宁波甬邦大厦项目空调系统CFD 气流温度场分析

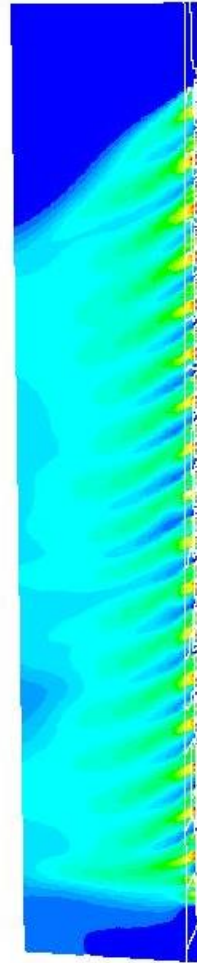
# Example 9: Velocity and temperature distribution simulation to improve design of air-conditioning system



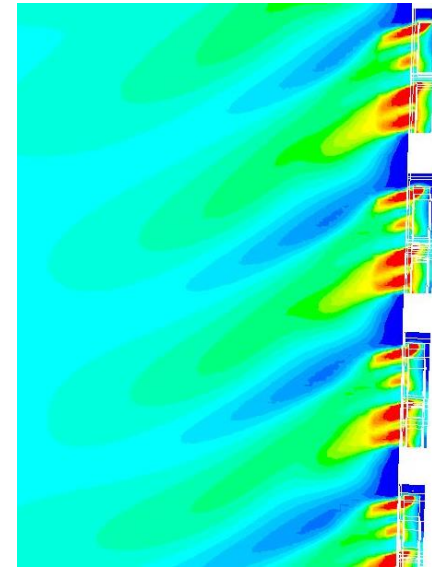
Out flow streamlines



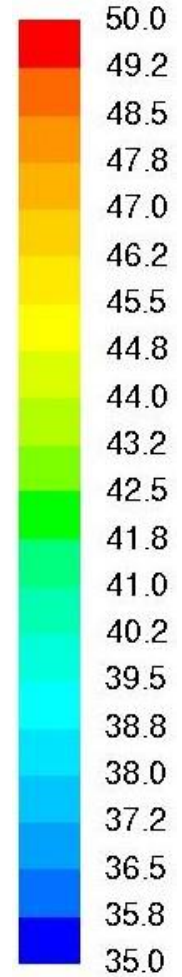
Out flow stream lines of 13F,14F,15F



Outflow air temperature clouds



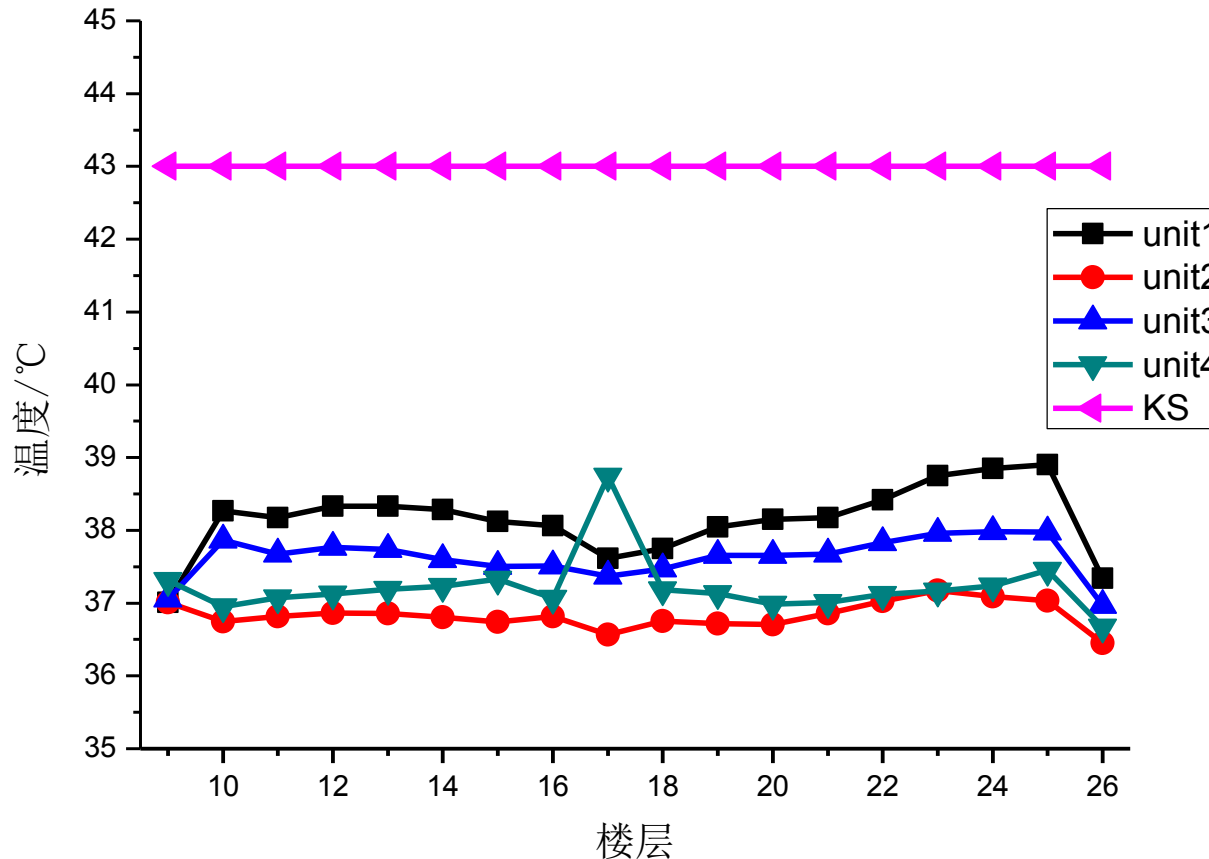
Temperature distributions of 13F,14F,15F,16F



Temperature scale: °C



## Effect of floor number on the inflow temperature of air for condenser

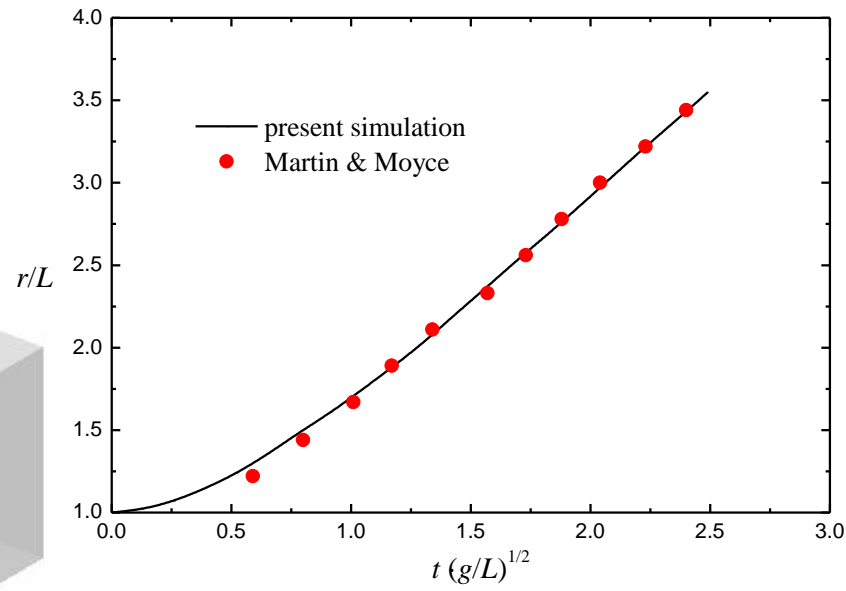
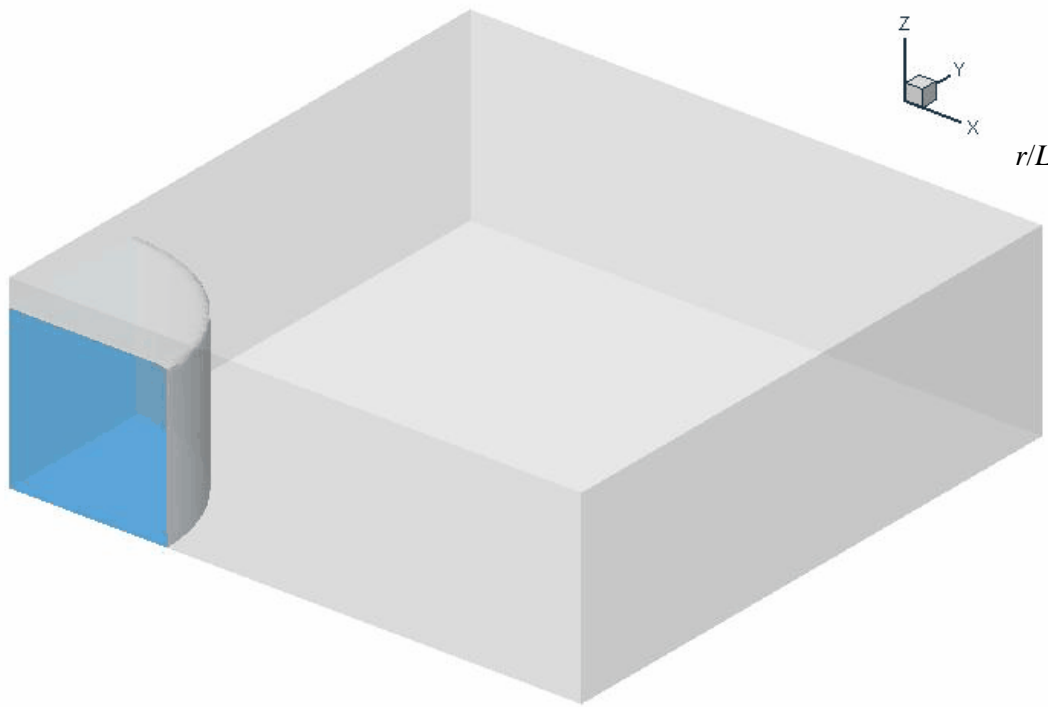


The allowed upper limit is 43 °C, thus the design is OK.

## Example 9: Simulation of multiphase (多相) flow

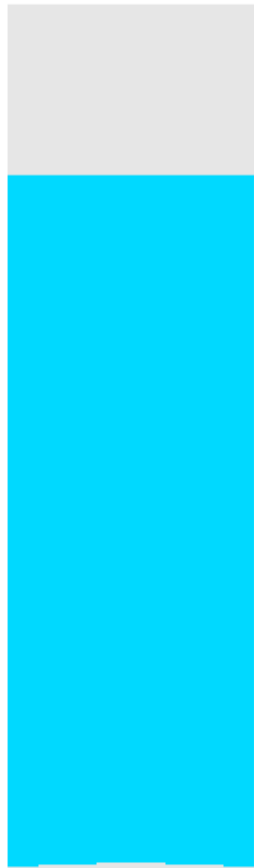
Visualization(可视化) of numerically predicted results:

1. Breaking down of a dam (溃坝).
2. Film boiling heat transfer (膜态沸腾) ;
3. Nucleate boiling in shallow liquid layer (浅液层中的核态沸腾)



Base radius vs. time

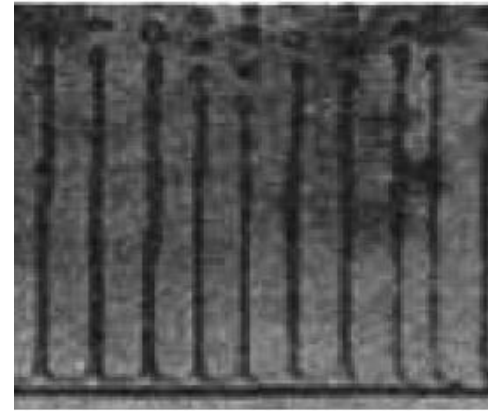
Evolution (演变) process of interface



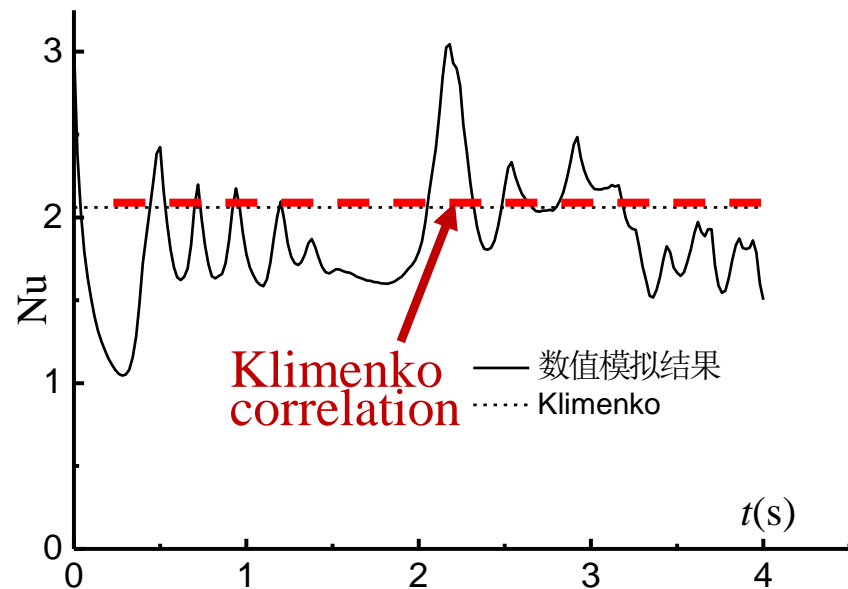
4K



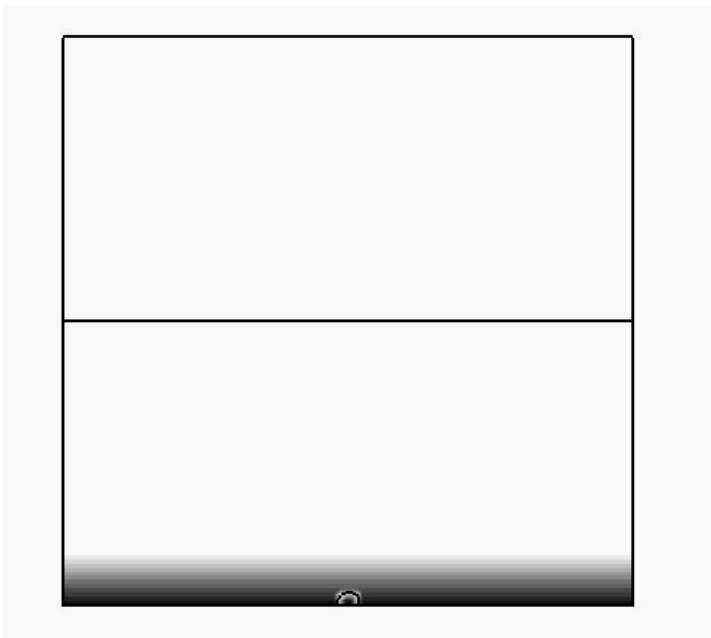
5K



Experiment by  
Reimann  
and Grigull  
(1975)



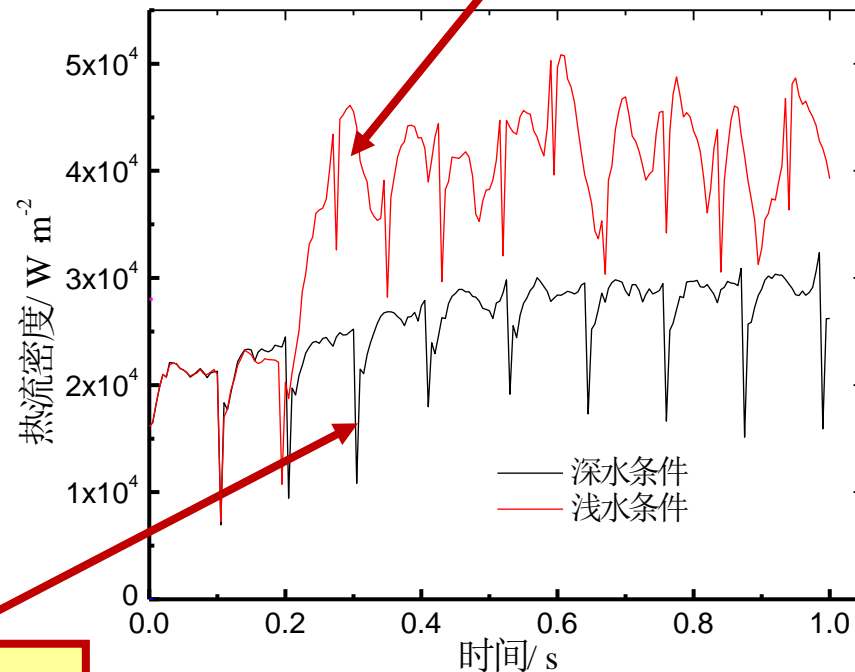
Guo D.Z., Sun D.L., Li Z.Y., Tao W.Q., Phase Change Heat Transfer Simulation for Boiling Bubbles Arising from a Vapor Film by VOSET Method. *Numerical Heat Transfer, Part A: Applications*, 2011, 59: 857-881



**Strong disturbance  
caused by bubble  
upward motion!**

**Deep (深)  
liquid layer**

**Shallow (浅)  
liquid layer**



**20160912**

Lin K, Tao WQ., Numerical simulation of nucleate boiling I shallow liquid. Asian Symposium on Computational Heat Transfer and Fluid Flow, 2015, Busan, Korea

## Summary

**It is now widely accepted that an appropriate combination of theoretical analysis, experimental study and numerical simulation is the best approach for modern scientific research.**

**With the further development of computer hardware and numerical algorithm (算法), the importance of numerical simulation will become more and more important!**

## 1.2.5 Some Suggestions

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

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

3. Practicing simulation method by a computer;

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

5. Adopting CSW(商业软件) with self-developed code.

# Brief review of 2016-09-12 lecture key points

## 1. General governing eqs. and boundary conditions of FF & HT problems

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

Three kinds of B.C.:

- (1) 1st : boundary value is known;
- (2) 2nd : boundary heat flux is known
- (3) 3rd : relationship between boundary value and boundary 1<sup>st</sup>-order normal derivative (导数) is known

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



## 2. Major concept of numerical simulation of HT & FF problems

**Domain discretization**

----replacing the continuum domain by a number of discrete points, called node or grid, at which the values of velocity, temp., etc., are to be solved;

**Equation discretization**

----replacing the governing equations by a number of algebraic equations for the nodes;

**Solution of algebraic eqs.**

----solving the algebraic equations for the nodes by a computer.

The differences in the three procedures (**过程**) lead to different numerical methods based on the continuum assumption.

## 1.3 Mathematical and physical classification of HT & FF problems and its effects on numerical solution

### 1.3.1 From mathematical viewpoint (观点)

1. General form of 2<sup>nd</sup>-order PDE (偏微分方程) with two independent variables (二元)
2. Basic features (特点) of three types of PDEs
3. Relationship to numerical solution method

### 1.3.2 From physical viewpoint

Conservative (守恒型) and non-conservative

# 1.3 Mathematical and physical classification of FF & HT Problems and its effects on numerical solutions

## 1.3.1 From mathematical viewpoint

### 1. General formulation of 2<sup>nd</sup> order PDEs with two IDVs

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

$a, b, c, d, e, f$  can be function of  $x, y, \phi$

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

## 2. Basic feature of three types of PDEs

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

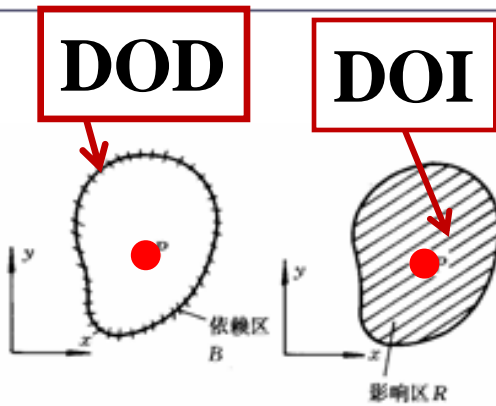
$b^2 - 4ac = 0$ , having one real characteristic line;

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

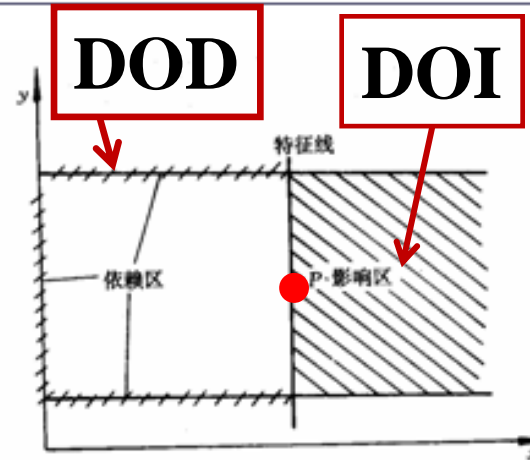
leading to the difference in **domain of dependence (DOD, 依赖区)** and **domain of influence (DOI, 影响区)**;

**DOD** of a node is an area 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.

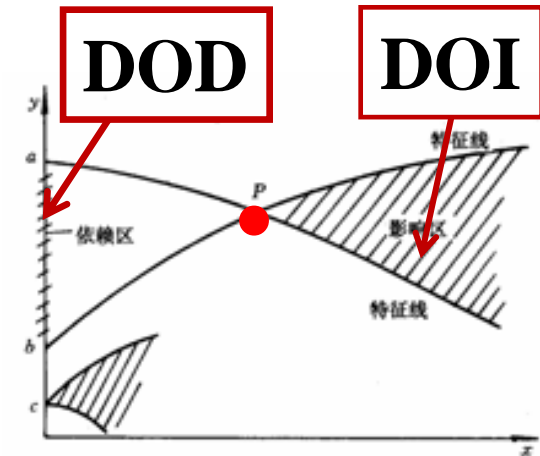
## Elliptic



## Parabolic



## Hyperbolic



$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

$$(a=1, b=0, c=1)$$

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

$$\frac{\partial T}{\partial t} = a \frac{\partial^2 T}{\partial y^2}$$

$$(a=0, b=0, c=a)$$

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \frac{\partial^2 u}{\partial y^2}$$

$$\frac{1}{a} \frac{\partial T}{\partial t} + \frac{1}{c^2} \frac{\partial^2 T}{\partial t^2} = \frac{\partial^2 T}{\partial y^2}$$

$$(a=1/c^2, b=0, c=-1)$$

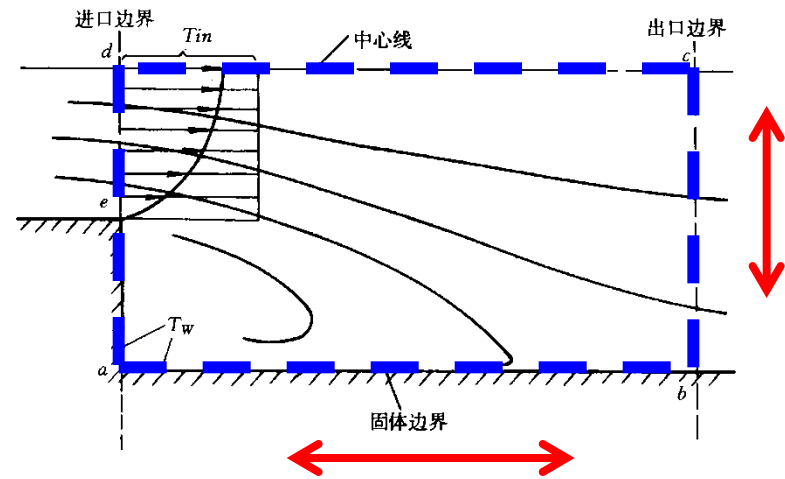
$$\frac{\partial^2 \phi}{\partial t^2} = C^2 \frac{\partial^2 \phi}{\partial y^2}$$

$$(a=1, b=0, c=-C^2)$$

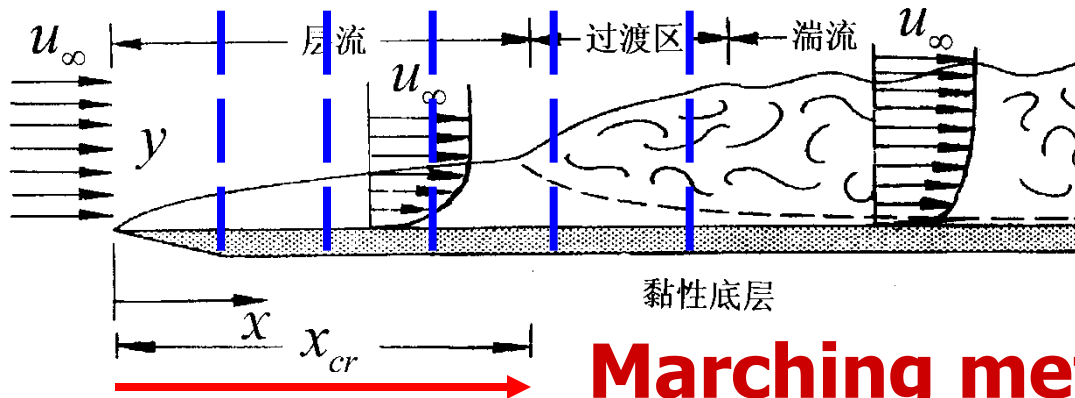
$$a\phi_{xx} + b\phi_{xy} + c\phi_{yy} \dots$$

### 3. Relationship with numerical methods

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



(2) **Parabolic**: flow **without** recirculation, solution can be conducted by marching method, greatly saving computing time!。



**Marching method**

## 1.3.2 From physical viewpoint

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

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

**Non-conservative:** those governing equation whose convective term is not expressed by divergence form is called **non-conservative governing equation** .

These two concepts **are only for numerical solution.**

## 2. Conservative GE can guarantee the applicability (可用性) of physical conservation law within a finite (有限大小) volume.

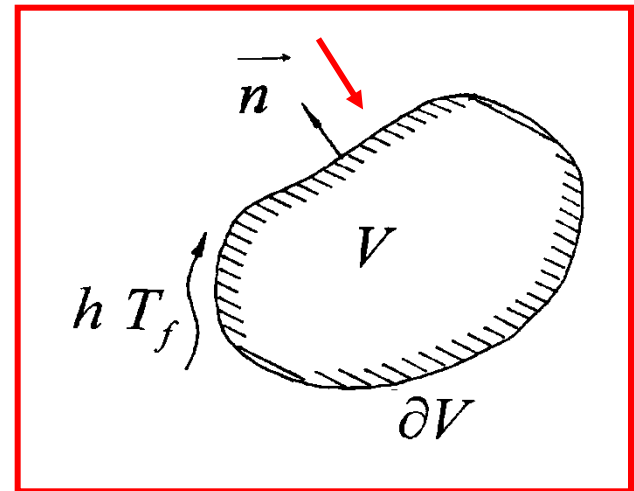
$$\frac{\partial(\rho c_p T)}{\partial t} + \text{div}(\rho c_p T \vec{U}) = \text{div}(\lambda \text{grad} T) + S_T c_p$$

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

From Gauss theorem

$$\int_V \text{div}(\rho c_p T \vec{U}) dv = \int_{\partial V} (\rho c_p T \vec{U}) \cdot \vec{n} dA$$

$$\int_V \text{div}(\lambda \text{grad} T) dv = \int_{\partial V} (\lambda \text{grad} T) \cdot \vec{n} dA$$



Dot product (点积)



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

**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!**

**Key to conservative form: convective term is expressed by divergence.**

**3. Generally conservation is expected. Discretization eqs. are suggested to be derived from conservative PDE.**

**4. Conservative or 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)!**

# 1.4 Recent advances in numerical simulation of HT & HH problems

## 1.4.1 Applicable region of continuum assumption (连续性假设的适用范围)

1) For liquids: Up to micrometer scale (微米尺度) the continuum based methods can be adopted.

2) For gases: Flow regimes (流态) are determined by Knudsen number: ratio of molecular mean free path (分子平均自由程) over characteristic length(特征长度) :

$$Kn = \frac{\lambda}{L} = \begin{cases} \leq 0.001 & \text{Continuum} \\ 0.001 \leq Kn \leq 0.1 & \text{Slip, jump region} \\ 0.1 \leq Kn \leq 10 & \text{Transition (过渡)} \\ \geq 10 & \text{Free molecule region} \end{cases}$$

## 1.4.2 Numerical methods at three levels

- 1) **Macroscale (宏观层次)** — Based on the continuum assumption: FDM, FVM, FEM, FAM
- 2) **Mesoscale (介观层次)** — lattice-Boltzmann method (LBM) ; Direct simulation of Monte Carlo method (DSMC)

LBM and DSMC belong to the mesoscale method: both methods adopt a concept of computational particle (计算粒子), which is much larger than a real molecule, but can be treated as a molecule in some sense (simulation molecule).

### 3) **Microscale** (微观层次—Molecular dynamics simulation (MDS)).

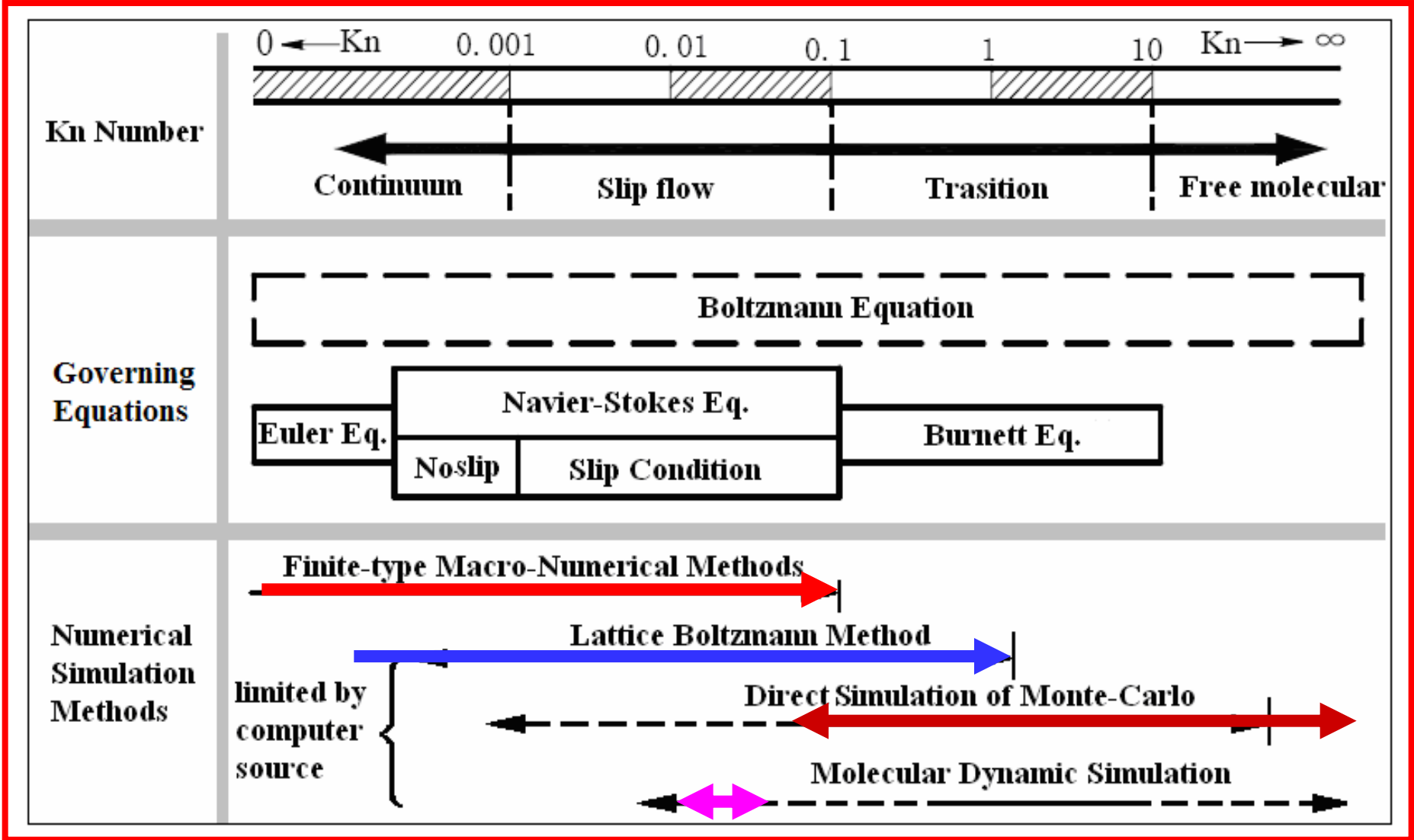
In MDS a domain contains a large number of molecules and each molecule moves according to Newton's 2<sup>nd</sup> law of motion.

There is one thing in common to the above three methods: macroscopic parameters (velocity, pressure, etc.) are obtained via some statistical (统计的) or averaged method.

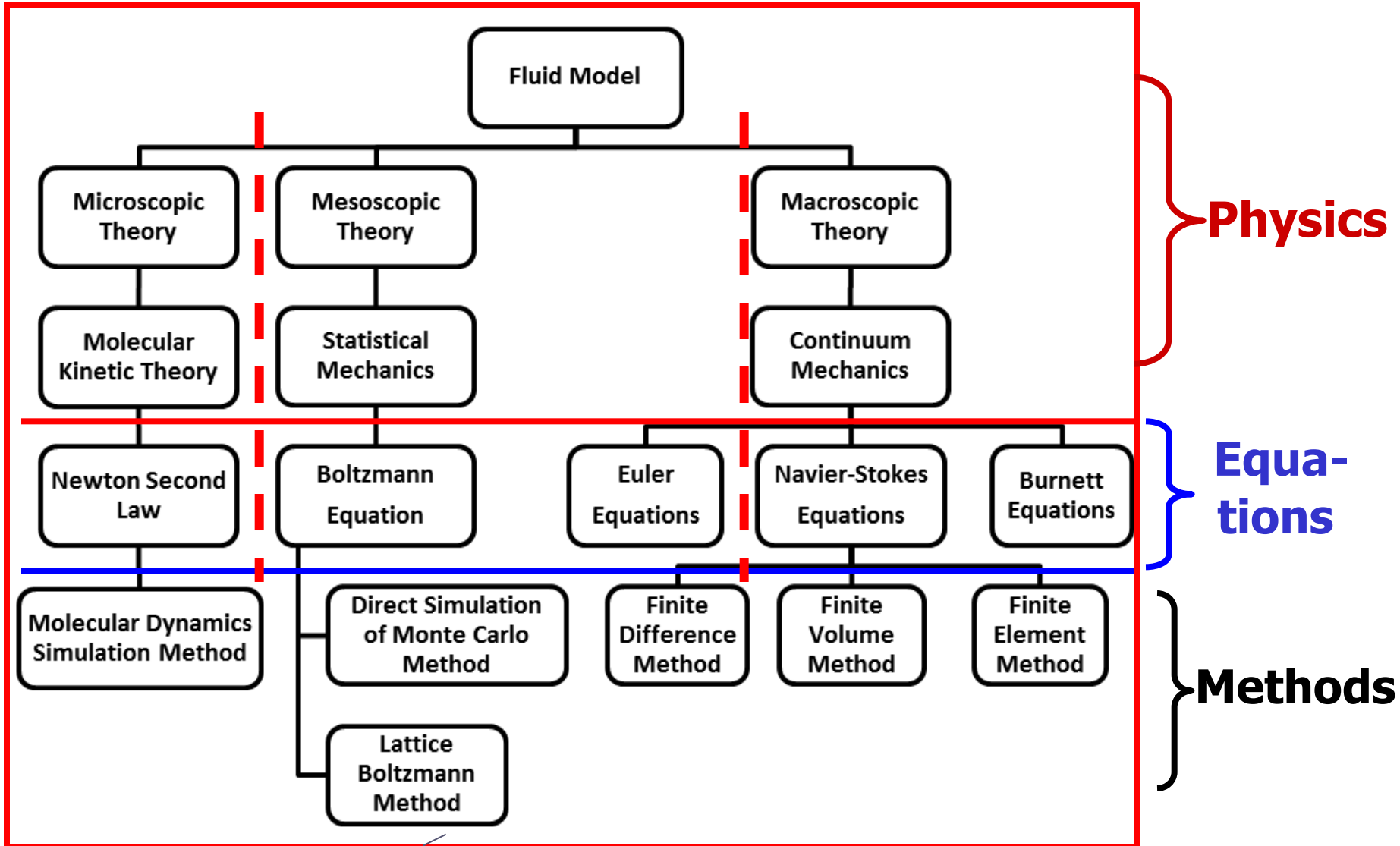
For numerical solutions of problems at different scales there is most applicable (适用) method to each scale.

Taking gas as an example, flow regime and related numerical method can be classified as follows according to the values of Knudson number:  $\lambda / L$





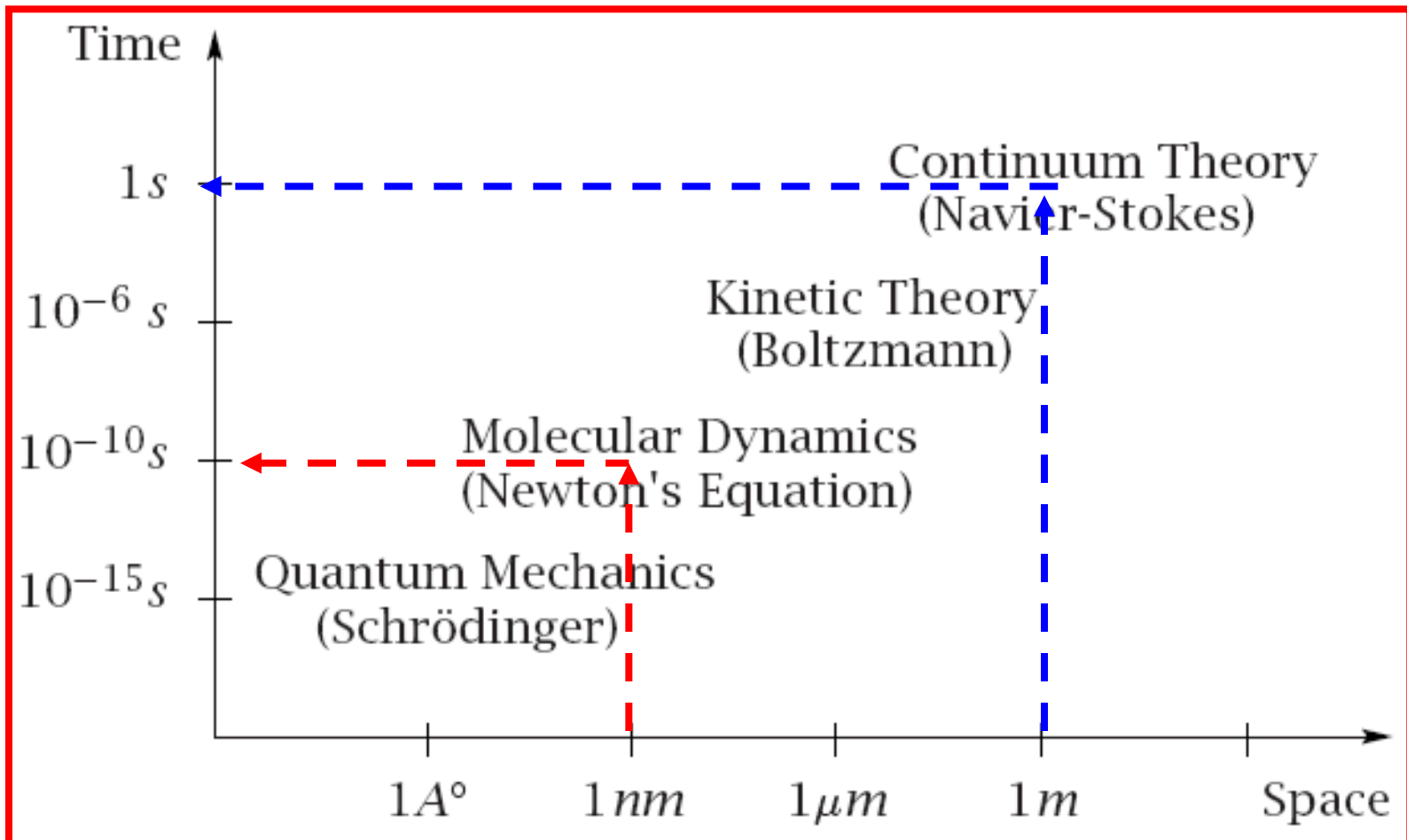
## Application feasibility(可用性) of different level numerical methods



**Physical background, govern,eqs. and numer. methods**

Ya-Ling He, Wen-Quan Tao, Multiscale simulations of heat transfer and fluid flow problems, ASME J. Heat Transfer, 2012, 134:031018

# The characteristic length and characteristic time are often closely related:



## 1.4.3 Multiscale simulation

In both engineering and nature, system or process often covers several geometric or time scales. Such system/process is called multiscale problem (**多尺度问题**) .

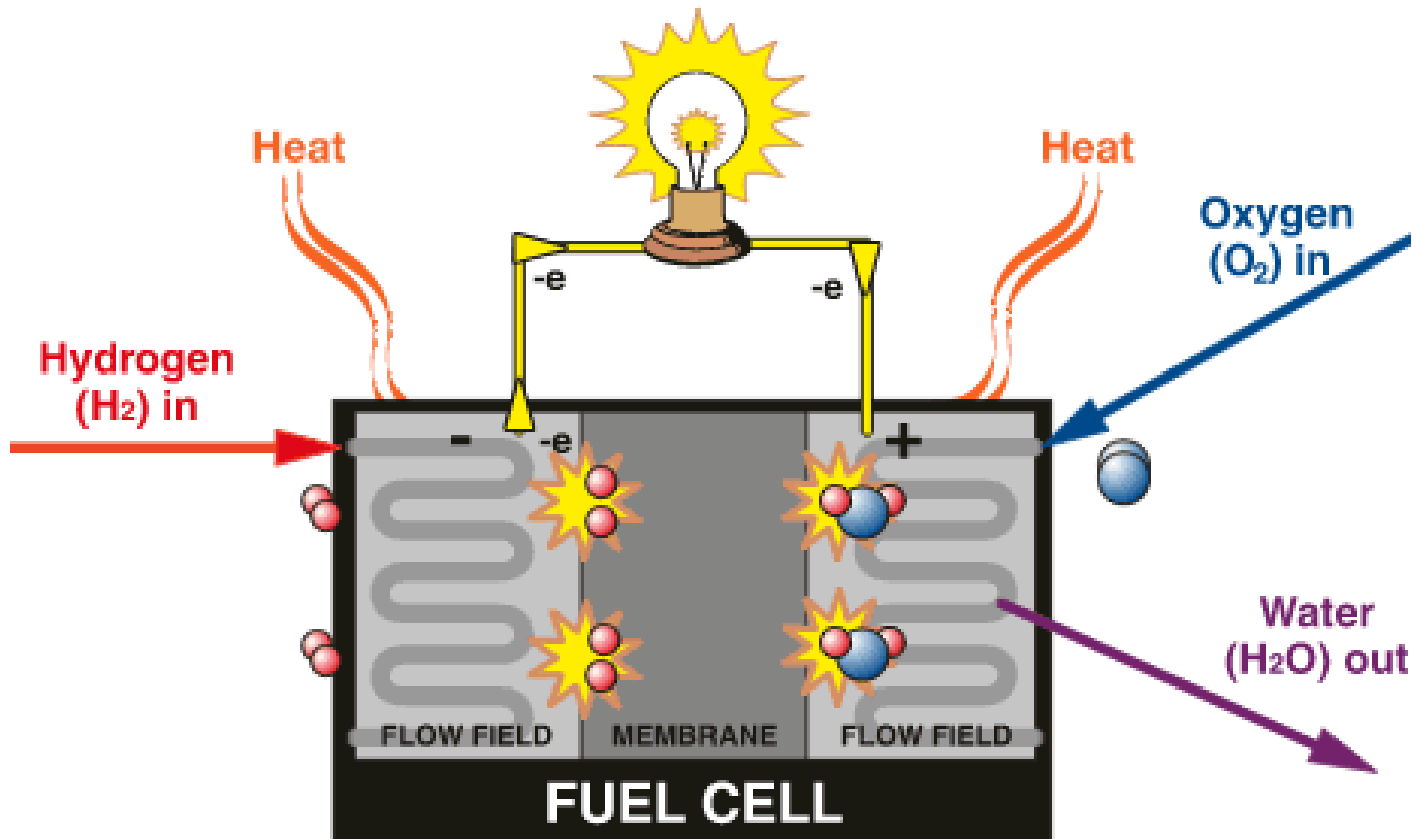
Actually almost all problems have multiple scales in nature (**有多尺度特性**) ;

Turbulent flow and heat transfer is a typically multiscale process where eddies (**涡旋**) at different scales are included and interact with each other.

Because of the limitations in the development of science and technology , previous studies were mainly concentrated **at individual scale level**.

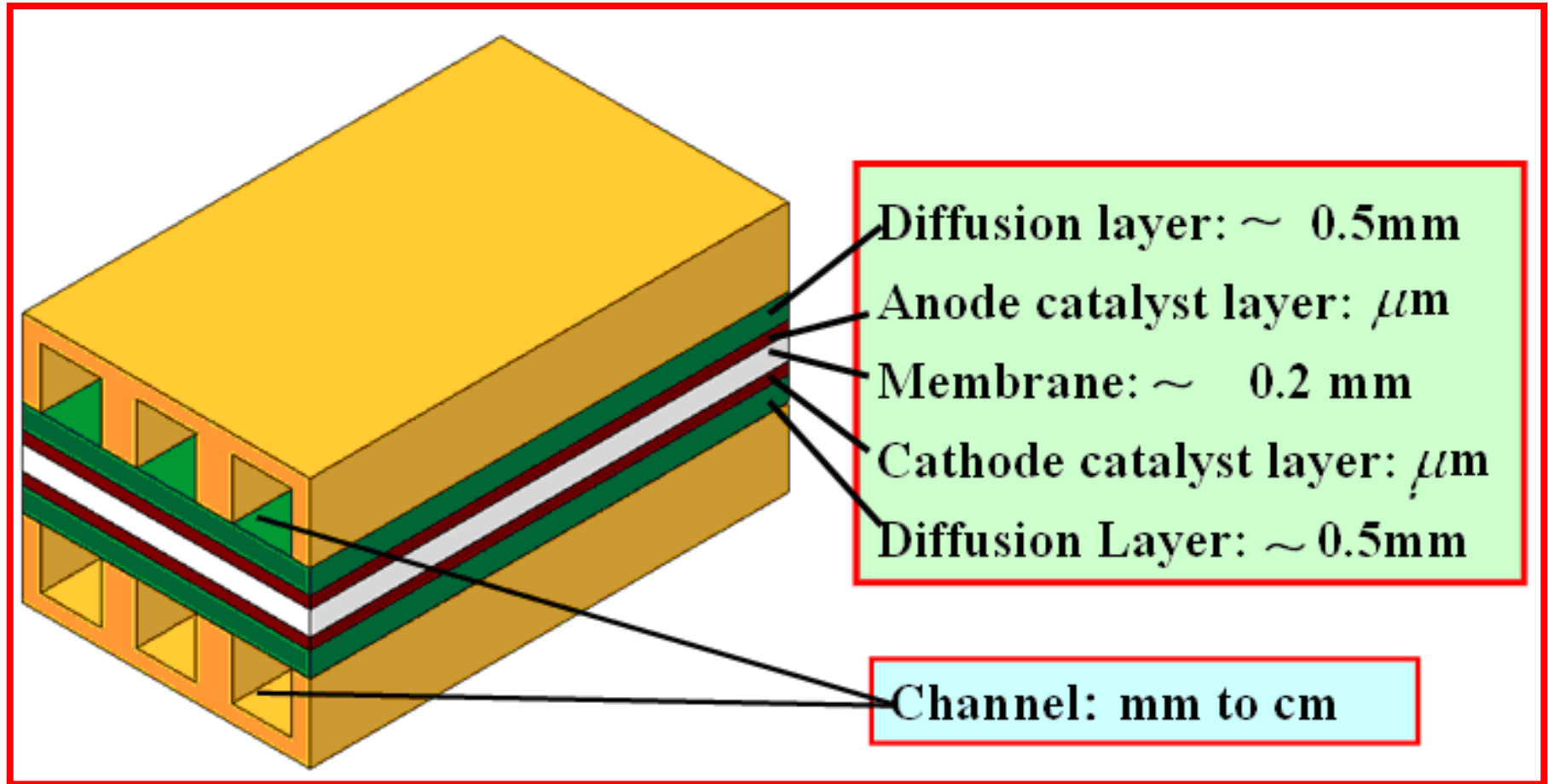


The transport process in PEMFC (质子交换膜燃料电池) covers several orders of geometries.



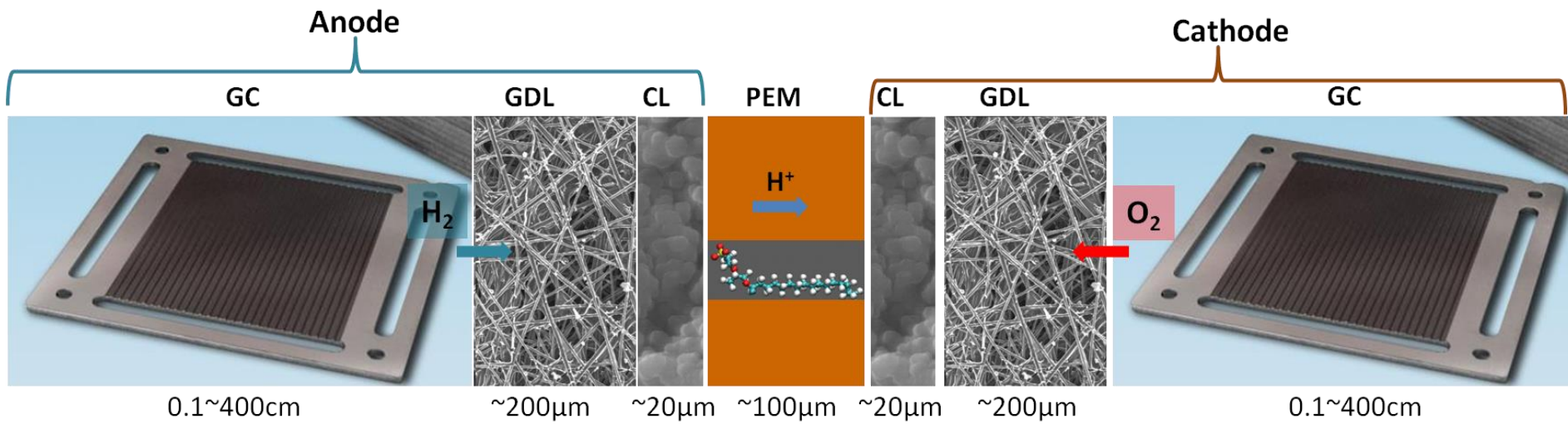
PEMFCs

# Transport process in PEMFC



Transport process in a PEMFC covers 3-4 orders of dimension.

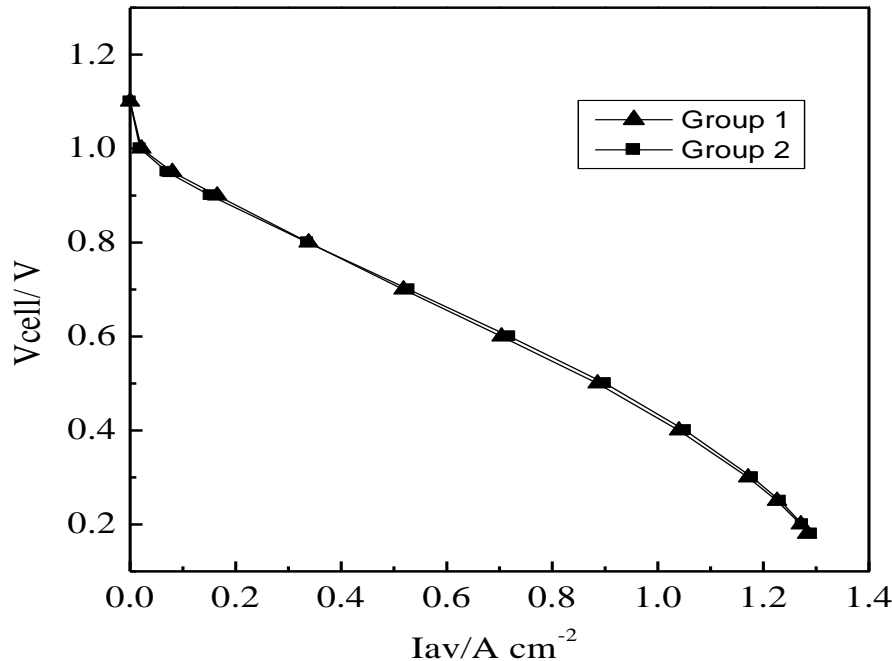
Anode-阳极    Cathode-阴极    Catalyst-催化剂



## Compositions of a PEMFC

In the present-day numerical simulation of PEMFC usually FVM is adopted, and **a number of empirical parameters (经验参数) are involved with their values being selected with great uncertain (不确定性)**. The V-I curve is usually taken to verify a simulation model.

This leads to following unpleasant situation:



With two different sets of empirical parameters we may obtain almost the same output curve.

**Only multiscale simulation can avoid (避免) such an un-pleasant situation!**

Tao W Q, Min C H, Liu X L, He Y L, Yin B H, Jiang W. Journal of Power Source, 2006, 160:359-373

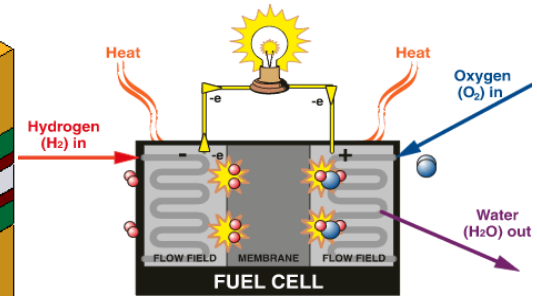
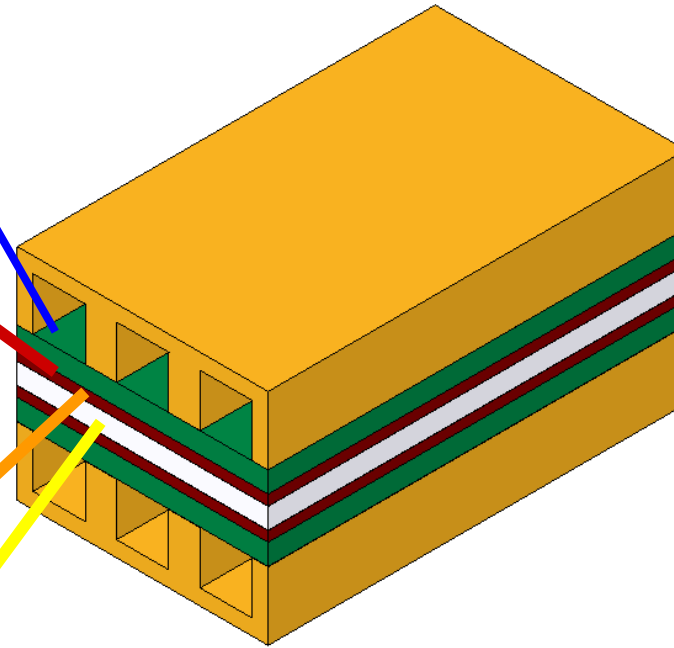
# Full multiscale simulation for PEMFC

Flow in channel  
by FVM

Transport in gas  
diffusion layer by  
LBM

Reaction in  
catalyst layer by  
MDS

Transport in  
membrane by  
MDS



Information is coupled at  
the interfaces of different  
regions.

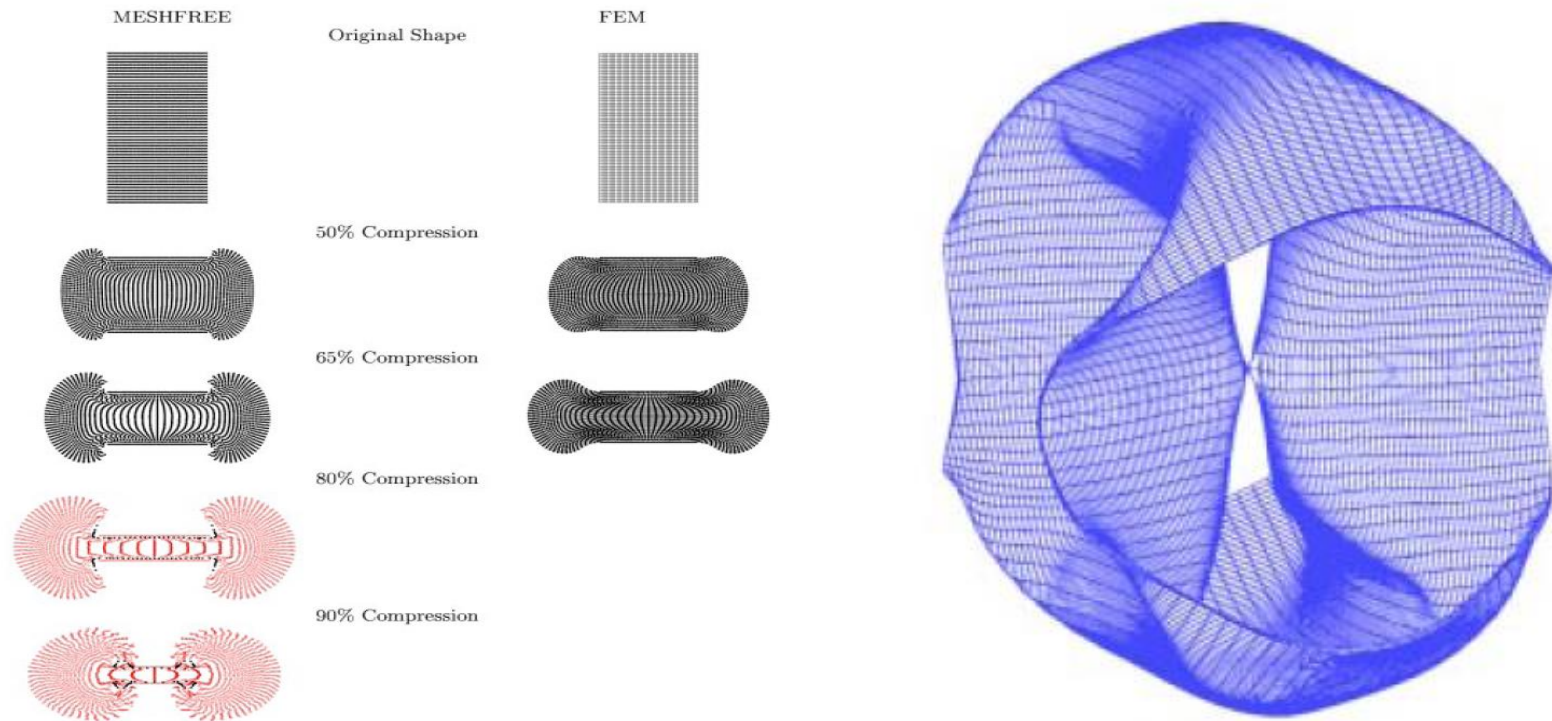
## 1.4.4 Mesh-less method

### 1. Mesh-less method (无网格方法)

In the grid generation two kinds of data or information are obtained: (1) positions of different nodes ; (2) relationship between neighboring nodes, influencing coefficient. The difficulty for grid generation of complicated geometry is in the establishment of the influencing coefficients.

In the mesh-less method the positions of nodes are still needed, however, the relationship between neighboring nodes are not required. This so much simplify the task of grid generation that researchers call it “mesh-less” method.

The conventional methods meet great difficulties when large deformation (形变) occurs during the simulation process. This happens in mechanical manufacturing process.



**Examples of sold large deformation**

## 1.4.5 Supper-computer and parallel computation

The rapid development of high performance supper computer (高性能超级计算机) has being greatly enlarged the applicable region of numerical simulation. Now we can say that almost every thing can be simulated by computers, with different reliability (可靠性) and accuracy (精度) .

**My dream:** there is one day in the future when computer simulation becomes the major tool for research and production design , and experiment measurement is only needed for validate (验证) some cases.



# 2010年11月世界TOP500超级计算机

排名	制造商	总核数	峰值/实测性能
1	中国国防科技大学	6核Intel 186368	4701万亿次 <b>2566万亿次 (2566T)</b>
2	<b>Jaguar</b> (美洲豹)	6核AMD 224162	2331万亿次 <b>1759万亿次</b>
3	<b>Nebulae</b> (星云) 曙光	6核Intel 120640	2984万亿次 1271万亿次
4	<b>Tsubame</b> (燕子) NEC/HP公司	6核Intel 73278	2287.6万亿次 1192万亿次
5	<b>Hopper</b> (跳跃者) <b>Cray</b>	12核AMD 294912	1188.6万亿次 1054万亿次

# 2013-11至2015-07世界TOP500超级计算机排名

排名	安装地点	制造商	峰值/实测	功耗
1	中国广州	国防科技大学	54900 <b>万亿(T)</b> 次 <b>33860万亿次</b>	17800kW
2	橡树林国家实验室 (Oak Ridge)	Cray	27110 17590	8200
3	劳伦斯国家实验室	IBM	20130 17170	7890
4	日本理化研究所	富士通	11280 10510	12660
5	阿贡国家实验室	IBM	10060 8580	3940

# Erratum

1. 第3页中间:  $-2/3$  应改为  $-2/3 \eta$
2. 第3页倒数第3行:  $-\frac{\partial p}{\partial x}$  应改为  $-\frac{\partial p}{\partial x} + \rho F_x$   
 倒数第1, 2行仿此修改。
3. 第4页倒数第3行:  $\lambda \operatorname{div} \mathbf{U}$  应改为  $\lambda (\operatorname{div} \mathbf{U})^2$
4. 第7页 式(1-18)中右端:  $\rho$  应改为  $p$
5. 第9页倒数第3、4行右端: 扩散项前的系数应为  $\nu$
6. 式(1-6),(1-8)中漏了重力项。

本章作业为习题1-7（补充不可压，常物性的条件），与第二章一起上交。

# Home Work 1

## Problem 1-7

**Adding following two assumptions:**

**Incompressible flow (不可压缩流体) ;**

**Constant thermo-physical properties (物性为常数)**

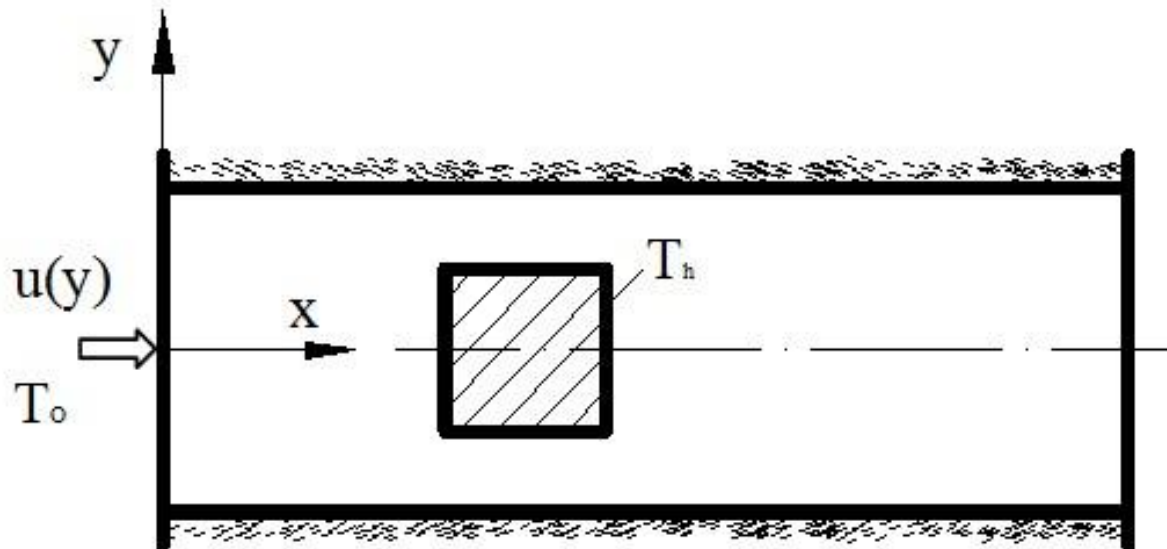
**Hand in with the home work of Chapter 2.**

**The pdf file of each chapter will be posted at our group website!**

## Problem 1-7

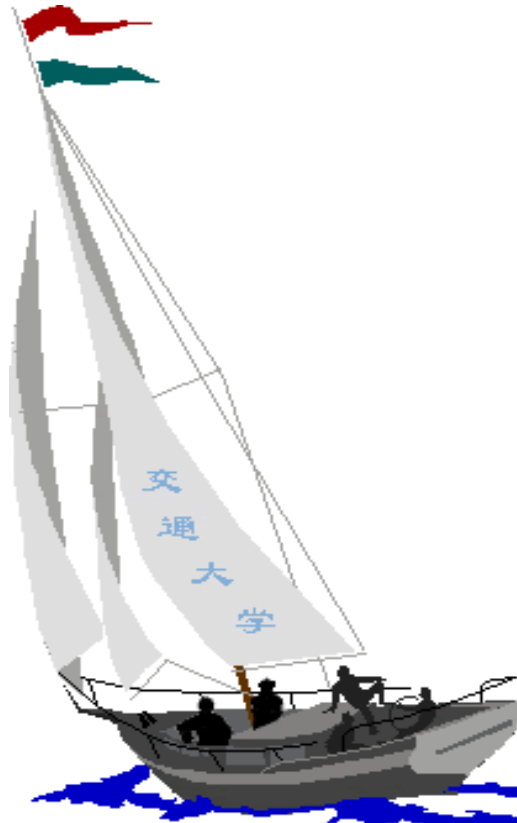
**A solid square having uniform temperature  $T_h$  is placed at center line of a two-dimensional parallel plate channel as shown in figure below. Flow is fully developed. The upper and lower side of the channel is insulated and therefore you may assume that these sides are adiabatic whereas outlet boundary is far from the solid square. Fluid enters the channel with a uniform temperature,  $T_{in} = C$ . Write down the governing equations for steady state, incompressible laminar flow with constant properties.**

**Also write down boundary conditions for the velocity and temperature for the given domain (It is preferable, at exit boundary, to take first derivative zero). Flow is incompressible and material properties are constants.**



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

For convenience of discussion, a **qq-group** has been set up:  
**573633261**



同舟共济  
渡彼岸!

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