

What is numerical simulation? And why should I care?

KYOTO UNIV GRAD SCHOOL OF ENERGY SCIENCE
ENERGY CONVERSION SCIENCE DEPT.

Master's student

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Self Introduction

- ▶ Name : Yusuke Ikemi
- ▶ Lab : Combustion and power engineering Lab
- ▶ Research : Heat transfer of impinging diesel spray
(Large eddy simulation : LES)
- ▶ Hometown : Shiga Pref
- ▶ Hobby : Bakery hopping

Today's topic

- ▶ Terminology
- ▶ Why not just testing?
- ▶ Numerical simulations around us
- ▶ Dig down CFD(Computational Fluid Dynamics)

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Definition of []

- ▶ Numerical Analysis

the study of algorithms that use numerical approximation for the problems of mathematical analysis



- ▶ Simulation

an approximate imitation of the operation of a process or system; that represents its operation over time

(often said as a training method)



- ▶ Numerical simulation

Calculation that is run on a computer following a program that implements a mathematical model for a physical system, whose models are too complex to provide analytical solutions.

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Why not just testing?

----In some case, you cannot test!!

For example... Testing

► Nuclear explosion

Dangerous, harmful

► Weather forecasting, earthquake

Too huge, you cannot make it happen

► Solar system

Too slow to observe

► Chemical reactions

Too fast and tiny to observe

With simulation...

Possible and safe

Calc whole earth

Fast forwarding

Close up and slow replay

Why not just testing? ----testing possible, but.....

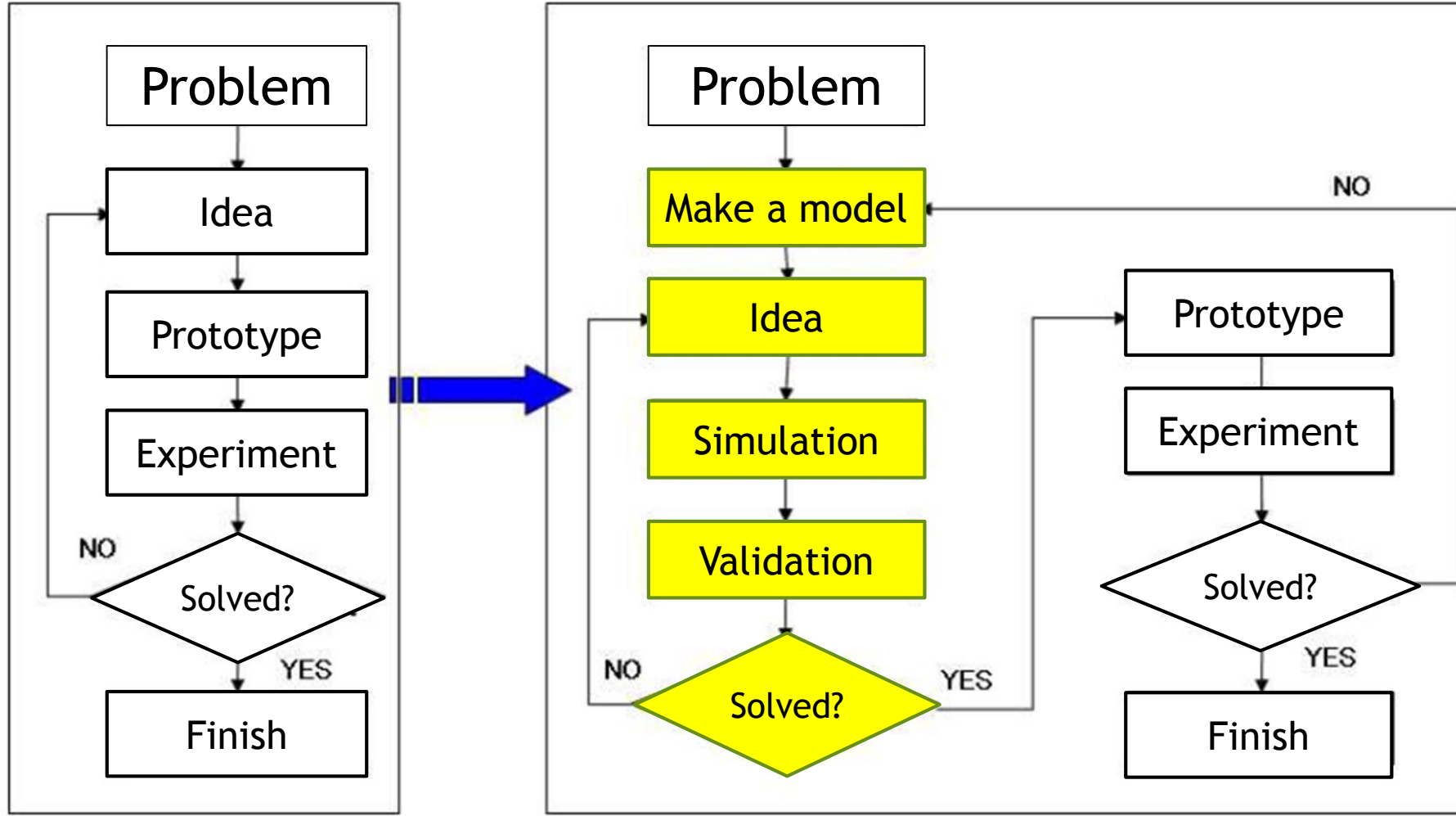
Case1: you wanna build a new car!

	Testing	Numerical Simulation
Costs	Material, Crafting, Expensive Apparatus,,,	Machine resource Software
Time	Build and analyze, again and again	Machine time (you can sleep)
Dangerousness	Flammables, Chemicals, Heavy stuff	No harm (You can sleep)
Reproducibility	Setting Environment costs a lot	Always you can control
Observability	Observation affects system Limited information	Full information of system



Numerical Simulation helps a lot!

Why not just testing?



Save your time and cost
by decreasing experiments

Today's topic

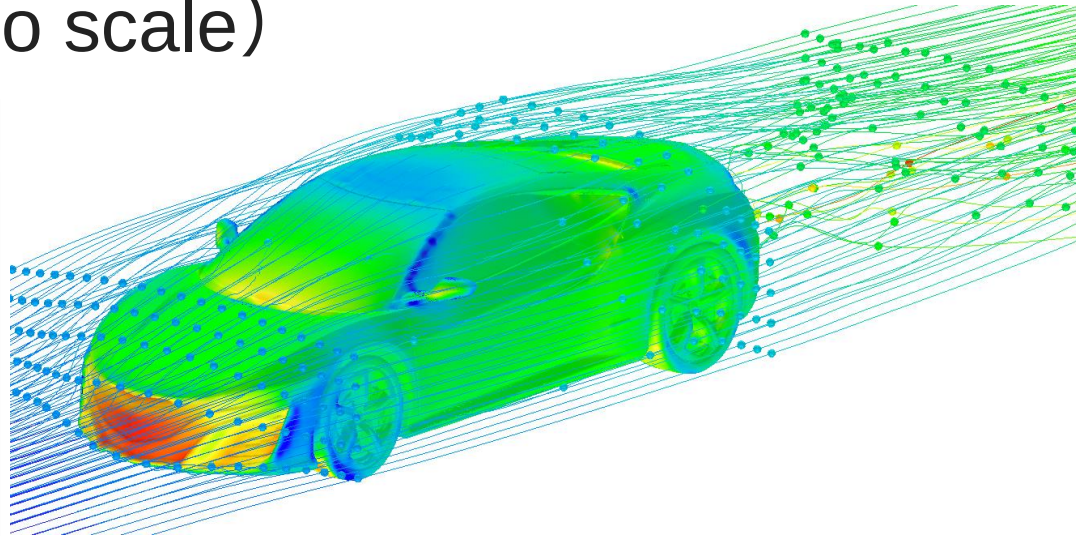
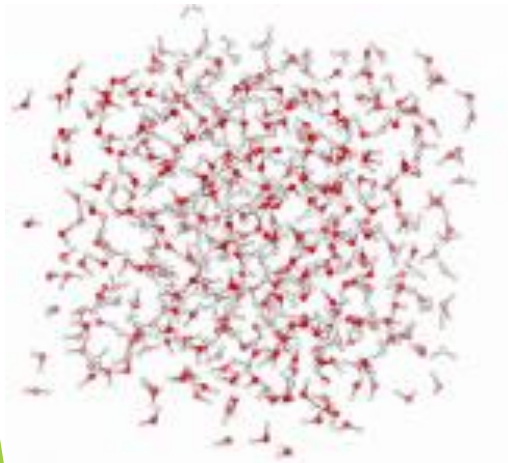
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Computer simulations are used in a wide variety of practical contexts, such as:

- analysis of [air pollutant](#) dispersion using [atmospheric dispersion modeling](#)
- design of complex systems such as [aircraft](#) and also [logistics](#) systems.
- design of [noise barriers](#) to effect roadway [noise mitigation](#)
- modeling of [application performance](#)^[14]
- [flight simulators](#) to train pilots
- [weather forecasting](#)
- simulation of other computers is [emulation](#).
- forecasting of prices on financial markets (for example [Adaptive Modeler](#))
- behavior of structures (such as buildings and industrial parts) under stress and other conditions
- design of industrial processes, such as chemical processing plants
- [strategic management](#) and [organizational studies](#)
- [reservoir simulation](#) for the petroleum engineering to model the subsurface reservoir
- process engineering simulation tools.
- [robot simulators](#) for the design of robots and robot control algorithms
- [urban simulation models](#) that simulate dynamic patterns of urban development and responses to urban land use and transportation policies. See a more detailed article on [Urban Environment Simulation](#).
- [traffic engineering](#) to plan or redesign parts of the street network from single junctions over cities to a national highway network to transportation system planning, design and operations. See a more detailed article on [Simulation in Transportation](#).
- modeling car crashes to test safety mechanisms in new vehicle models.
- [crop-soil systems](#) in agriculture, via dedicated software frameworks (e.g. [BioMA](#), OMS3, APSIM)

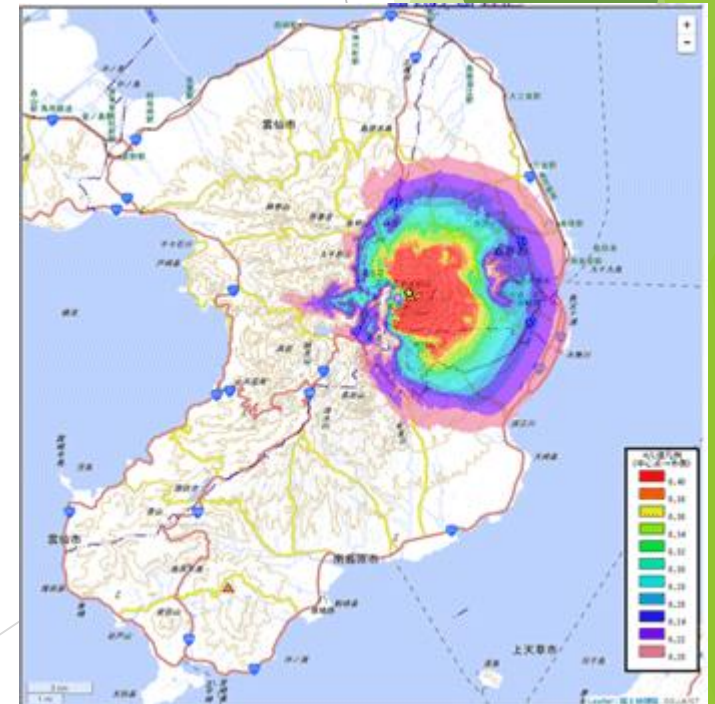
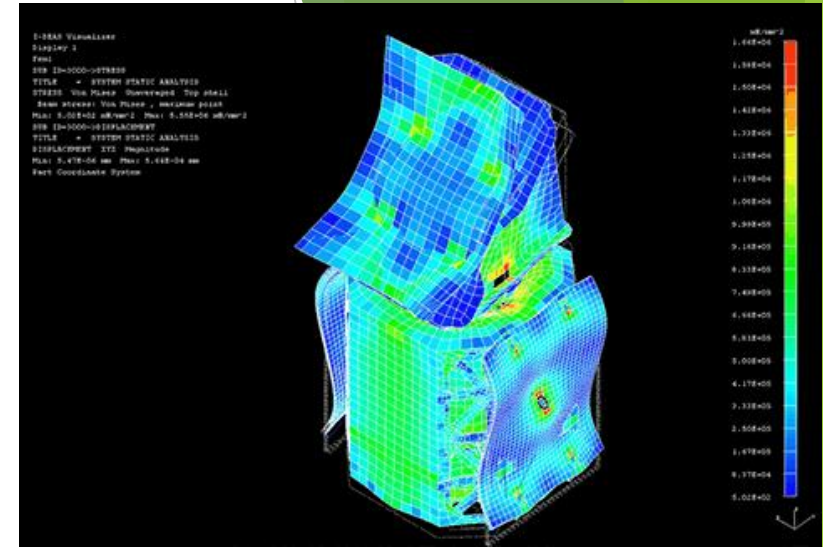
Numerical simulations around us (Examples)

- Deep understanding of known
(Natural Disaster)
- Optimization of scenario
(Decision, engineering processes)
- Prediction of unknown
(Weather, nano scale)



Almost anything...

Aero Space



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- ▶ Dig down CFD(Computational Fluid Dynamics)
How it works inside a computer. As an example.

Dig down CFD(Computational Fluid Dynamics)

► Computational Fluid Dynamics (CFD)

the simulation of fluids engineering systems using modeling and numerical methods

► Governing equation : Navier-Stokes

→a partial differential equation that describes the flow of viscous fluid substances.

The nonlinearity makes most problems difficult to solve analytically

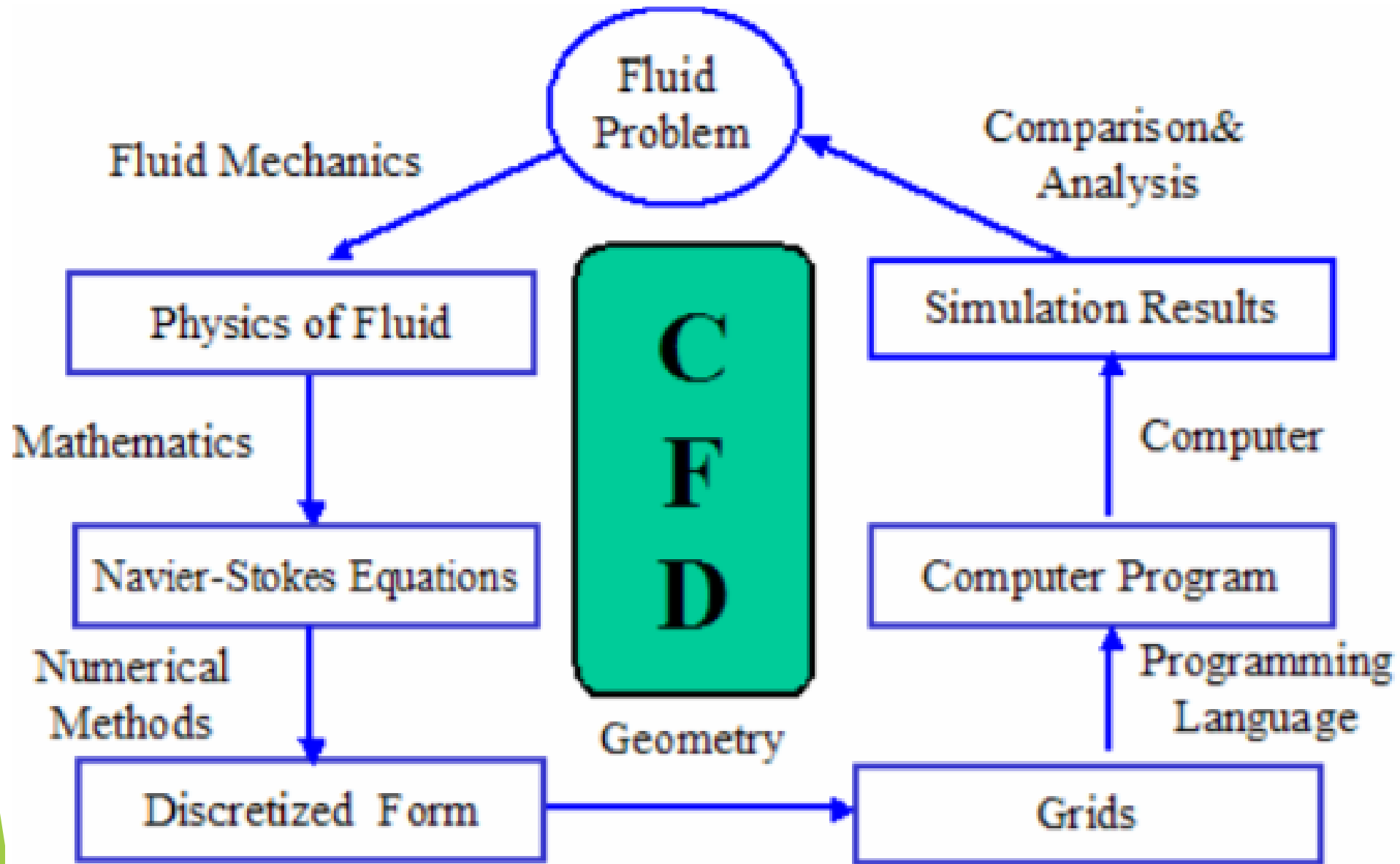
Navier-Stokes

$$\rho \frac{\partial \vec{v}}{\partial t} + \rho (\vec{v} \cdot \nabla) \vec{v} = -\nabla P + \vec{\gamma} \rho + \mu \nabla^2 \vec{v}$$

Diagram illustrating the Navier-Stokes equation with labels for its terms:

- Local Acceleration: $\rho \frac{\partial \vec{v}}{\partial t}$
- Convective Acceleration: $\rho (\vec{v} \cdot \nabla) \vec{v}$
- Pressure Gradient: $-\nabla P$
- Body force term: $\vec{\gamma} \rho$
- Viscous term: $\mu \nabla^2 \vec{v}$

Dig down CFD(Computational Fluid Dynamics)



Dig down CFD(Computational Fluid Dynamics)

Example

► Basic Equations

Divide calculation domain into tiny cells.

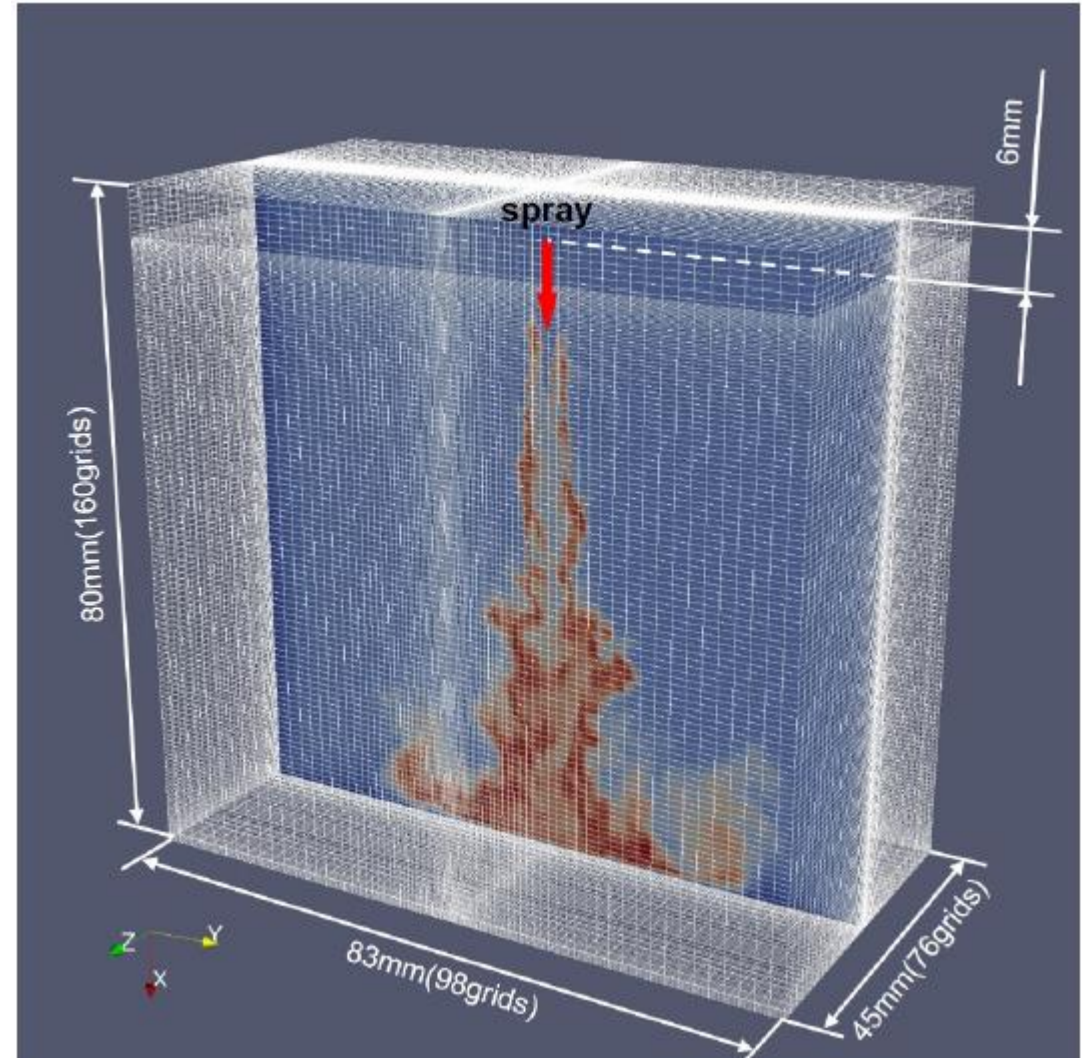
$$\frac{\partial \bar{\rho} V_f}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = \bar{\dot{\rho}}^s, \quad (1)$$

$$\frac{\partial \bar{\rho} \tilde{u}_i V_f}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_i \tilde{u}_j + \tau_{ij}^{SGS})}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \bar{F}_i^s, \quad (2)$$

$$\frac{\partial \bar{\rho} \tilde{f}_m V_f}{\partial t} + \frac{\partial (\bar{\rho} \tilde{f}_m \tilde{u}_j + j_{i,m}^{SGS})}{\partial x_j} = -\frac{\partial}{\partial x_j} \bar{j}_{j,m} + \bar{\omega}_m + \bar{\dot{\rho}}_m^s, \quad (3)$$

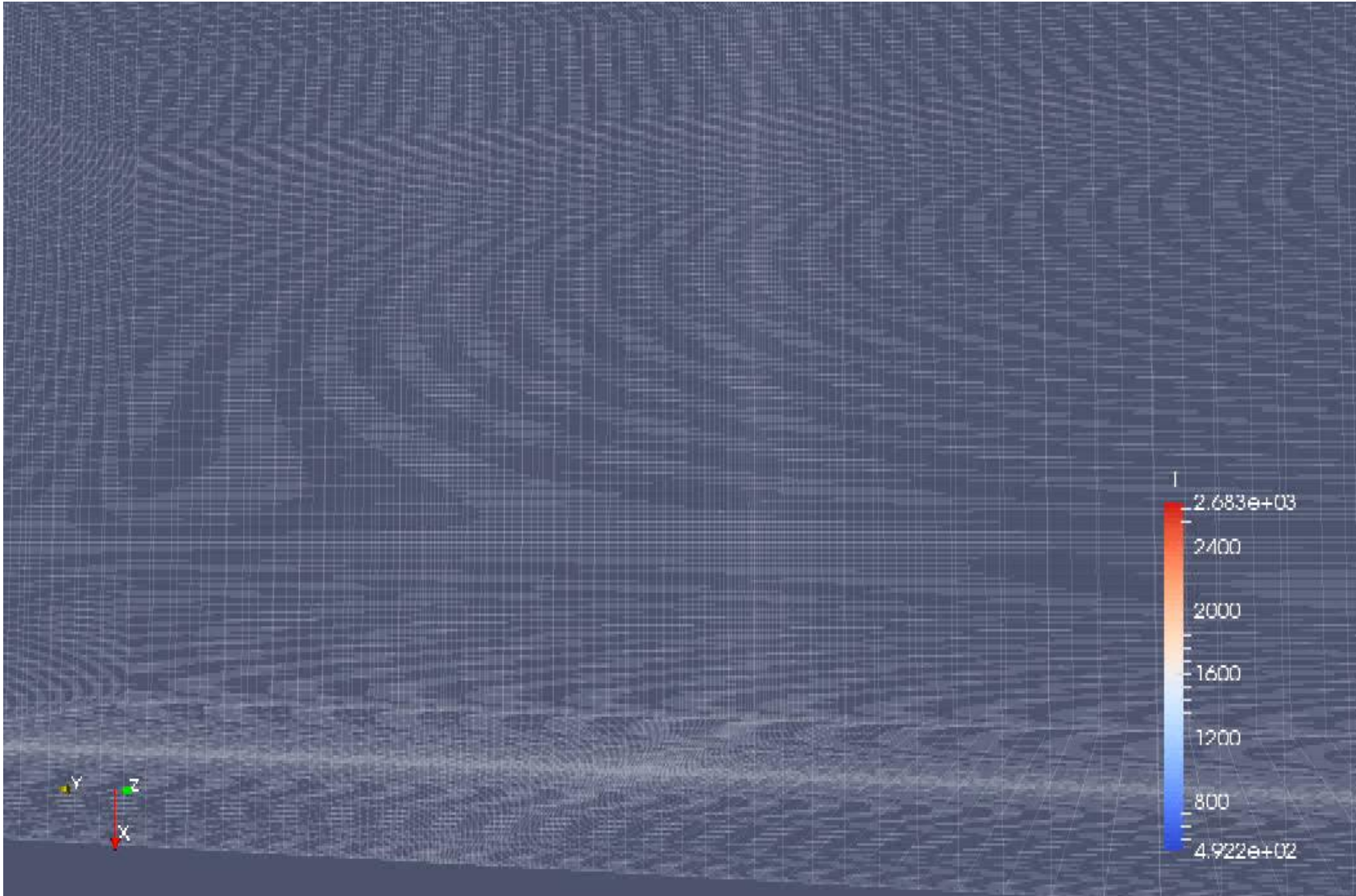
$$\frac{\partial \bar{\rho} \tilde{h} V_f}{\partial t} + \frac{\partial (\bar{\rho} \tilde{h} \tilde{u}_j + q_j^{SGS})}{\partial x_j} = -\frac{\partial p_0 V_f}{\partial t} - \frac{\partial}{\partial x_j} \bar{q}_j + \bar{\dot{Q}}^s, \quad (4)$$

About a half million cells



Dig down CFD(Computational Fluid Dynamics)

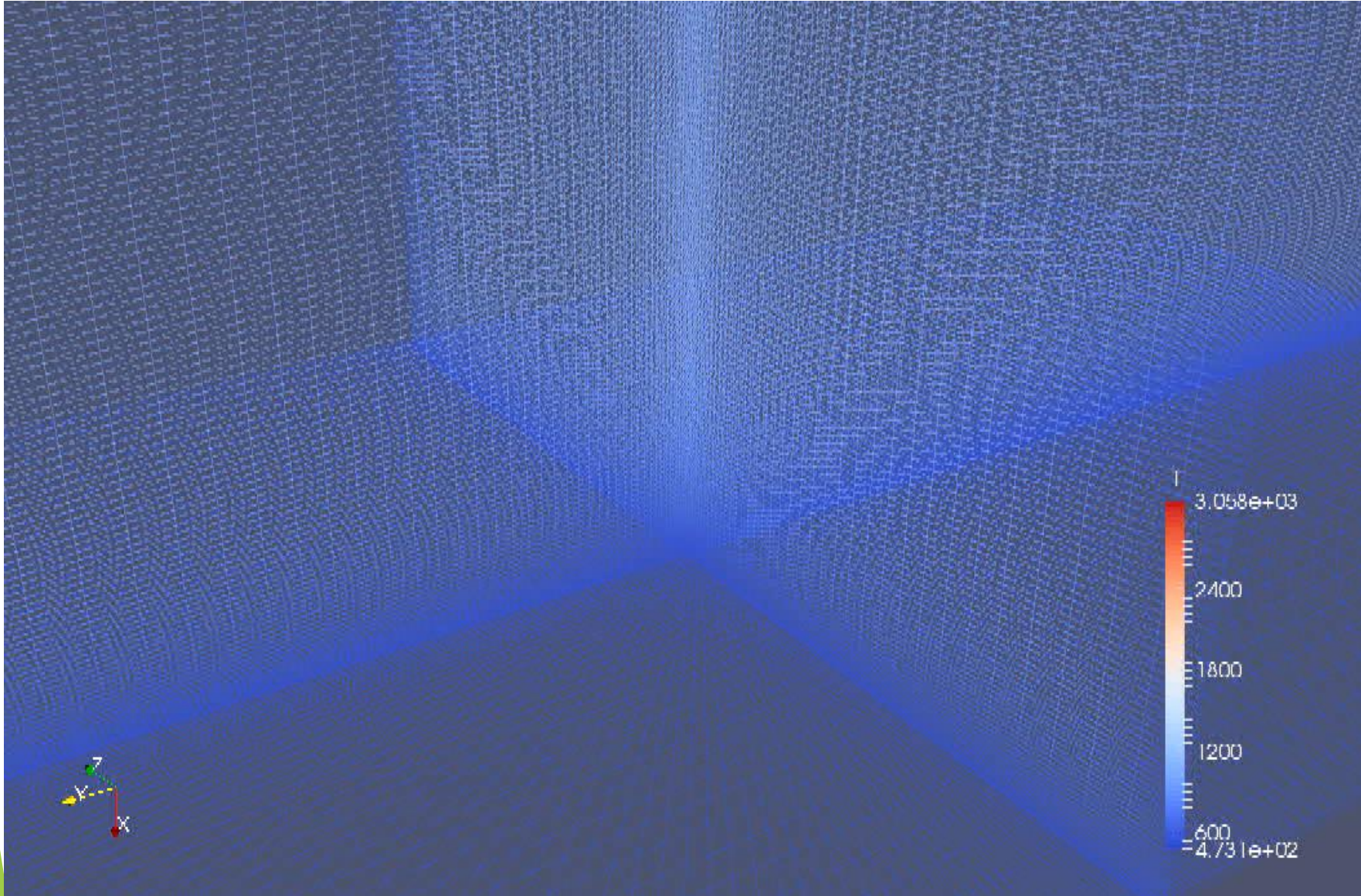
► Transient + Burning Flow



It took 6days
to calc
4ms combustion
With
Xeon 20 cores
workstation

Dig down CFD(Computational Fluid Dynamics)

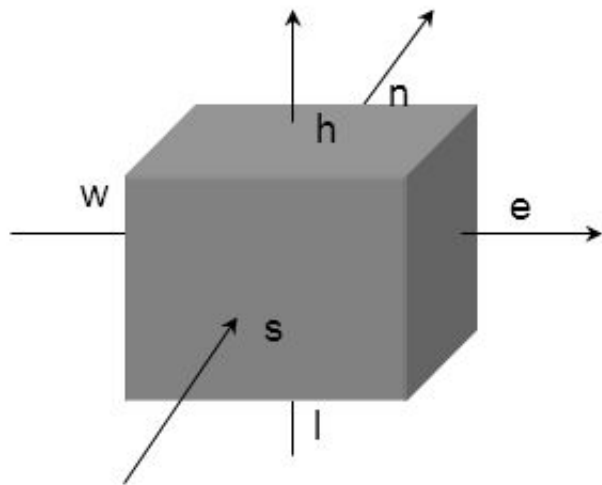
► Transient + Burning Flow



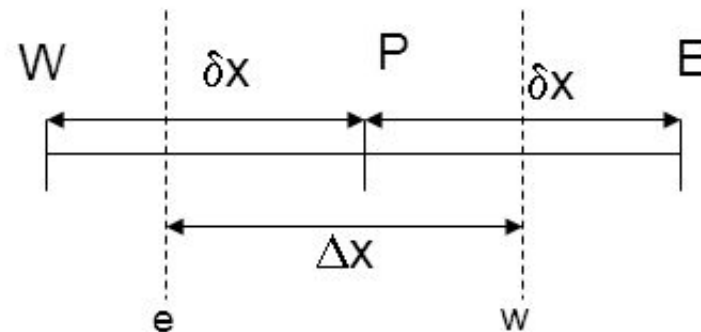
Finite Volume Method (Discretization)

- Conservation of ϕ for the finite volume

Divide the whole computation domain into sub-domains



One dimension:



Must Include some error

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

- Finite volume is a *fixed* space in the flow domain with imaginary boundaries that allow the fluid to flow in and out.
- Integral conservation of the quantities such as mass, momentum and energy.



Dig down CFD(Computatio

Example

► Basic Equations

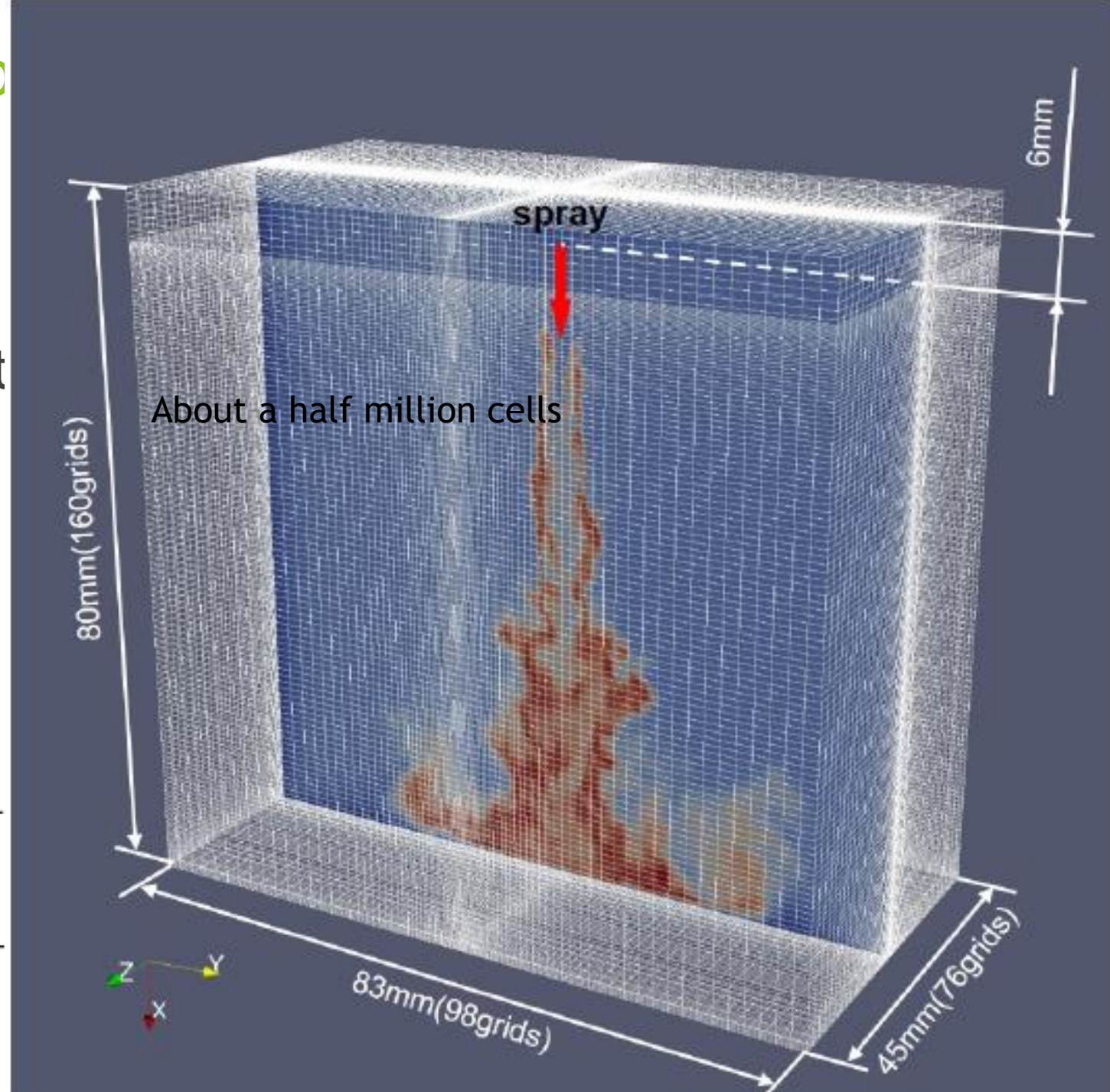
Divide calculation domain into cells.

$$\frac{\partial \bar{\rho} V_f}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = \bar{\dot{\rho}}^s,$$

$$\frac{\partial \bar{\rho} \tilde{u}_i V_f}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_i \tilde{u}_j + \tau_{ij}^{SGS})}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \bar{F}_i^s,$$

$$\frac{\partial \bar{\rho} \tilde{f}_m V_f}{\partial t} + \frac{\partial (\bar{\rho} \tilde{f}_m \tilde{u}_j + j_{i,m}^{SGS})}{\partial x_j} = -\frac{\partial}{\partial x_j} \bar{j}_{j,m} + \bar{\omega}_m +$$

$$\frac{\partial \bar{\rho} \tilde{h} V_f}{\partial t} + \frac{\partial (\bar{\rho} \tilde{h} \tilde{u}_j + q_j^{SGS})}{\partial x_j} = -\frac{\partial p_0 V_f}{\partial t} - \frac{\partial}{\partial x_j} \bar{q}_j +$$



3D problem

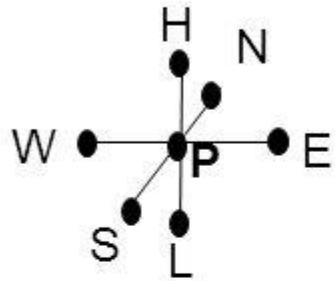
Navier-Stokes

$$\rho \left[\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} u + \frac{\partial u}{\partial y} v + \frac{\partial u}{\partial z} w \right] = -\frac{\partial p}{\partial x} + \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + \rho g_x$$

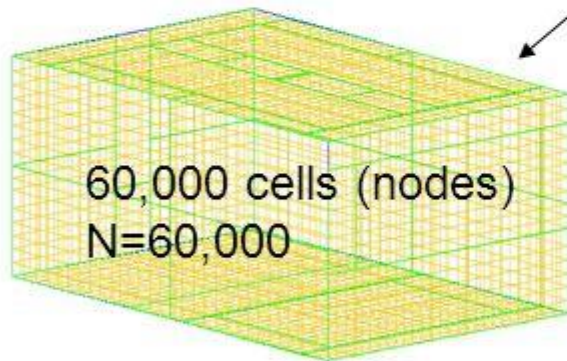
Equation in the general format:

$$a_P \Phi_P + a_E \Phi_E + a_W \Phi_W + a_S \Phi_S + a_N \Phi_N + a_H \Phi_H + a_L \Phi_L = f$$

Discretization



Write this equation for each discretization volume of your discretization domain



7-diagonal matrix

This is the system for only one variable (Φ)

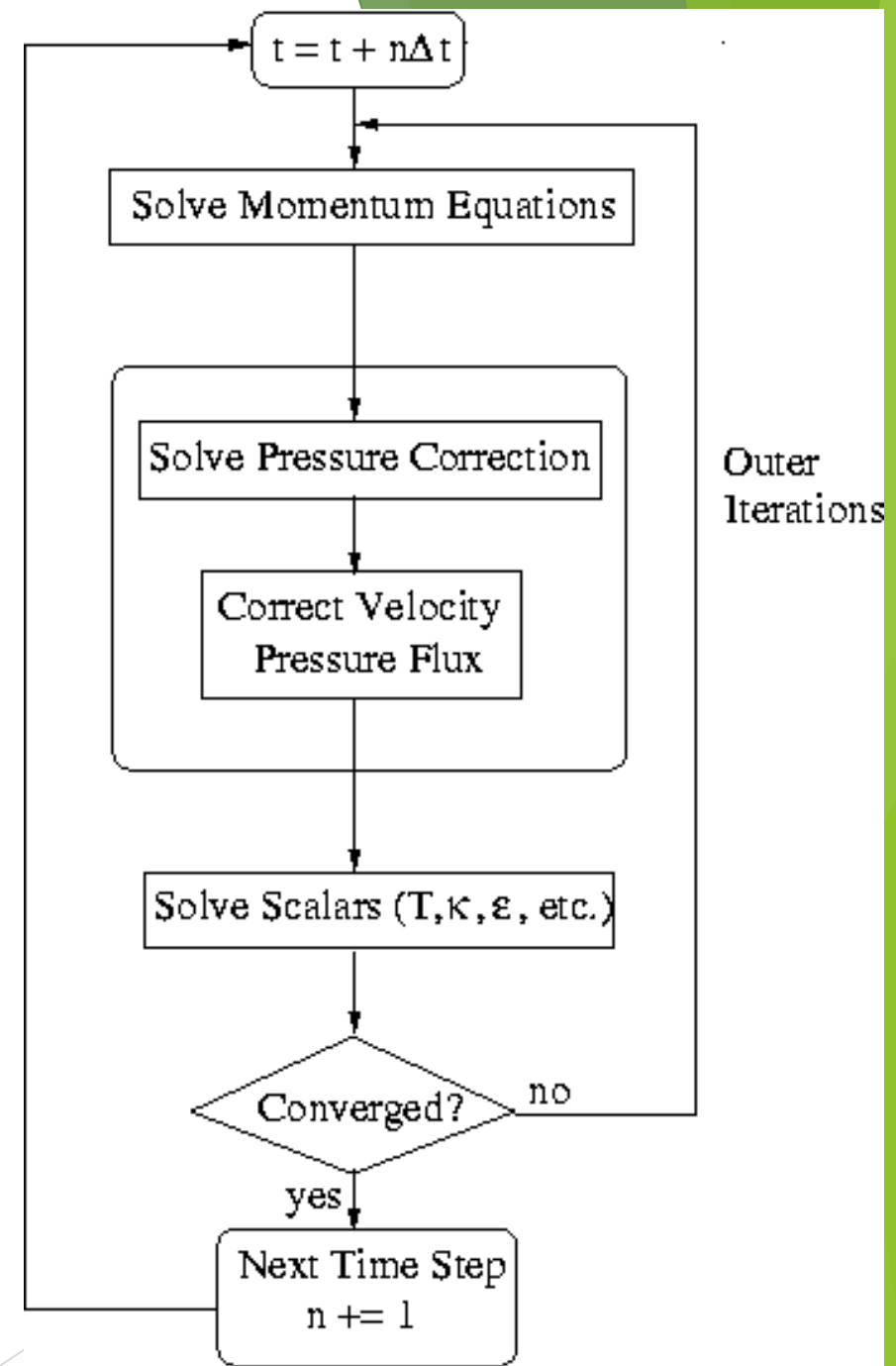
$$\begin{matrix} \xrightarrow{A} \\ \text{60,000 elements} \end{matrix} \quad \begin{matrix} \Phi \\ \times \end{matrix} = \begin{matrix} F \end{matrix}$$

Just use Matrix-Solver

CFD Flow

- Give initial condition.
- Solve conservation equation of all the cells.
- Check if its converged, if not, do it again
- If its converged (or if we get small enough error), go to next time step.
- Use last time variables as an initial condition.

$$N = \left[O \left(\frac{L}{l} \right) \right]^3 = O(Re^{9/4})$$



Summary

- ▶ All [numerical simulation] has its [mathematical model] .
- ▶ Numerical simulation is regarded as important as testing.
you must know how it works.
- ▶ There's always a certain range of error in calculation.
But experiment has also....
- ▶ Because of improvement of calc power, nowadays
complex NS is possible with low time cost.
It makes development faster!!

Thank you Any Question??