Advanced Numerical Methods

Minping Wan

Tel: 0755 8801 8278
Email: wanmp@sustc.edu.cn

Course Information

- Lectures:
  Wed 2:00pm-3:50pm (Odd week), Friday 10:20am-12:10pm,
  102 2nd Building Lychee Hill (Li Yuan)

- Office:
  507 5th Building, Wisdom Valley (Hui Yuan)

- Teaching Assistants:
  Xiaotian Zhang（张孝天）
  Email: 11756011@mail.sustech.edu.cn

Course Objectives

1. To learn numerical methods for data analysis, optimisation, linear algebra and ODEs;

2. To learn MATLAB/Python skills in numerical methods, programming and graphics;

3. To apply 1,2 to Mathematical problems and obtain solutions;

4. To present these solutions in a coherent manner for assessment.

Topics Covered (tentative)

- Solution of nonlinear equations
- Solution of linear systems
- Interpolation and polynomial approximation
- Curve fitting
- Numerical differentiation
- Numerical integration
- Numerical optimization
- Solution of differential equations
- Solution of partial differential equations

Course Grading

- Weighting for the various components of the course

Mid-Term Exam	20%
Final Exam	40%
Homework	20%
Projects	20%

万敏平 教授
博士生导师

- 1998-2002，清华大学工程力学系 学士
- 2002-2008，约翰霍普金斯大学机械工程系 硕士、博士
- 2008-2011，特拉华大学物理与天文系 博士后
- 2011-2015，特拉华大学物理与天文系 Research Associate
- 2015-2020，南方科技大学力学与航空航天工程系 副教授
- 2020至今， 南方科技大学力学与航空航天工程系 教授

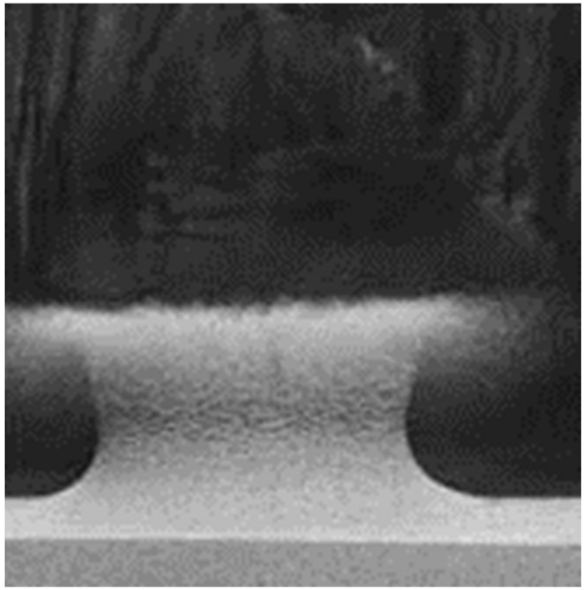
流体物理与湍流研究实验室

Fluid Physics and Turbulence Research Lab

研究对象是什么？

99.9%以上的宇宙物质是流体

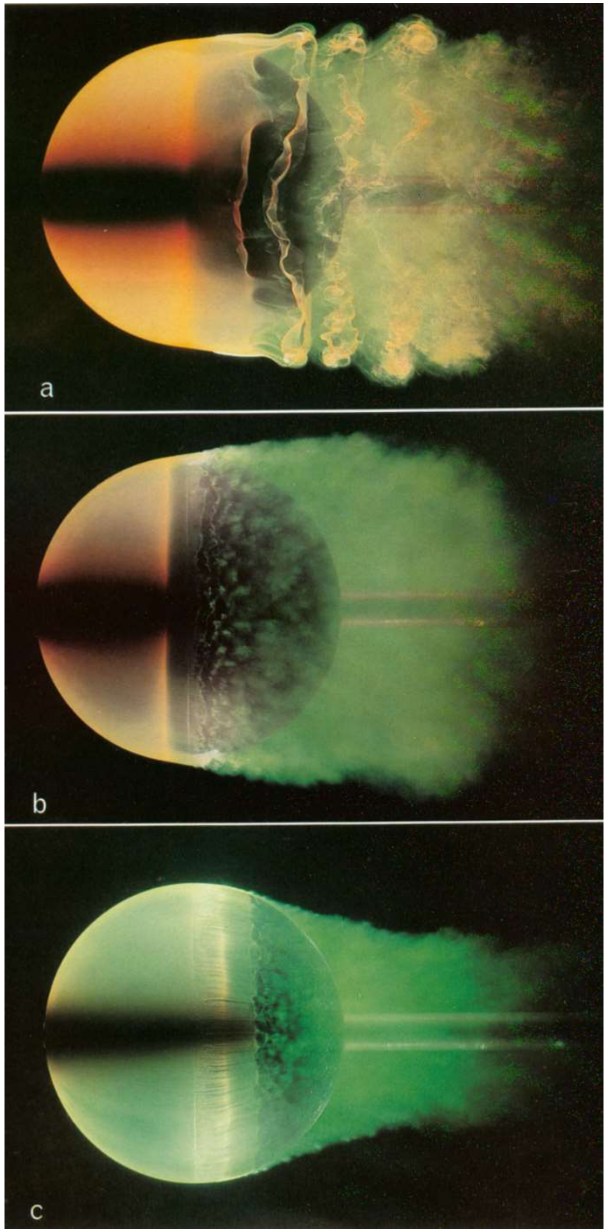
--Milton Van Dyke



研究的物理过程是什么？

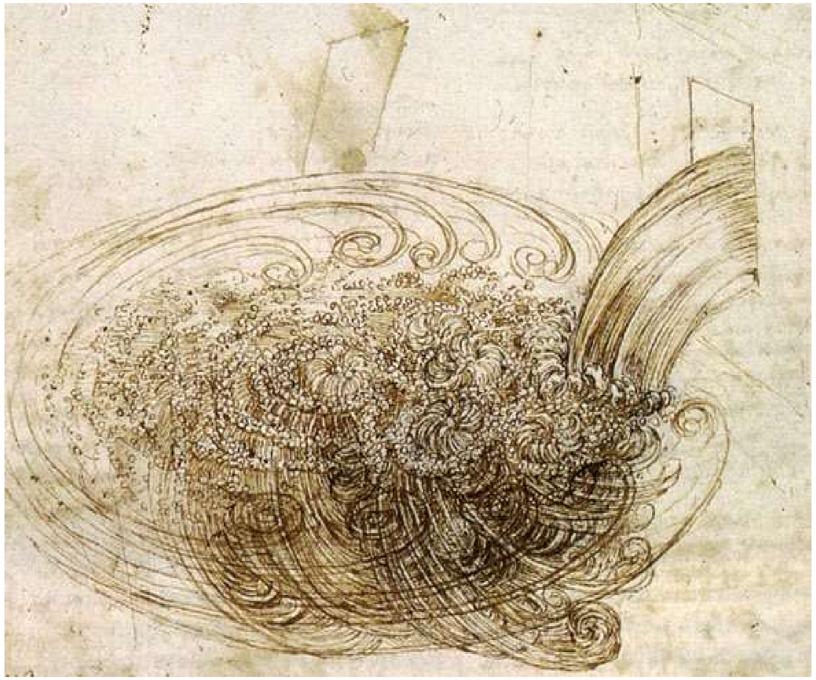
湍流（Turbulence）

- Heisenberg想问上帝两个问题：
  一个是为什么广义相对论如此奇怪？
  另一个是怎么解释湍流？
- R. Feymann：湍流是宏观物理学最后的难题。
- 分离-失稳-转捩-湍流。
- 难在极多尺度、高度非线性、混沌。



什么是湍流？

What is turbulence?



Leonardo da Vinci,
1508-9

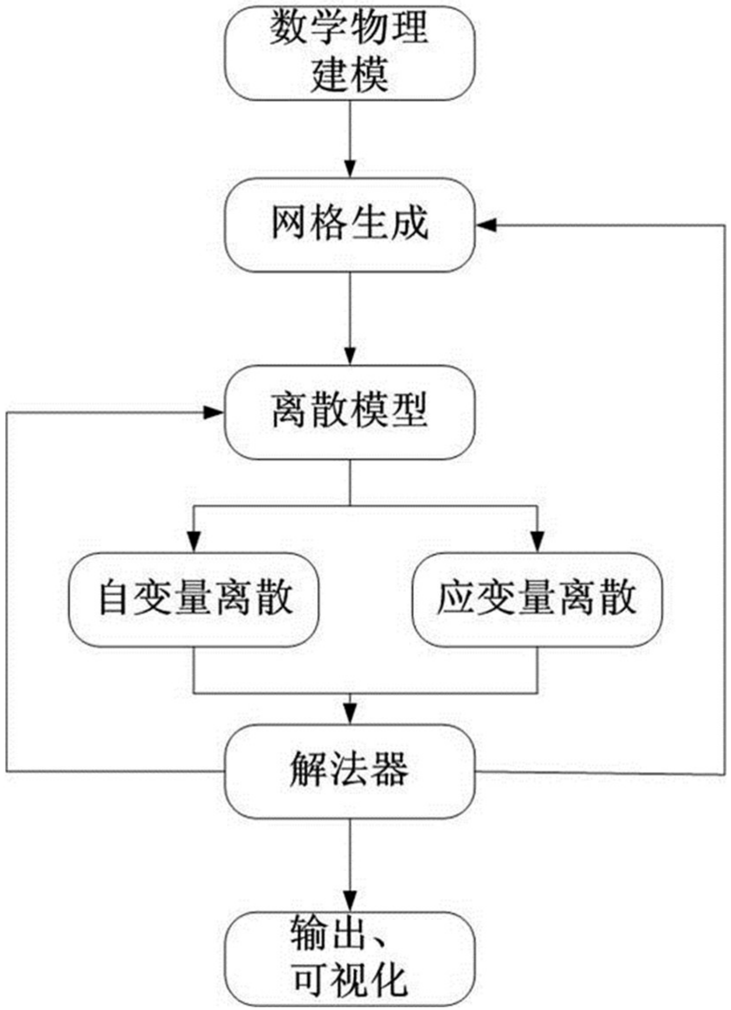
“Observe the motion of the surface of the water, which resembles that of hair, which has two motions, of which one is caused by the weight of the hair, the other by the direction of the curls; thus the water has eddying motions, one part of which is due to the principal current, the other to random and reverse motion”. [Leonardo da Vinci, “Study of water falling into still water”.]

为什么研究流体湍流？

采用什么研究工具？

计算流体力学 CFD

Computational Fluid Dynamics

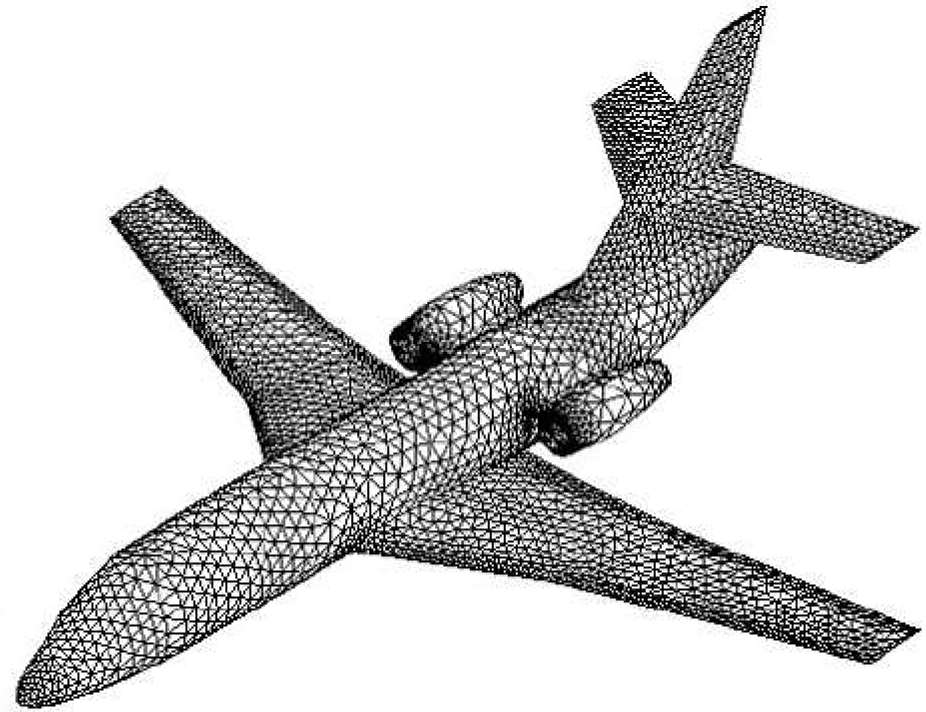


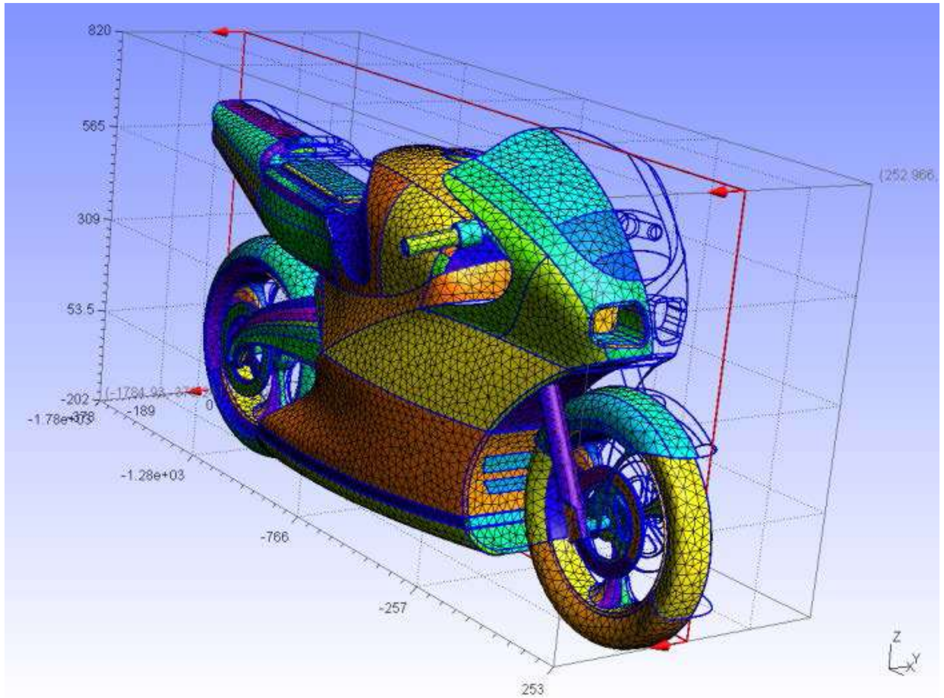
- CFD集流体力学、数值计算方法以及计算机图形学于一体

- 前处理
- 流场计算
- 后处理

采用什么研究工具？

- 网格生成



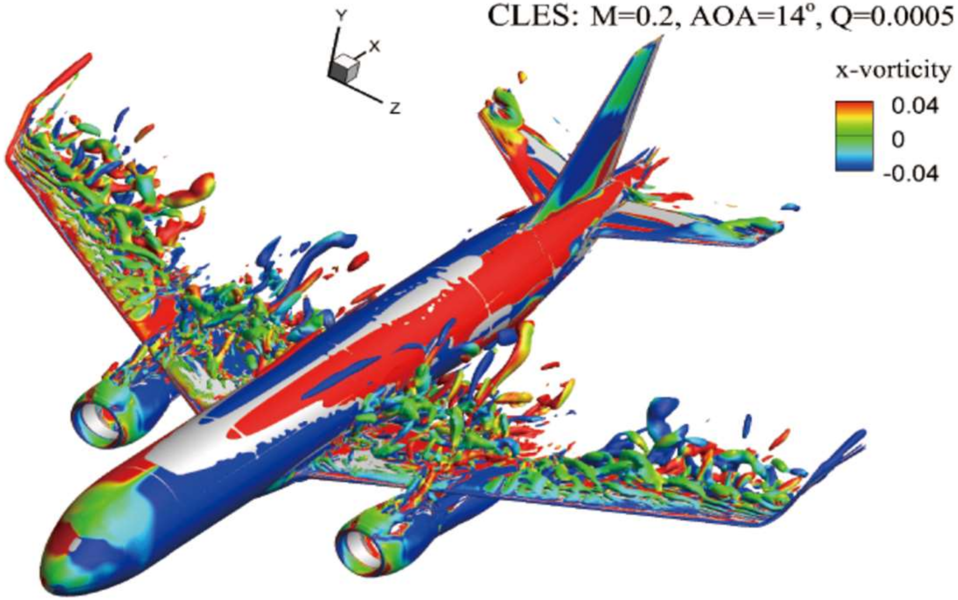


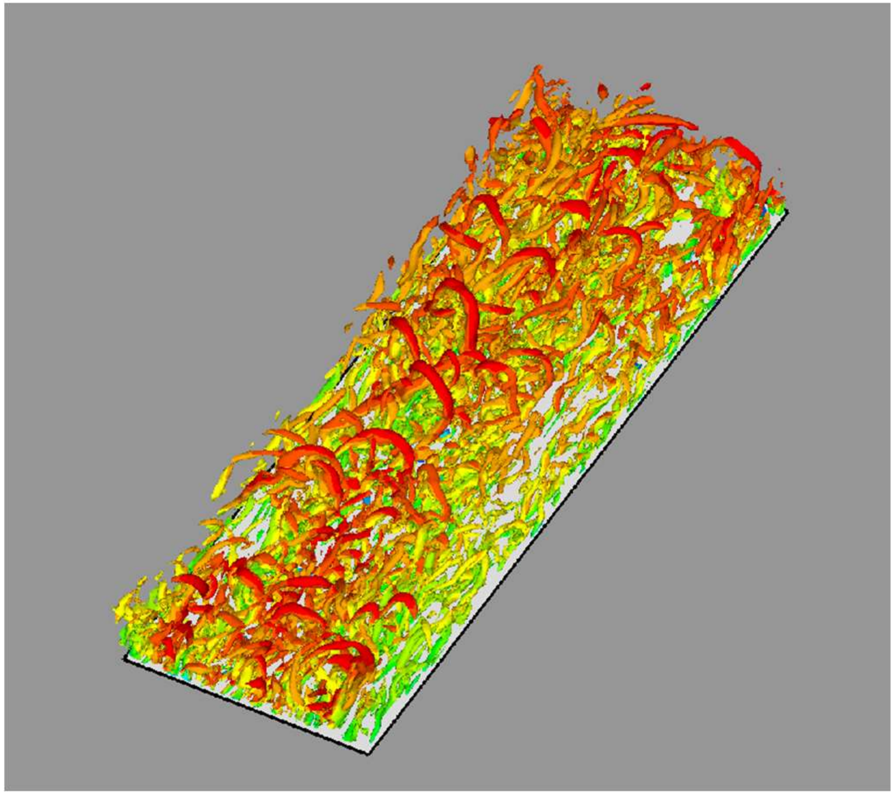
采用什么研究工具？

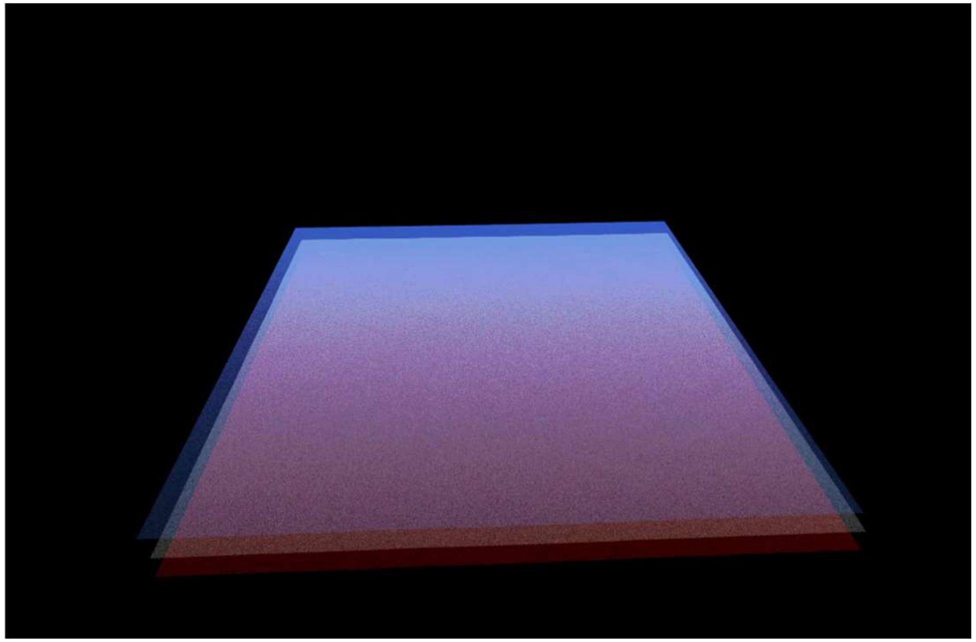
■ 流场计算及可视化

Navier-Stokes方程

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = \boldsymbol{f} - \frac{1}{\rho}\nabla p + \nu\nabla^2\boldsymbol{u}$$

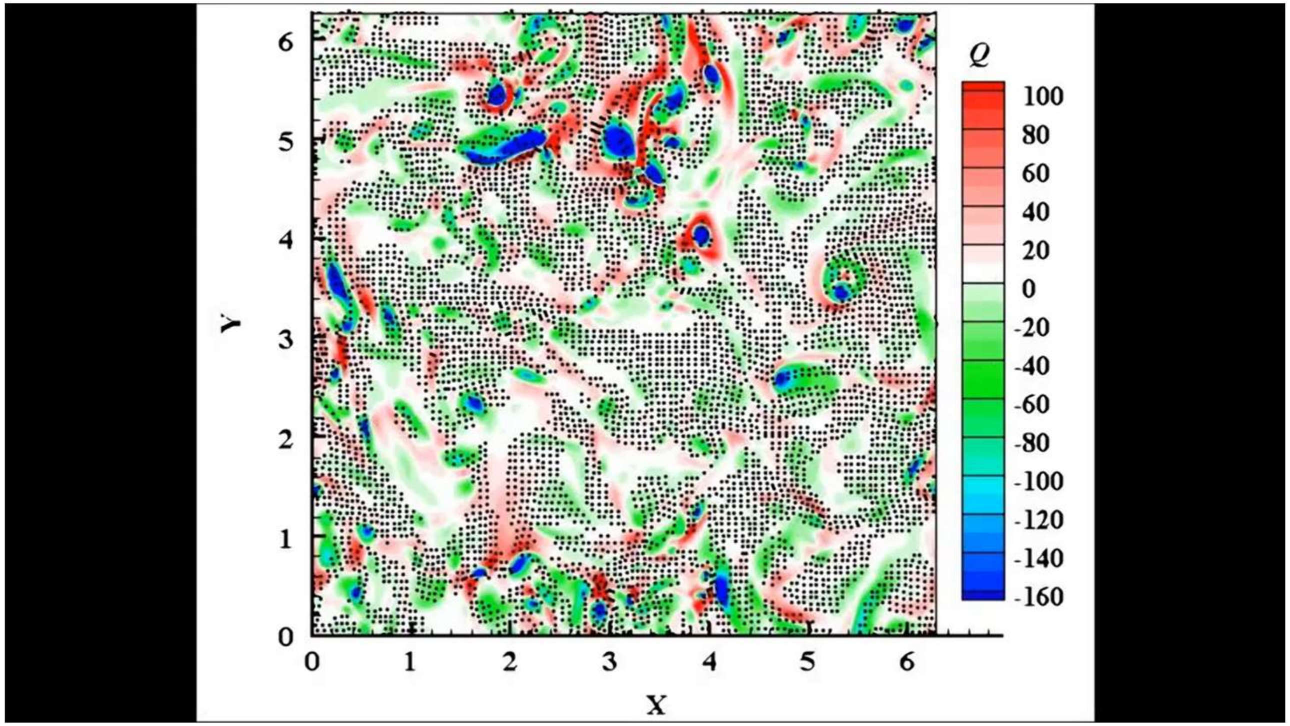






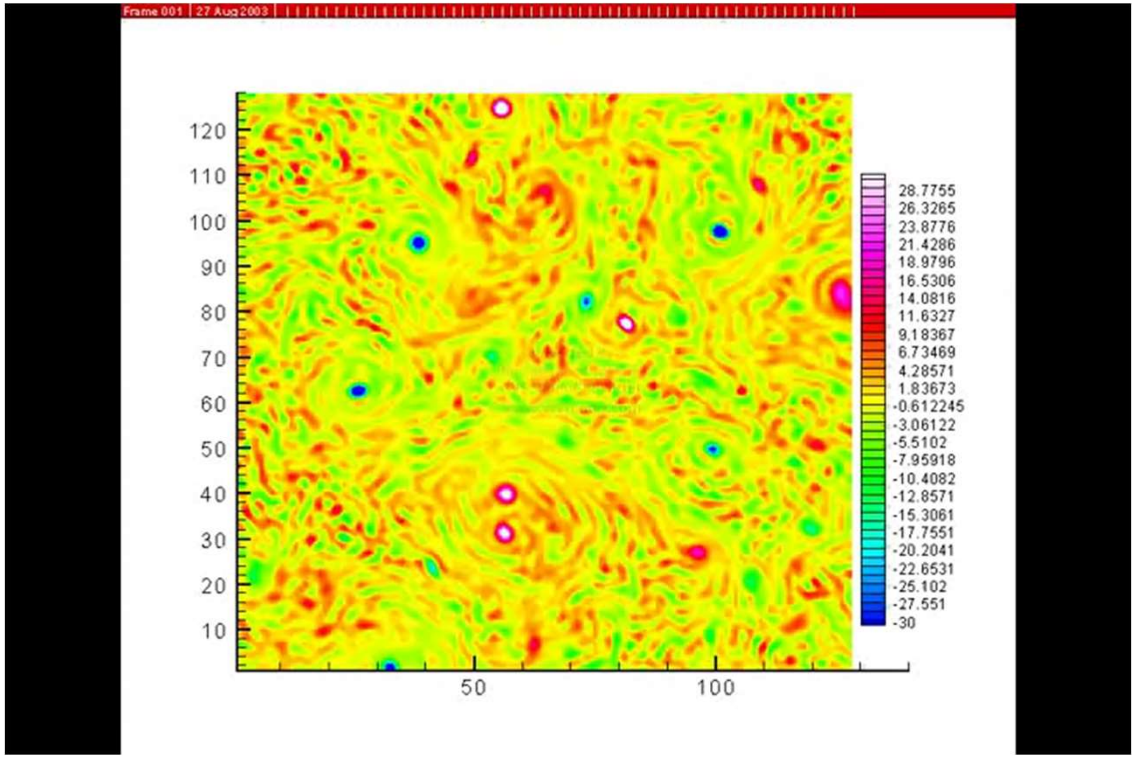
我们的研究课题（1）

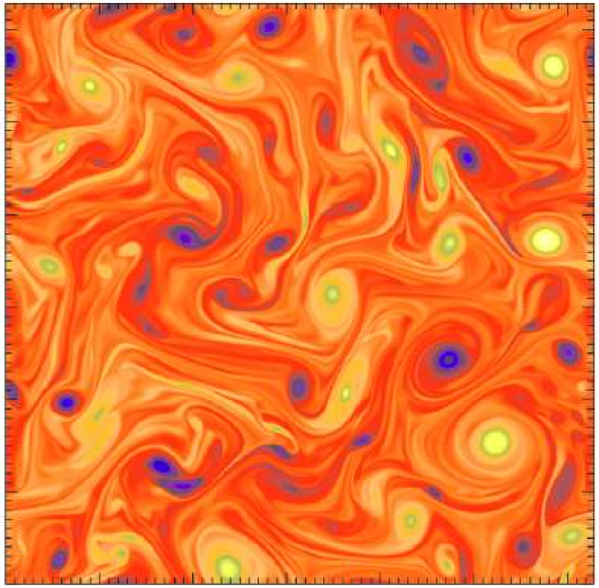
- 湍流中惯性颗粒的扩散与输运



我们的研究课题（2）

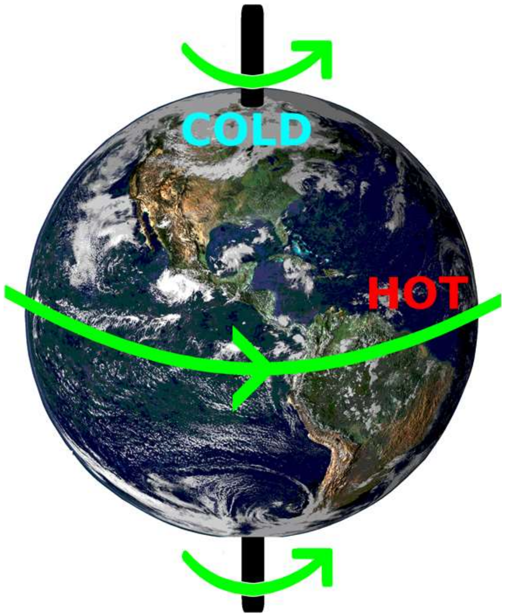
- 二维湍流



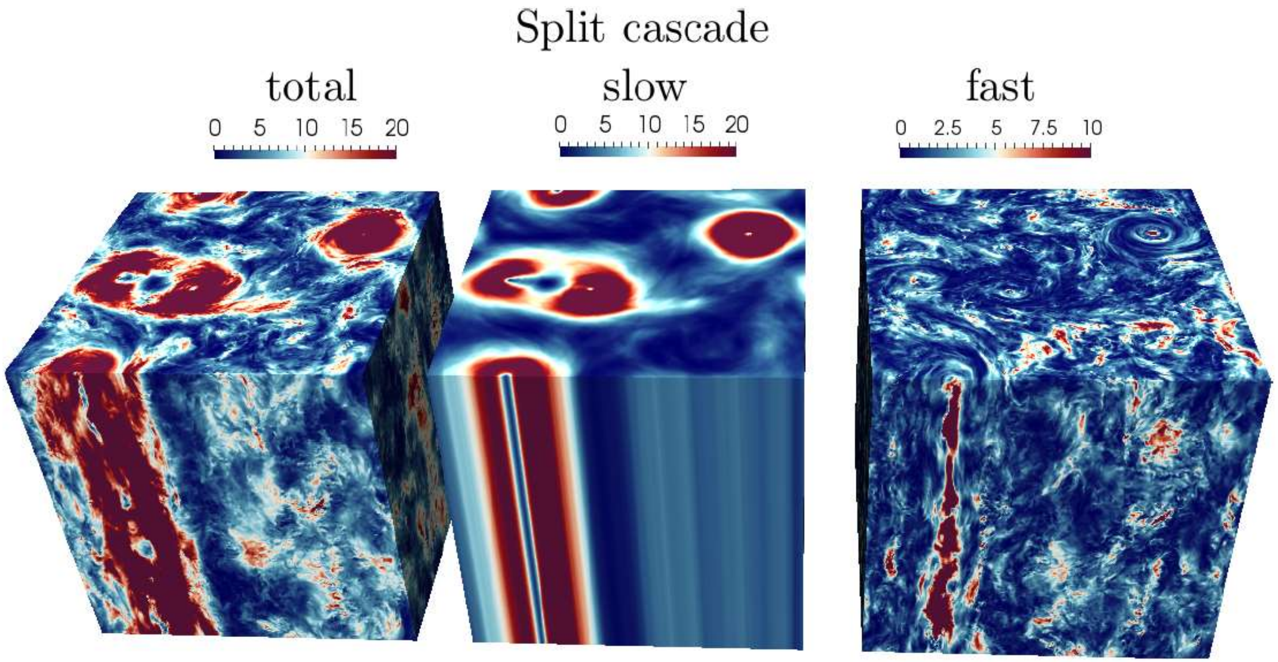


我们的研究课题（3）

- 旋转分层湍流

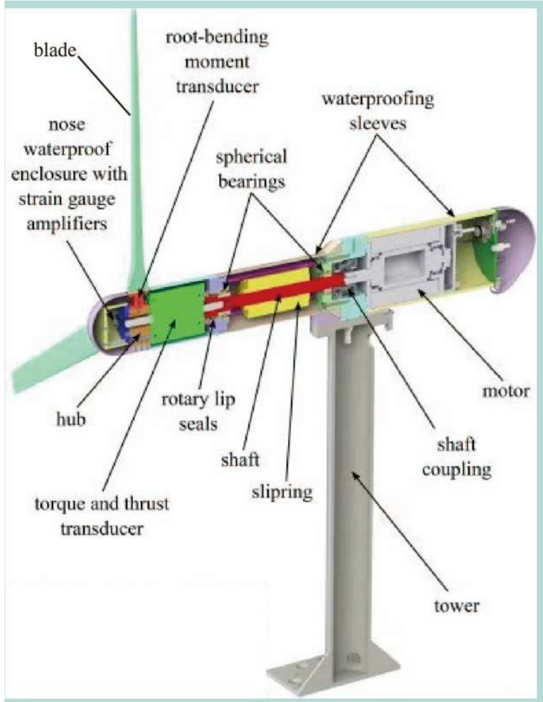


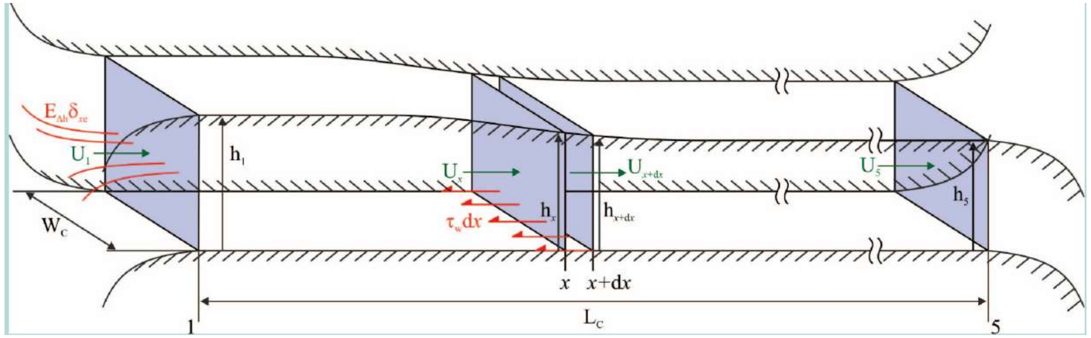
$$E(k) = E_F(k) + E_S(k)$$
$$= E_F(k) + E_{2D}(k) + E_\theta(k)$$

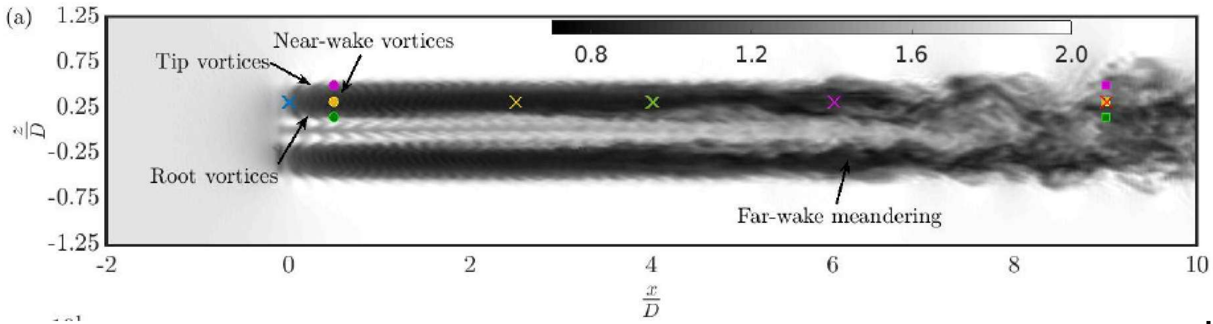


我们的研究课题（4）

■ 潮汐能：潮流涡轮发电的数值研究与优化

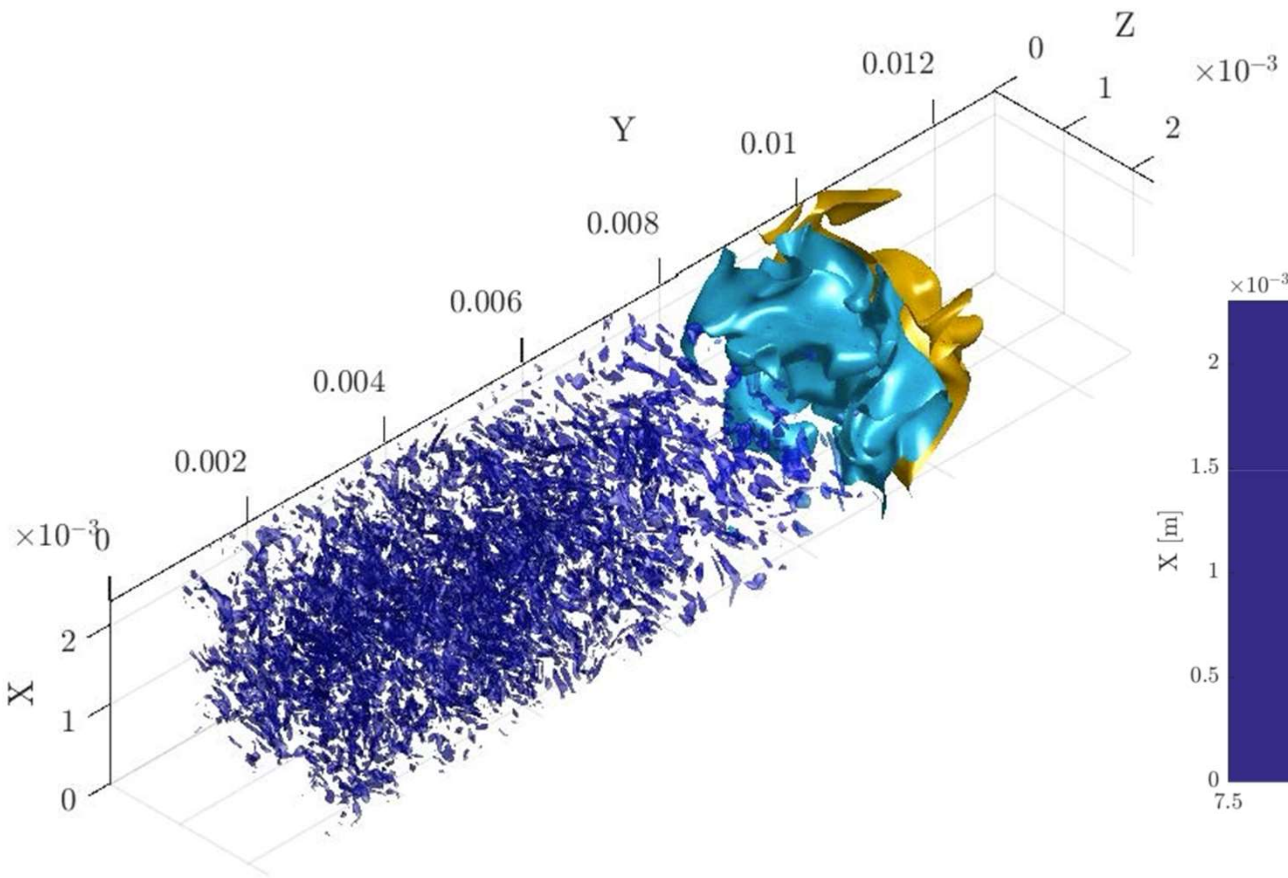




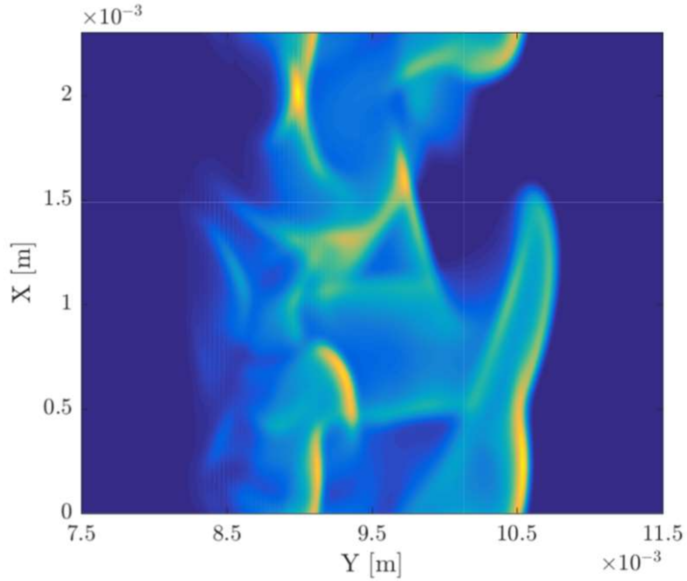


我们的研究课题（5）

- 湍流燃烧



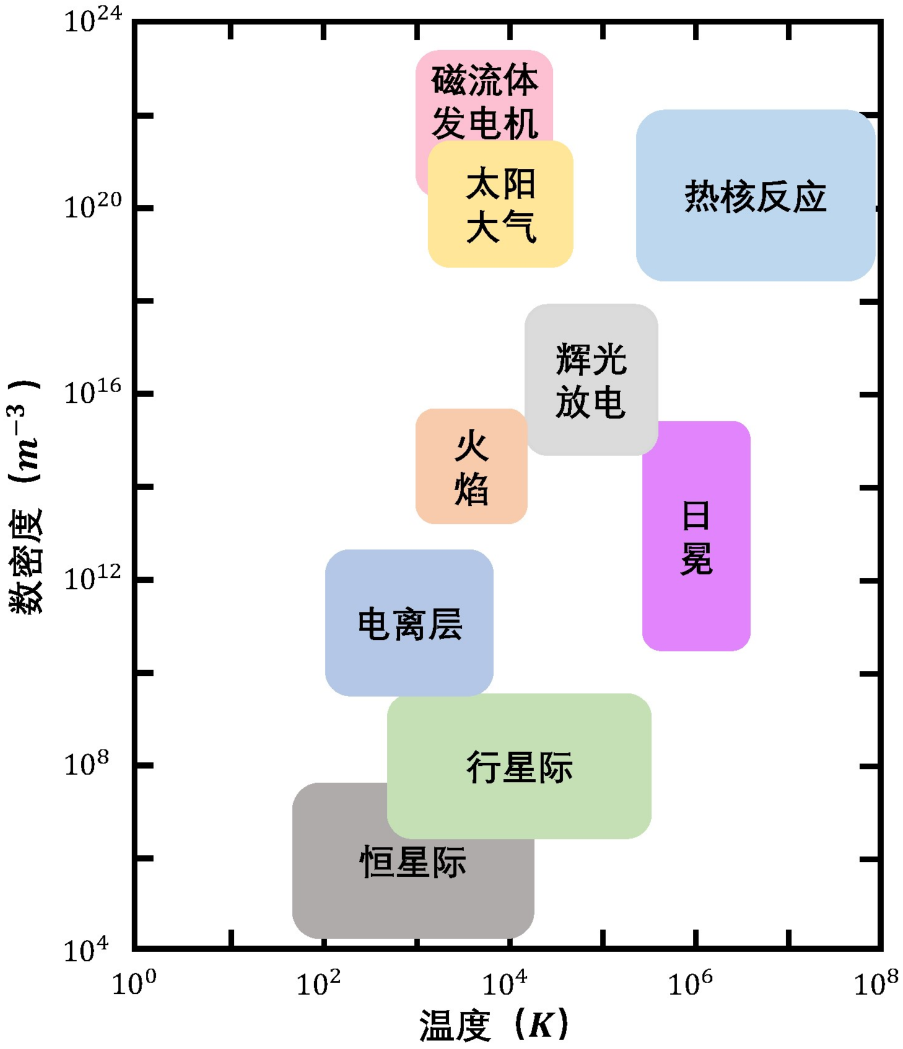
Q-criterion colored by temperature [K]. The two surfaces were extracted at T=800 and T=1400 K.

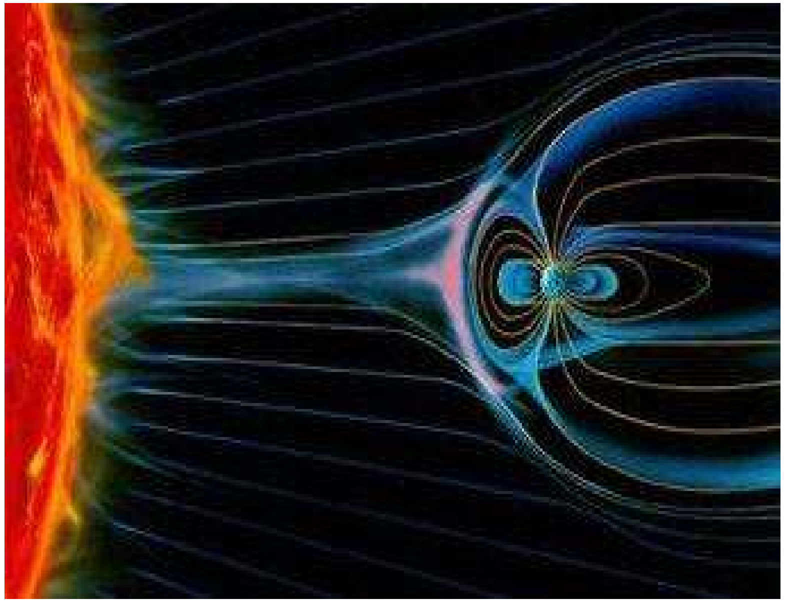


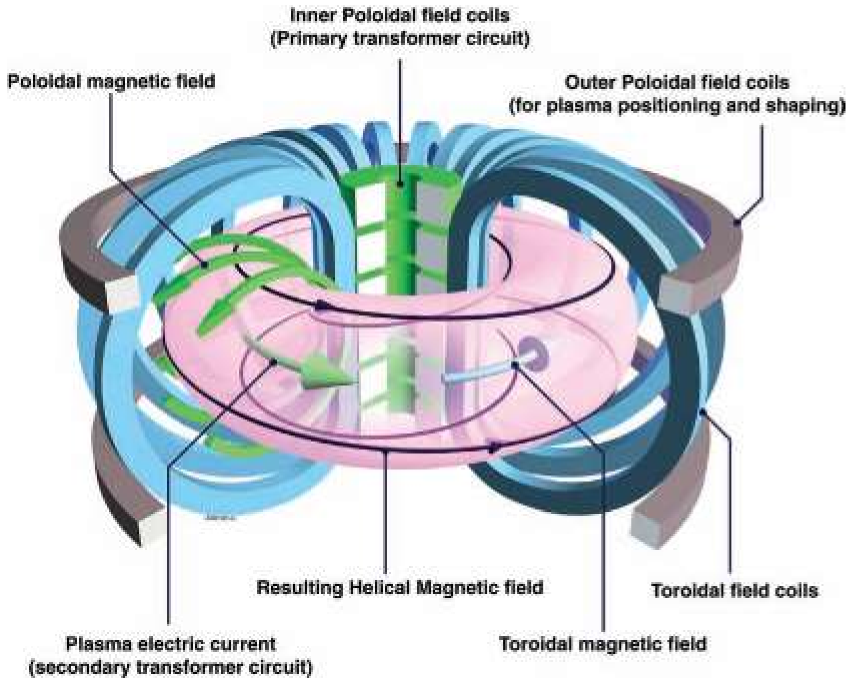
the consumption rate of the fuel species, $C_{12}H_{26}$.

我们的研究课题（6）

■ 磁流体、等离子体湍流

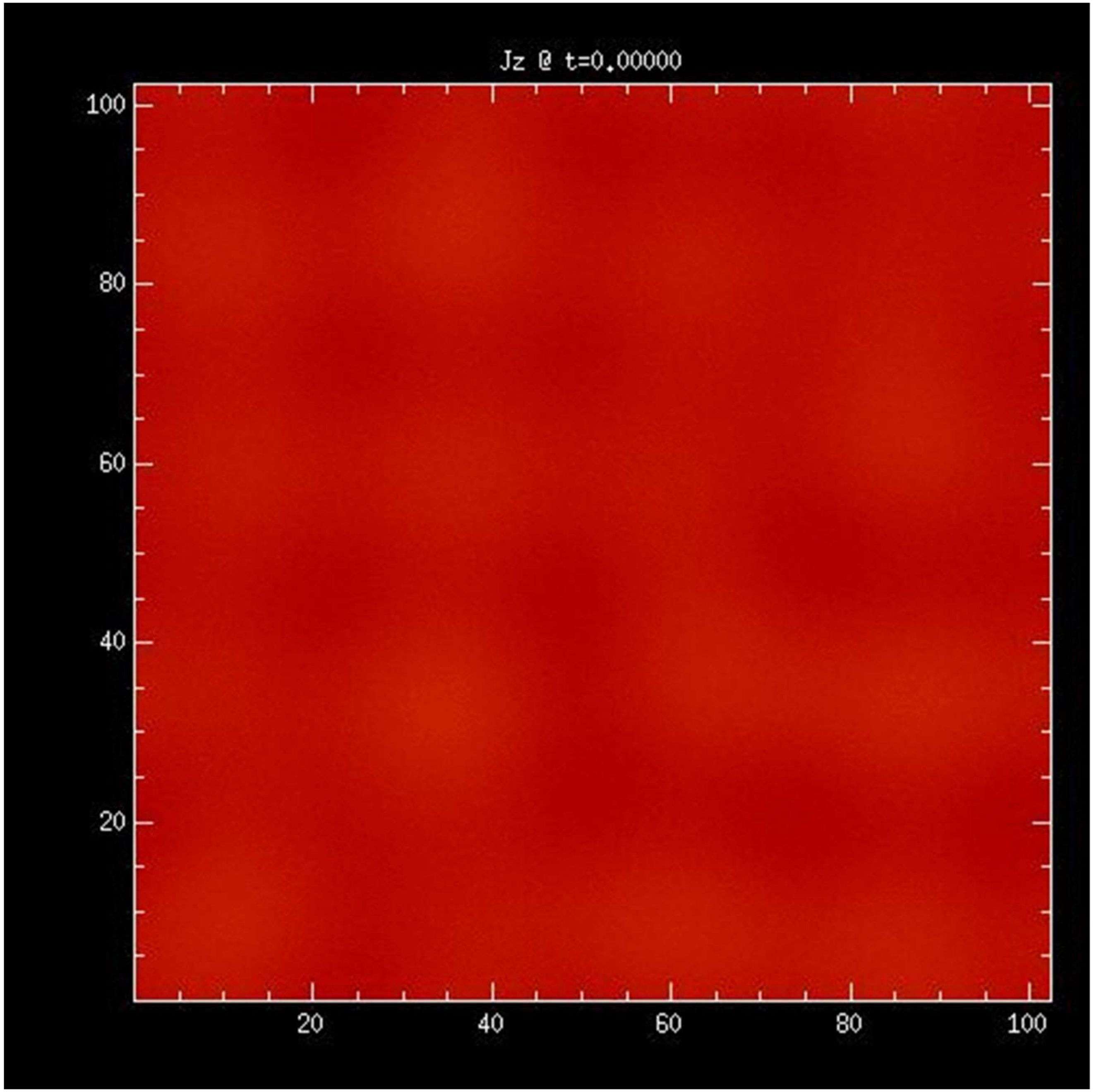






PIC simulation of shear driven turbulence (K-H instability)

PIC simulation of decaying plasma turbulence



2.5 D

8192^2 grid,

300 particles/cell;

Mass ratio 25

System size 102.4 d_i

Introduction to Numerical Method

- Most engineering/industrial/scientific problems require the computational solution of a variety of problems. The solution process generally involves three stages.

1. Front end: Problem description in easy manner.

2. Main computational effort. Various tasks including:
   Data input
   Data manipulation . Image and signal processing
   Linear Algebra
   Optimization
   Solution of ordinary/partial DEs
   Approximation

3. Output: Typical 3D graphics. Often now animated.

Introduction

- This course will aim to teach computational mathematics and numerical methods in the overall context of 1,2,and 3 through:

  - The use of MATLAB/Python.

  - Understanding of the mathematical principles behind how the various algorithms in MATLAB/Python work and their limitations.

  - Learning some ideas of structured programming through using the MATLAB/Python language.

  - Looking at all theory and methods in the context of case studies found from real applications.

Introduction

- In summary, the approach behind the implementation of a numerical method to an industrial/engineering/science problem can be summarized as follows:

  - Solve the right problem . . .make sure your model is right;

  - Solve the problem right . . . use the best methods;

  - Don’t reinvent the wheel . . .Be aware of the existence of good software and be prepared to use it.

  - Keep a healthy skepticism about your answers.

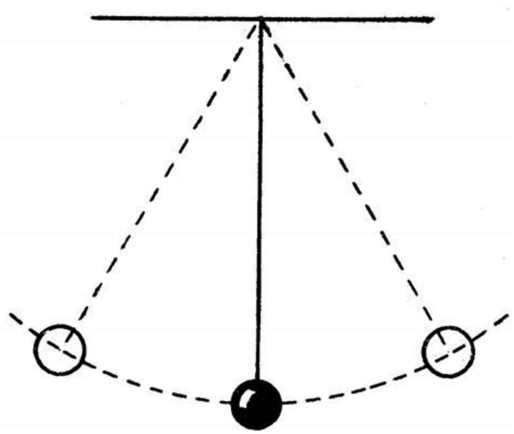
An example of this approach

- A famous system: **the pendulum**, which is described by the following second order ordinary differential equation

$$\frac{d^2\theta}{dt^2} + \sin(\theta) = 0$$

- Initial conditions:

for example $\theta = \theta_0$ and $\frac{d\theta}{dt} = 0$ at $t = 0$



The Traditional Mathematical Approach

- Change/simplify problem to

$$\frac{d^2\theta}{dt^2} + \theta = 0$$

- Solve this analytically to give

$$\theta(t) = A\sin(t) + B\cos(t)$$

- This approach is fine for small swings, but is bad for large swings

Traditional Numerical Method

- Rewrite the system as:

$$d\theta/dt = v$$
$$dv/dt = -\ sin(\theta)$$

- Divide time into equal steps $t_n = n \triangle t$ and approximate $\theta(t), v(t)$

$$\theta_n \approx \theta(t_n),\ V_n \approx v(t_n)$$

- Discretize the system. For example, using the Euler method:

$$\frac{\theta_{n+1} - \theta_n}{\triangle t} = V_n$$
$$\frac{V_{n+1} - V_n}{\triangle t} = -\sin(\theta_n)$$

- Finally write a program (typically as a loop) that generates a sequence of values (θ_n, V_n) plot these and compare with reality.
- Problem: we need to write a new program every time we want to solve an ODE.

Software Approach (I)

- Instead of doing the discretization “by hand” we can use a software package. We will now see how we can use MATLAB to solve this
- Firstly, create a function file func.m with the ODE coded into it

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%                                                   %
%  MATH0174 : function file func.m                  %
%                                                   %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%
% This file sets up the equations for
%           theta'' + sin(theta) = 0
%
% To do this it takes thet(1)| = theta and thet(2) = theta'
% It then sets up the vector thetprime so that
%
%  thetprime(1) = theta'
%  thetprime(2) = theta''
%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%
%  function func.m
%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function thetprime=func(t,thet)
thetprime=[thet(2);-sin(thet(1))];
```

$$\theta_1' = \theta_2, \quad \theta_2' = -\sin(\theta_1)$$

Software Approach (II)

- Now set the initial conditions, and the time span t ∈ [0, 10]
- Next use the MATLAB command ode45 to solve the ODE over the time span; This implements a Runge-Kutta routine to the ODE with a Dormand-Price error estimator. You can specify the error tolerance in advance

```
%
%  We specify an interval of t in [0,10]
%

tspan = [0 10];

%
%  We specify the initial conditions [thet,v] = [0 1]
%

start = [0;1];

%
% Options sets the tolerance to 1d-6
%

options = odeset('AbsTol',1d-6);

%
% Now solve the ODE using the Dormand-Price explicit Runge-Kutta
% method


[t,thet] = ode45('func',tspan,start,options);
```

Software Approach (III)

- Finally plot the result. This will look like plot(t,thet) or plot(thet(:,1), thet(:,2))

```
%
% Now plot the solution
%

plot(t,thet)

pause

%
%  Now plot the phase plane
%

theta = thet(:,1);
v     = thet(:,2);

plot(theta,v)
axis('equal')
```