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Evolution In High Performance Computing And Its Effects On Extreme-Scale Simulations

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Thursday, September 12 at 15:30

Introduction

There are many factors that constrain the performance of the applications of HPC systems when going to large core count, both within the compute node and across the whole system. Major simulations require a lot of computing time: from days to even weeks but only a few (maybe) hours are needed on a supercomputer.

Rapid progress in high performance computing enables us to investigate deep into the behavior of natural phenomenon of physics. e.g.

1. Complex flow in CFD(complex flow simulation enabled the researchers to model complex jet engine environments which cannot be observed firsthand, using one million compute cores),
2. Turbulent flow analysis (20 percent of world energy consumption is traceable by turbulent flow analysis and the energy it dissipates),
3. Neural-network simulation (A neural network simulation of 1.73 billion nerve cells connected by 10.4 trillion synapses was performed, which is only 1 percent of the neuronal network in the brain.) etc.

Every architecture has a certain significance, depending on its size, speed, and scale.
The future is bright for HPC's but challenges loom as we go from Peta-Flops to Exa-Flops even Zeta-Flops.
How do we program for $10^{8\text{-}10}$ cores, especially if the cores are different?

Most of the scientific communities prefer Green computers .
Some economically efficient HPC's provide highest efficiency in performance with the lowest energy consumption..
The supercomputer SANAM redefines power-efficiency, securing the 4th rank in the global Green500™ List, as well as 52nd on the Top500 Super Computer List in June 2013.

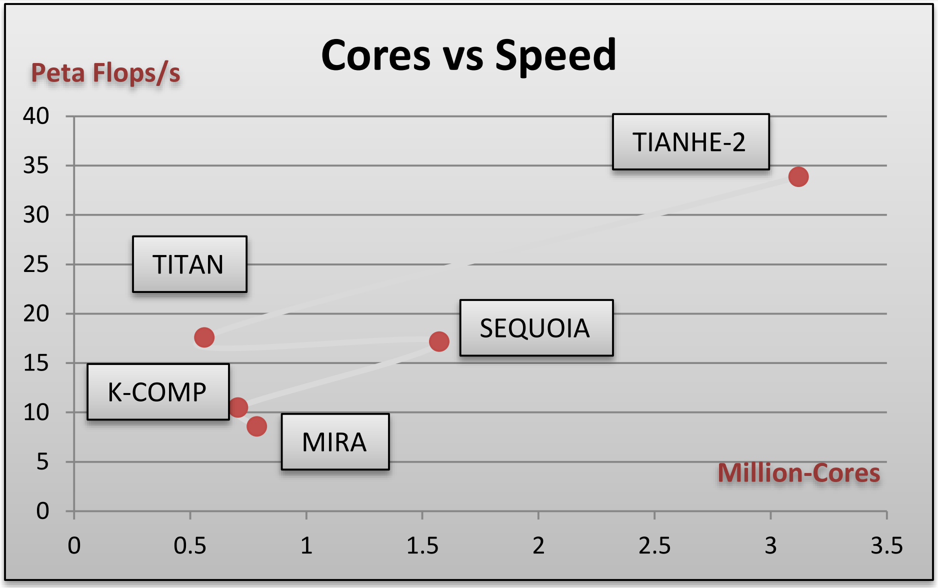
Examples of World's HPC Centers

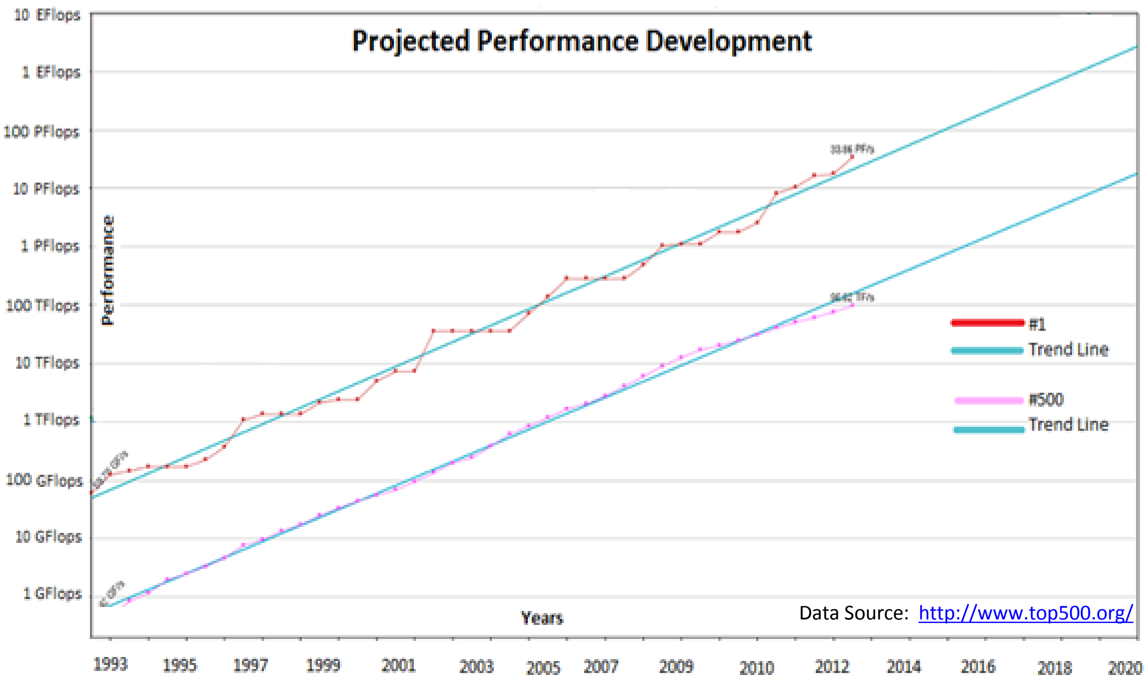
1. Tianhe-2 (China)

Location: National University of Defense Technology
Speed : 33.9 petaflops
Application areas: Airplanes, processing "big data," and aiding in government security.

2. Titan (CRAY-USA)

Location: Oak Ridge National Laboratory
Speed: 17.6 petaflops
Application areas: Climate change, bio fuels and nuclear energy.





3. Sequoia (IBM-USA)

Location: DOE's Lawrence Livermore National Laboratory
Speed: 17.17 petaflop/s
Application Areas: Life sciences, public safety and transportation.

4. K computer (Fujitsu-Japan)

Location: RIKEN Advanced Institute for Computational Science (AICS)
Speed: 10.51 Pflop/s
Application areas: energy ,healthcare , climate change , industries and space.

5. Mira (IBM-USA)

Location: Argonne National Laboratory
Speed: 8.59 petaflop/s
Application areas: Exploding stars, nuclear energy, climate change, and jet engines.

Data Source: http://www.top500.org

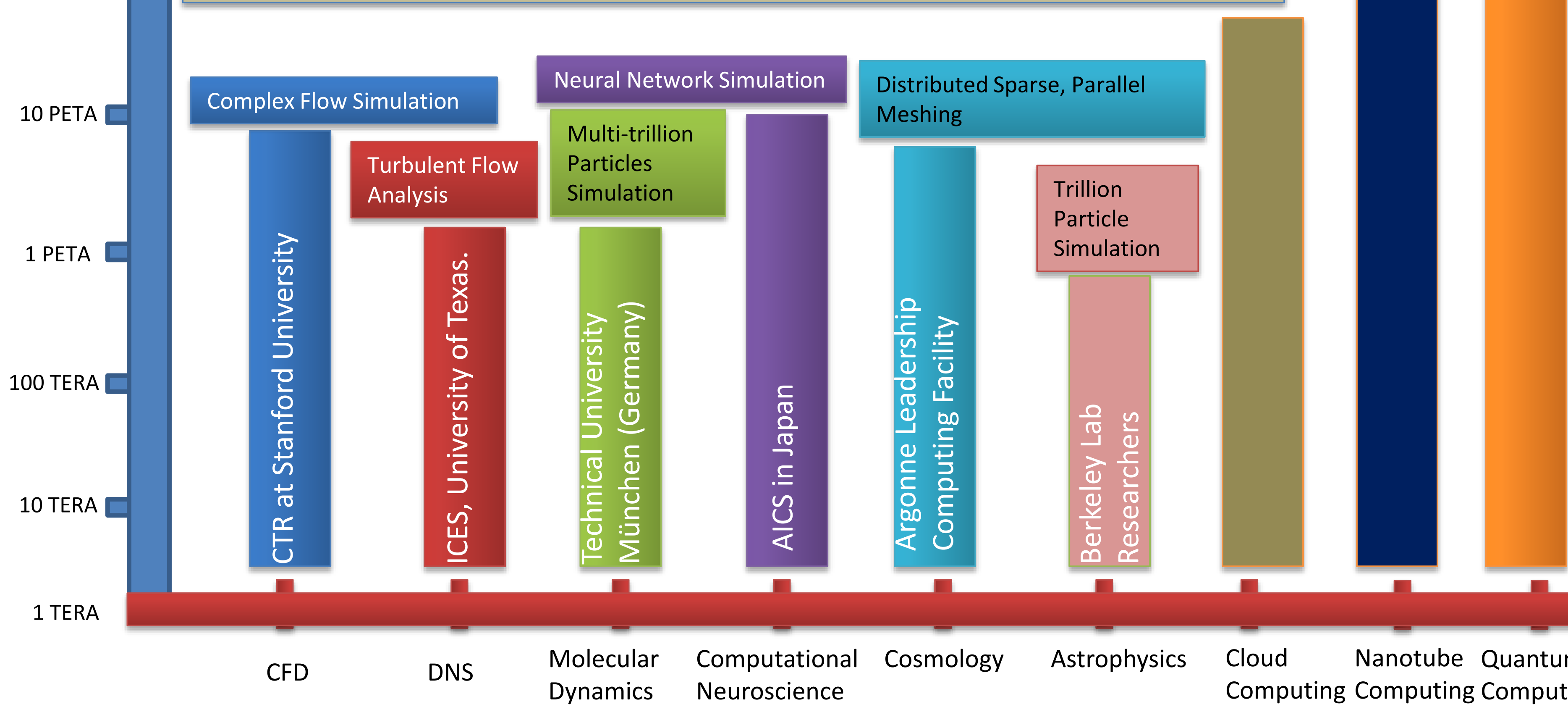
Extreme-Scale Computing

Extreme-Scale Computing acts as a scientific and technological driver enabling science through simulations in the Peta-scale performance range and beyond at unprecedented size and fidelity

Quantum Computing: Through quantum computing/computers we can solve a polynomial of 10^{24} within sec.[1]

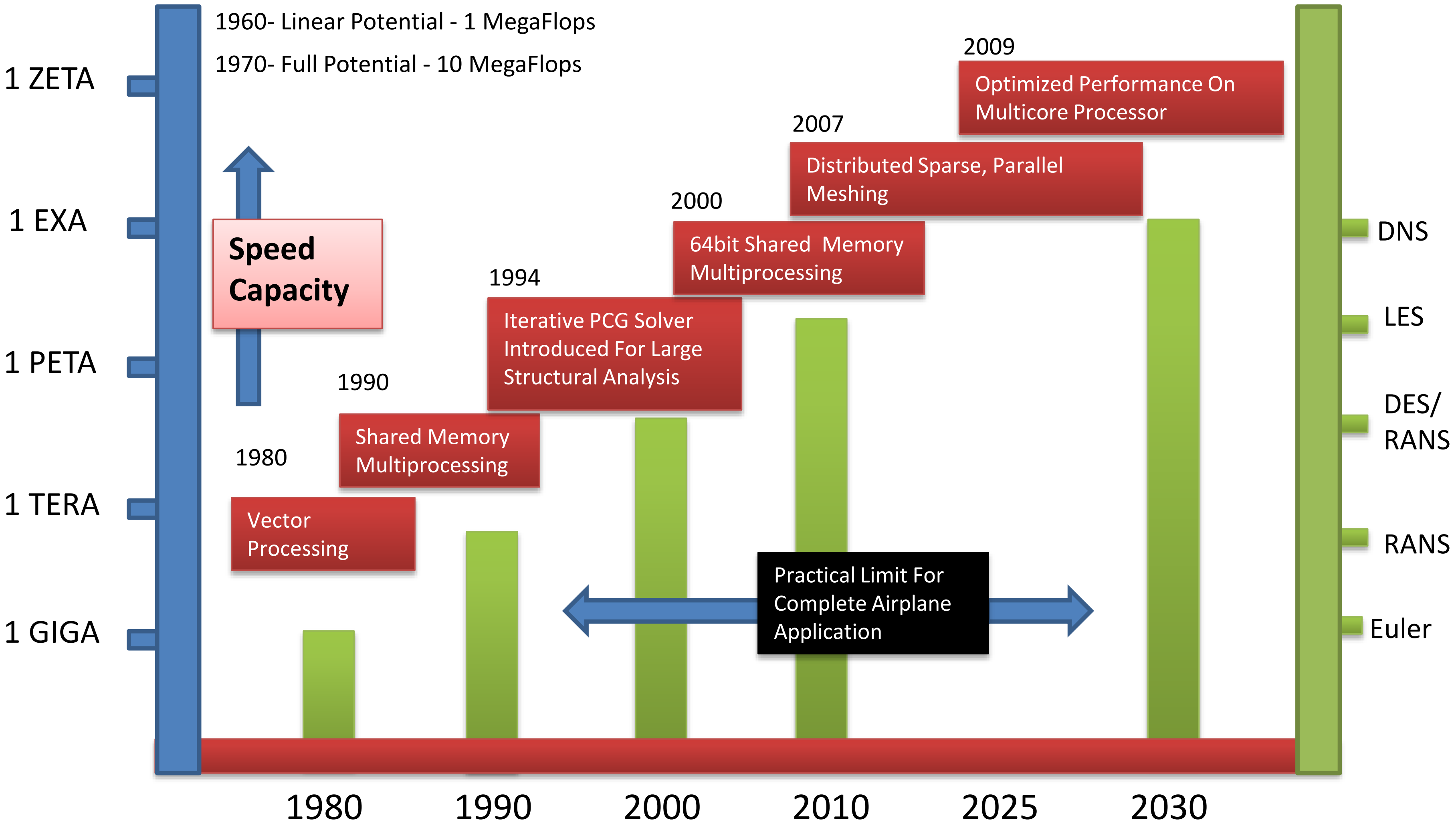
Nanotube Computing: Current circuit elements are 45nm wide, and the next-generation technology will be 32nm.It would efficiently make chips crammed with millions of transistors .[1]

Cloud computing can be considered as a step towards extreme computing as delivery of a service which may be an infrastructure, platform or software rather than a product.[1]



[1] - Data Source: Wikipedia.org

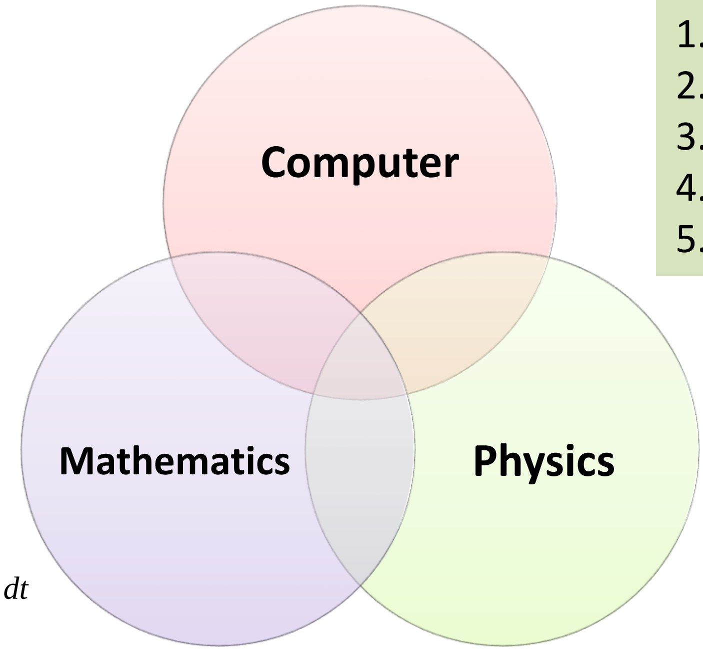
Increasing Computational Complexity, Decreasing Experiment



How HPC fits into CFD?

C++, Fortran, MPI / OpenMP
Opengl, Cuda,Parallel Libraries
And more

1. Linear Algebra
2. Numerical Methods
3. Discretization
4. Meshing Methods



1. Navier-Stokes Equations
2. Euler Equations
3. Large Eddy Simulation
4. Linear and Full Potential
5. And more

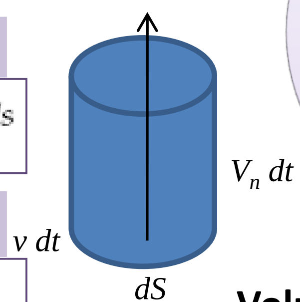
Constitutive Equations

$$F(p, \rho, \theta) = 0$$
$$T = (\mathrm{tr}(D)\lambda - p)\, I + 2\mu D$$
$$\vec{q} = -k \vec{\nabla} \theta$$
$$u = u(\theta, \rho)$$

$$\tau = \mu \frac{\partial u}{\partial y},$$

Stokes theorem:

$$\int_S \mathbf{n}.(\nabla \times \mathbf{v}) dS = \int_C \mathbf{t}.\mathbf{v} ds$$



Green's theorem

$$\int_S f n_i dS = \int_V \frac{\partial f}{\partial x_i} dV$$

Divergence theorem

$$\int_S v_i n_i dS = \int_V \frac{\partial v_i}{\partial x_i} dV,$$
$$\int_S \mathbf{v}.\mathbf{n} dS = \int_V \nabla.\mathbf{v} dV,$$
$$\int_S \mathbf{n} \times \mathbf{v} dS = \int_V \nabla \times \mathbf{v} dV,$$

Volume Flux $\int_S \mathbf{v}.\mathbf{n} dS = \int_S v_j n_j dS$

Mass Flux $\int_S \rho \mathbf{v}.\mathbf{n} dS = \int_S \rho v_j n_j dS$

Momentum Flux $\int_S \rho \mathbf{v}(\mathbf{v}.\mathbf{n}) dS = \mathbf{i}_k \int_S \rho v_k v_j n_j dS$

Kinetic Energy Flux $\int_S \frac{1}{2} \rho v^2 (\mathbf{v}.\mathbf{n}) dS = \int_S \frac{1}{2} \rho v_i v_i v_j n_j dS$

Drag Equation

$$D = \frac{1}{2} c_d \rho A v^2$$

Ideal Gas Law

$$pV = nRT$$

Sutherlands Law

$$\mu = \mu_{ref} \left(\frac{T}{T_{ref}} \right)^{3/2} \frac{T_{ref} + S}{T + S}$$

Computational Fluid Dynamics

1. Fluid flows are governed by partial differential equations which represent conservation laws for the mass, momentum, and energy.
2. CFD is the simulation of fluid engineering applications, using modeling and numerical methods (CAD, Pre processing, discretization, solvers, numerical parameters, and grid generations, post processing etc.)

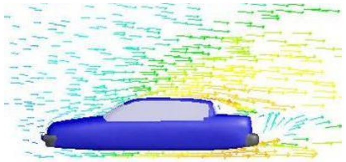
Governing Equations of CFD

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho u_j\right] = 0$$

Momentum equations:

$$\frac{\partial}{\partial t}\left(\rho u_i\right) + \frac{\partial}{\partial x_j}\left[\rho u_i u_j + p\delta_{ij} - \tau_{ji}\right] = 0,$$



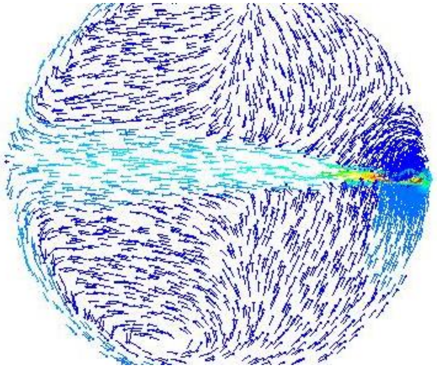
Energy equation:

$$\frac{\partial}{\partial t}\left(\rho e_0\right) + \frac{\partial}{\partial x_j}\left[\rho u_j e_0 + u_j p + q_j - u_i \tau_{ij}\right] = 0$$

Applications and Examples of CFD

1. Full scale simulations (airplanes, automotives etc)
2. Simulate of physical fluid phenomena that are difficult for experiments
3. More cost effective and more rapid than EFD (Explicit Formula Database)
4. High-fidelity database for diagnosing flow field
5. Environmental effects (oil, wind, weather, etc)
6. Hazards (Explosions, radiation, pollution etc)

Simulation



CFD Simulation Phases

Governing Partial Differential Equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}[\rho u_j] = 0$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}[\rho u_i u_j + p\delta_{ij} - \tau_{ji}] = 0,$$

$$\frac{\partial}{\partial t}(\rho e_0) + \frac{\partial}{\partial x_j}[\rho u_j e_0 + u_j p + q_j - u_i \tau_{ij}] = 0$$

Discretization

- ✓ **The finite volume method has the broadest applicability (~80%)**
- ✓ **Finite element (~15%)**
- ✓ **There are certainly many other approaches (5%), including:**

Finite difference, Spectral methods,
Boundary element. Vorticity based methods, Lattice gas/lattice Boltzmann, Smooth Particle Hydrodynamics
And more!

System Of Algebraic Equations

Upwind Scheme

$$\mathrm{Pe}\,\frac{u_i - u_{i-1}}{\Delta x} - \frac{u_{i-1} - 2u_i + u_{i+1}}{(\Delta x)^2}$$

Central Scheme

$$\mathrm{Pe}\,\frac{u_{i+1} - u_{i-1}}{2\Delta x} - \frac{u_{i-1} - 2u_i + u_{i+1}}{(\Delta x)^2} = 0$$

FD - Scheme

$$T_j^{n+1} \models T_j^n + \frac{\alpha \delta t}{(\delta x)^2}\left(T_{j-1}^n - 2T_j^n + T_{j+1}^n\right)$$

All discretization Schemes lead to:

Linear system $\boxed{Au = F}$ $A \in \mathbb{R}^{N-1 \times N-1}$ $u, F \in \mathbb{R}^{N-1}$

$$A = \frac{1}{(\Delta x)^2}\begin{bmatrix} b & c & & & \\ a & b & c & & \\ & a & b & c & \\ & & & \dots & \\ & & & a & b \end{bmatrix} u = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ . \\ u_{N-1} \end{bmatrix} F = \begin{bmatrix} 0 \\ 0 \\ 0 \\ . \\ -\frac{c}{(\Delta x)^2} \end{bmatrix}$$

Stability

- ▪Ability of a discretization to produce approximations
- ▪If a solution is stable = It does not magnify the errors

➢Temporal problem - bounded solution
➢Iterative problem - solution does not diverge

- **Gaussian Elimination Techniques**
  - ✓Gaussian Elimination Method
  - ✓Gaussian Elimination Method with partial pivoting
  - ✓Gauss-Jordan Method
- **Lu Factorization Method**
  - ✓Cholesky Method
  - ✓Thomas Algorithm
- **Iterative Methods**

Jacobi Method, Gauss-Seidle method , SOR-Method, UR-Method

Approximate Solution

CPU	Decimal Places
32Bit	16 Approx
64Bit	34 Approx
128Bit	72 Approx

Single Precision Method gives 7 decimal places
Double Precision method gives 16 decimal places
Convergence Criteria : E^-4 / E^-5

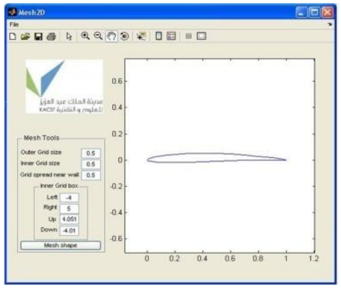
Convergence

Exact Solution!!

p,u, v, w, mach,ρ, α, η, etc.

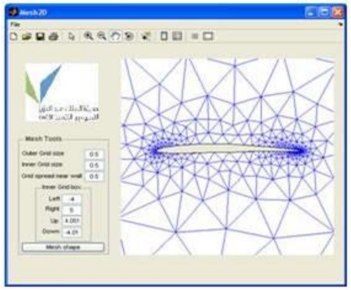
When do we need a Mesh?

A mesh is needed when, We want to solve a given problem on a computer using a method which requires a discrete representation of the domain



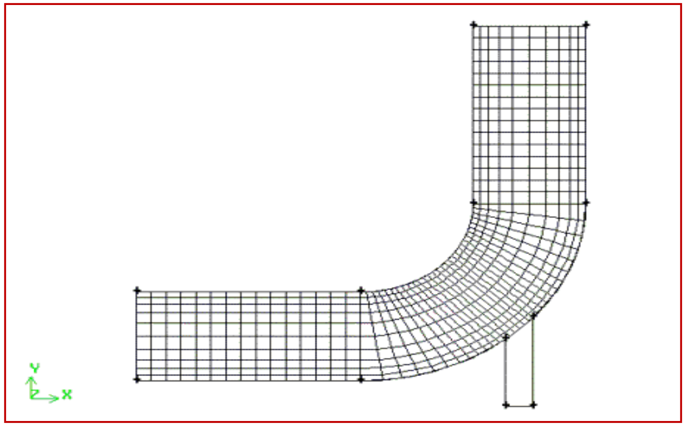
What defines a Mesh?

- A mesh is defined as a discrete representation Ω_h of some spatial domain Ω
- A domain can be subdivided into ‘K’ smaller non-overlapping closed sub domains. Ω_h^k.
- The mesh is the union of such sub domains $\Omega_h = \bigcup_{k=1}^{K} \Omega_h^k$



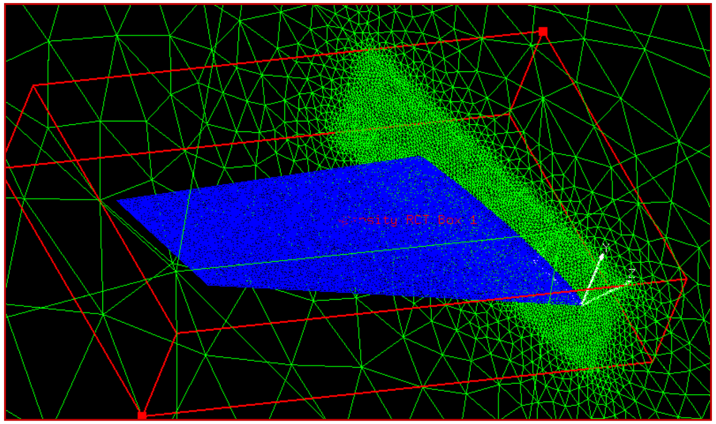
Structured Meshes

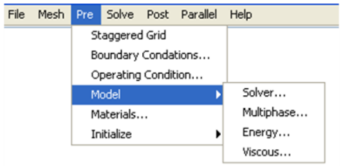
Requires geometry to conform to specific characteristics

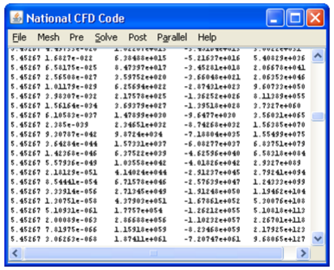


Unstructured Meshes

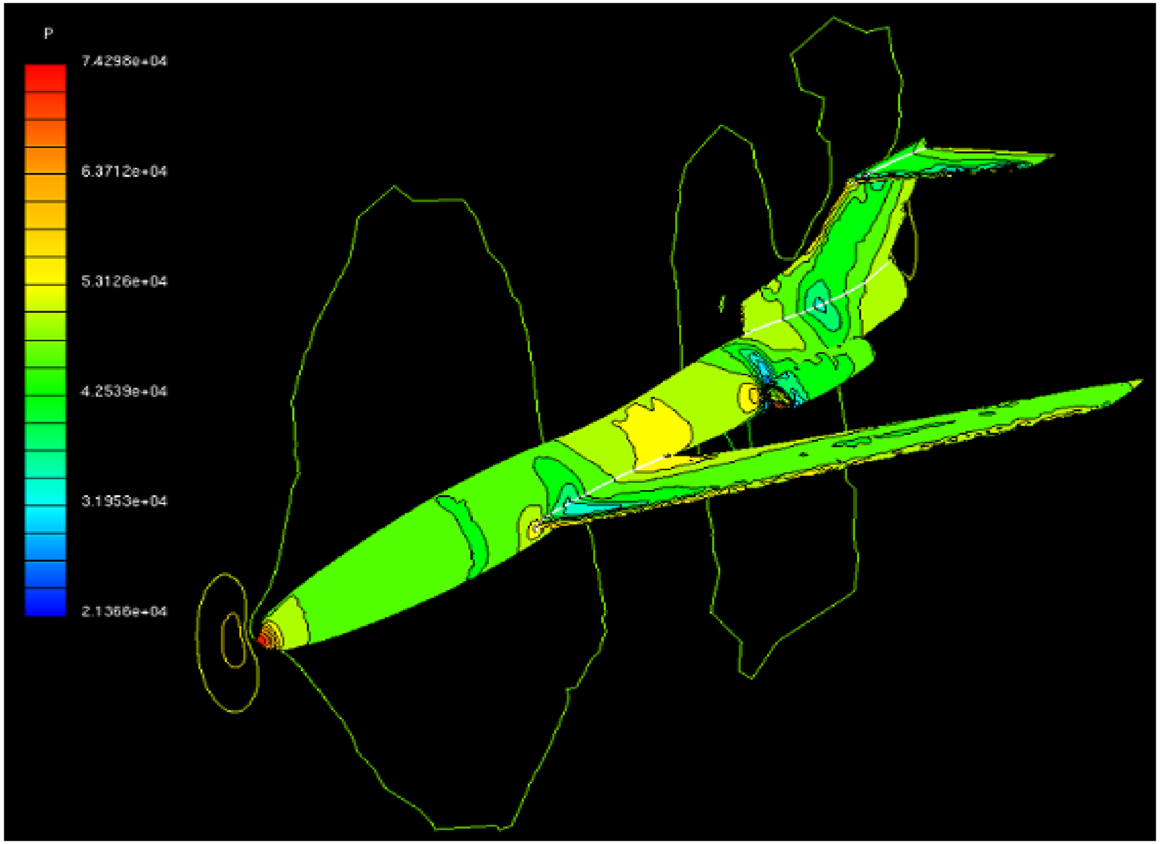
No specific requirements for geometry







Application Of CFD



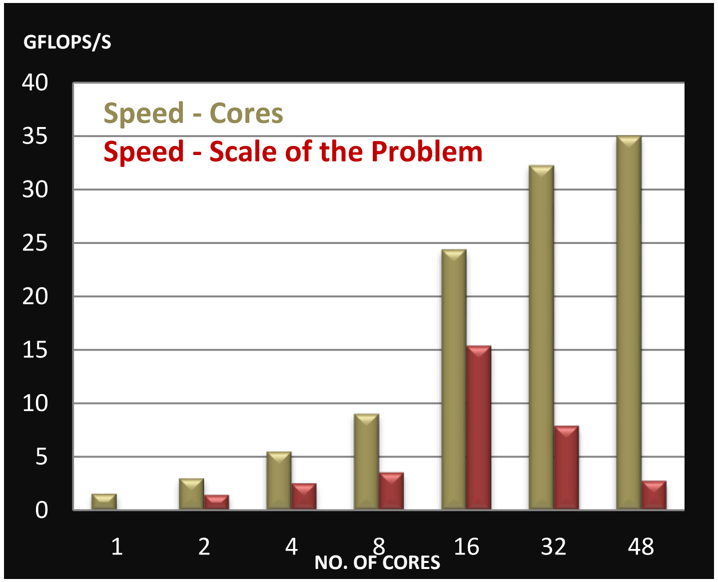
Airplane Transonic Study

Free Stream Flow Conditions

- Free Stream Mach Number = 0.90
- Chords Reynolds number = 5 million
- Angle of Attack = 4^0
- Reference Temperature = 310.92 k

Solver Setup

- Steady state, Density based
- Sparat – Allmaras

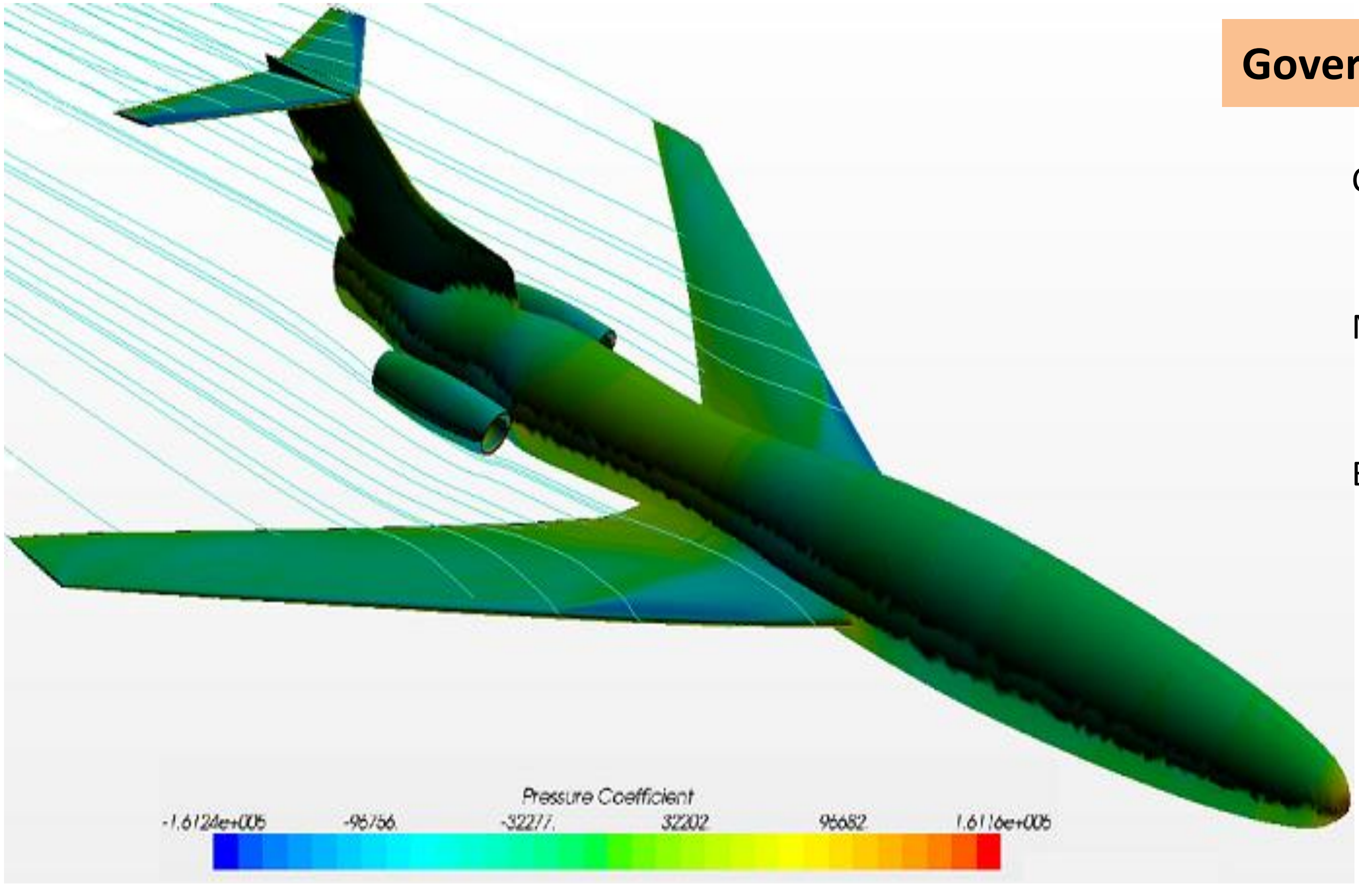


Grid Generation

- Unstructured Tetrahedral and Prism Mesh
- 6,405,679 mixed cells
- Increased number of cells around wing body to capture boundary layer effects

Application Of CFD

- In CFD the prediction of aerodynamic drag is a big challenge.
- The accuracy in drag prediction is highly dependent on the mesh resolution.
- In order to meet the computational requirement for solution of such problems the role of HPC is vital.
- The research is still in progress on common grid study for more accurate predictions of drag which highly depends on the grid refinement .



Governing Equations of CFD

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Energy equation:

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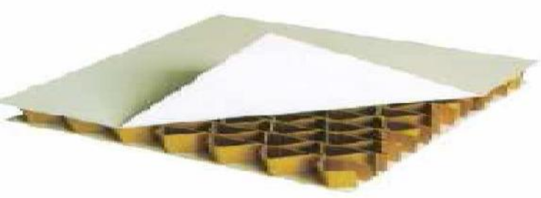
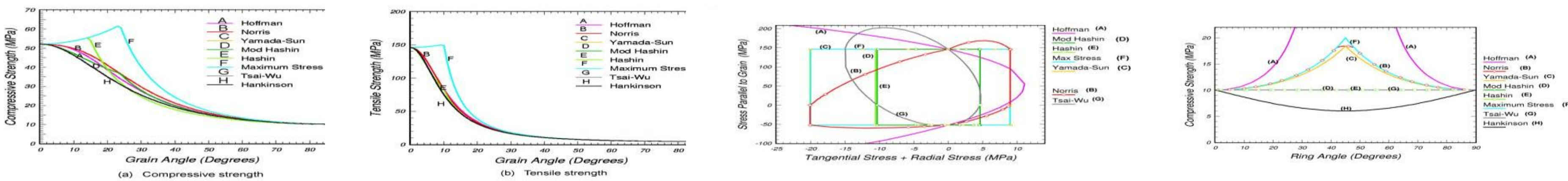
Airframe Design FEM-FSI

Composites - Strength verification



airframe design in composite carbon and glass fibers materials. Composite sandwich panels are characterized by high stiffness and low weight. Composites are transversely isotropic materials with distinct failure modes in the parallel (fiber) and perpendicular (transverse fiber) directions.

Numerous failure criteria are available for modeling the yield strength of composite materials. Below is the comparison of various failure modes.

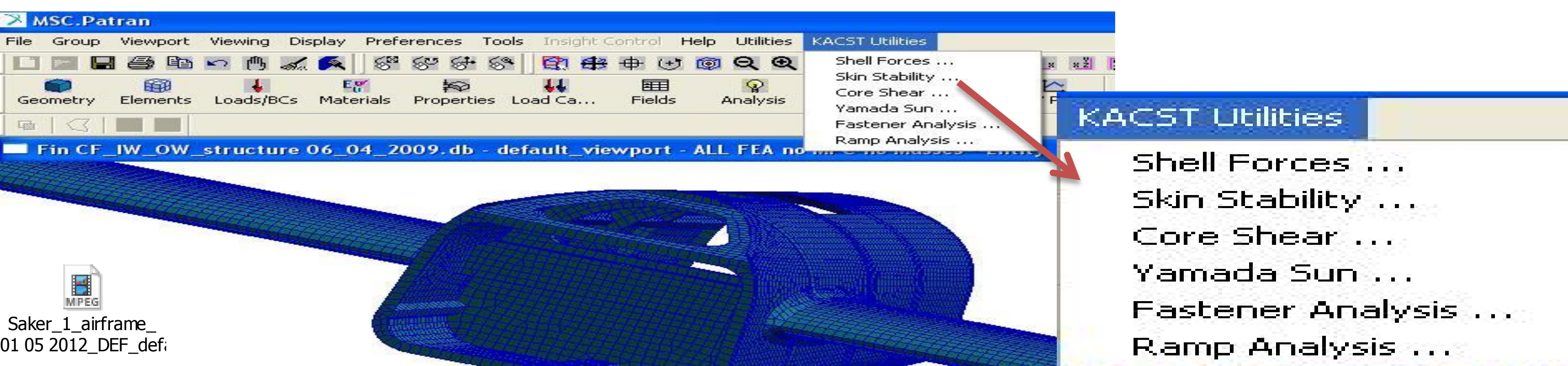


The program utilizes the Yamada – Sun failure criteria

This criterion predicts that the normal and shear stresses are mutually weakening (the presence of shear stress reduces the strength below that measured in uniaxial stress).

$$\frac{\sigma_{11}^2}{X^2} + \frac{\sigma_{12}^2}{S^2} \geq 1$$

KACST Utilities program was developed in-house in order to calculate Reserve Factors (RF) for Yamada – Sun failure criteria . The program is directly imbedded in PATRAN software and directly interfaced with NASTRAN Finite Element Analyses results.



Airframe Design FEM-FSI

CFD Optimization KACST Light Helicopter

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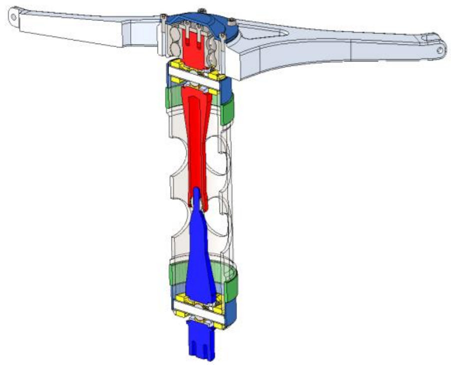
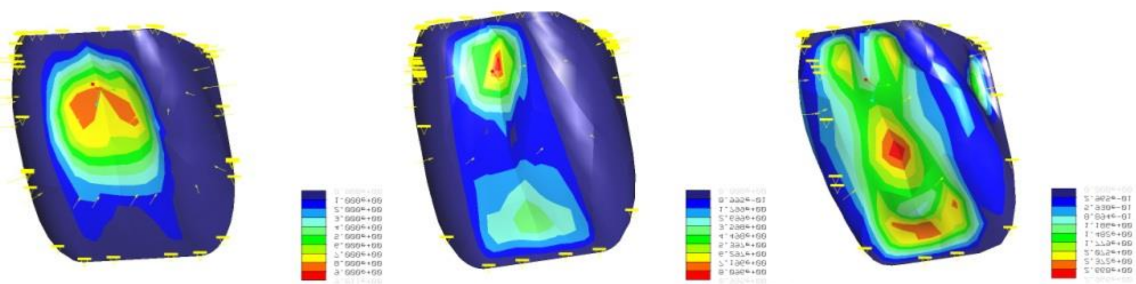
Features:

- Luxury 4-Seater Cabin.
- Turbine Engine.
- Carbon Composite Fuselage.
- Dual-Controls.
- NOTAR Anti-Torque System.
- Low-profile Rotor Hub.
- Infinite Life Composite Rotor Blades.



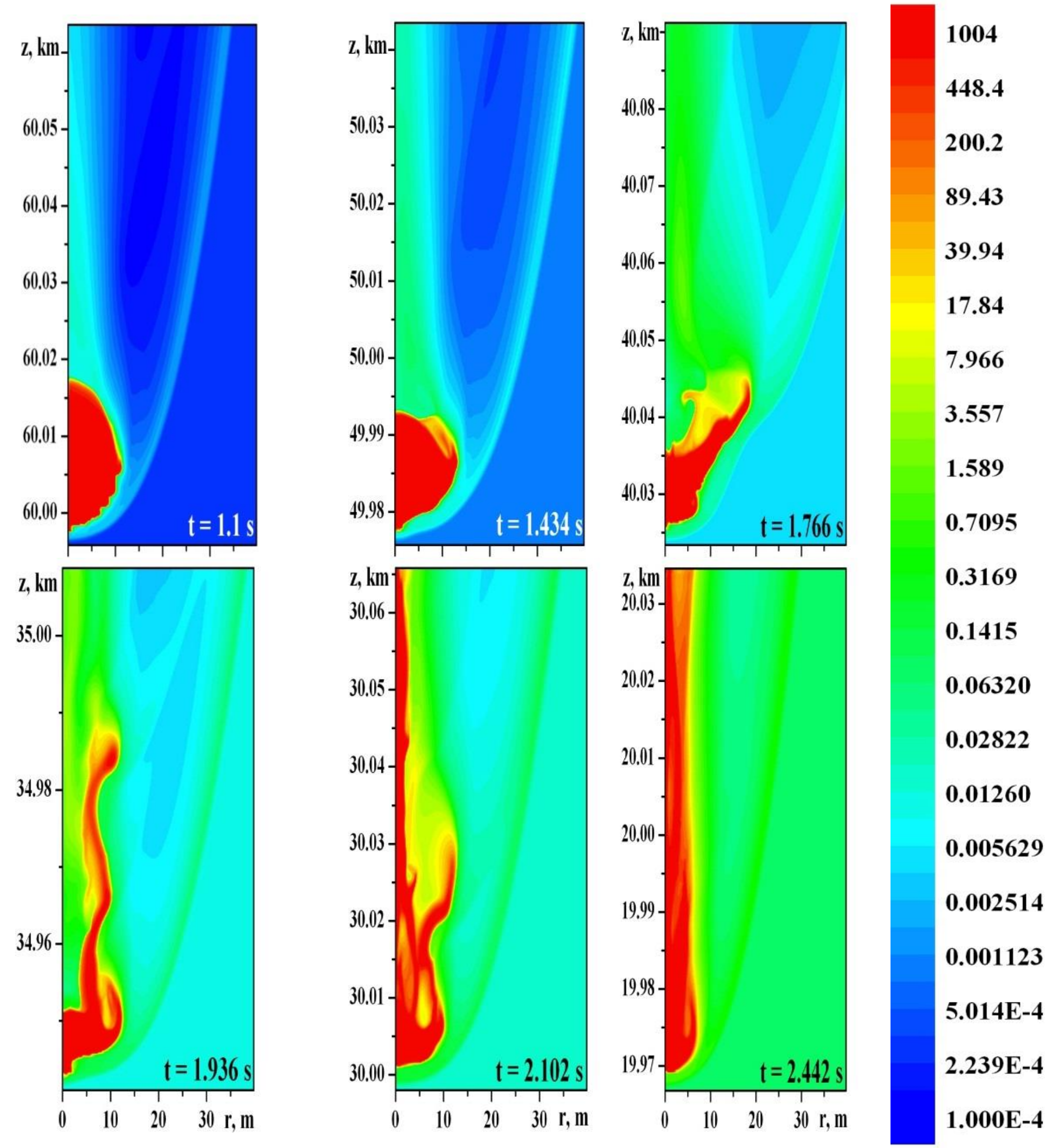
Main Rotor Diameter:	10.40m
Fuselage Length:	9.29m
Fuselage Width:	1.64m
Overall Height:	2.56m
Ground Clearance:	0.39m
Cabin Height:	2.08m
Skid Gear Width:	2.00m



COMPUTATIONAL EXPERIMENT IN THE PROBLEMS OF HAZARDS DUE TO COMETS AND ASTEROIDS

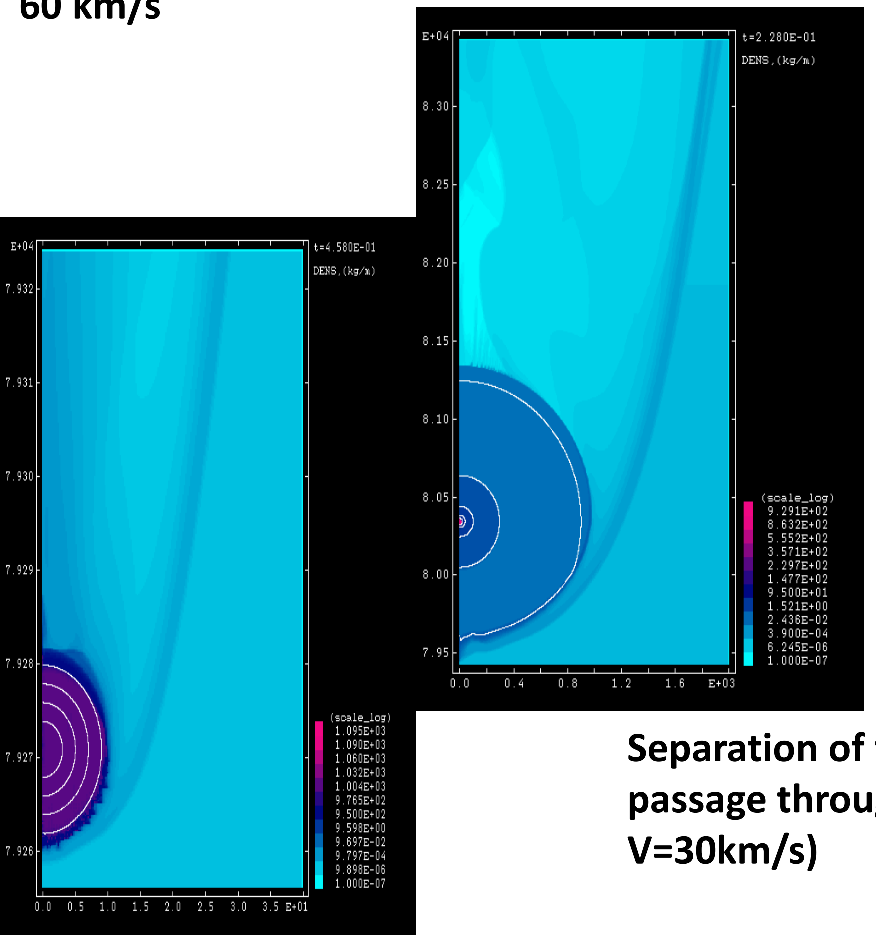
- **Development of physical and mathematical models of a falling large space body through dense layers of atmosphere and their impact on a surface of planets.**
- **Development of the applied software for carrying out of computing experiments in the field of tasks of asteroid hazard.**
- **Development of the applied software for visualisation of results of computing experiments.**
- **Carrying out of computing experiments and the analysis of the derived results.**

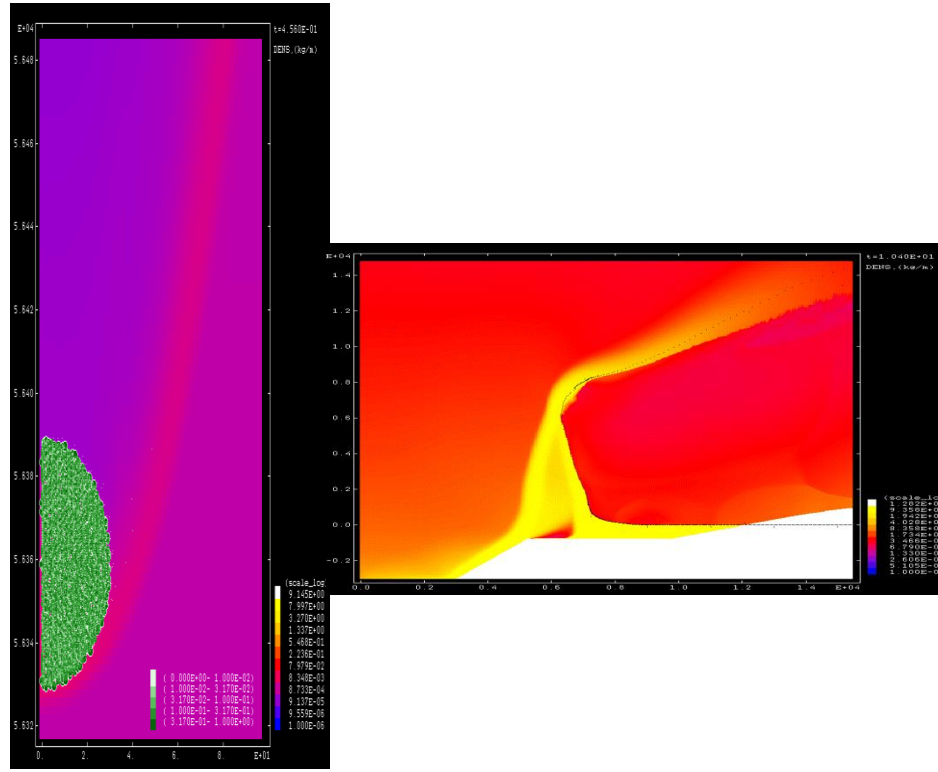
Density fields for a meteoroid with a radius of 10 m with velocity 30 km/s .



Numerical Simulation of Collision & Fragmentation of Cosmic Bodies

Density fields of a comet-like object of radius 1000 m (the density is in kg/m3) with velocity 60 km/s





Separation of fragments of a space object in passage through the atmosphere (R=30m, V=30km/s)

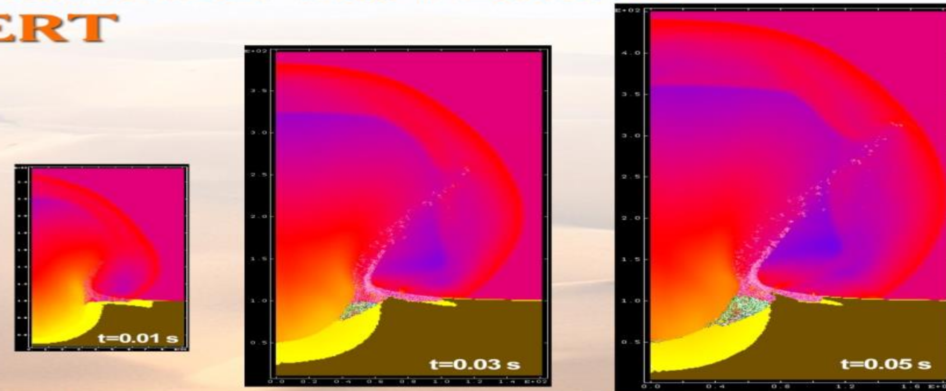
FALL OF THE SMALL ASTEROID ON TO A DESERT

The initial data:

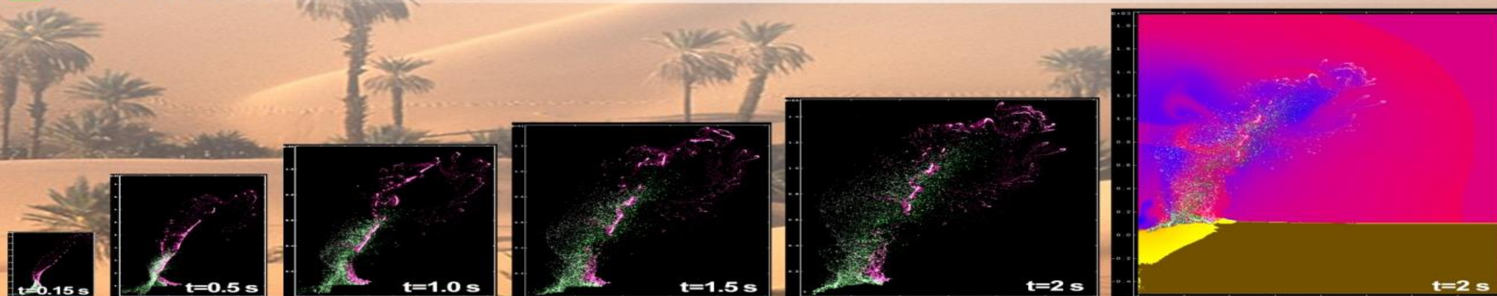
asteroid diameter 10 m
asteroid speed 60 km/s
altitude 100 m
sand and dust 15 m

sand & dust
(0.000E+00 - 2.000E-06)
(2.000E-06 - 1.000E-05)
(1.000E-05 - 1.000E-04)
(1.000E-04 - 1.000E-03)

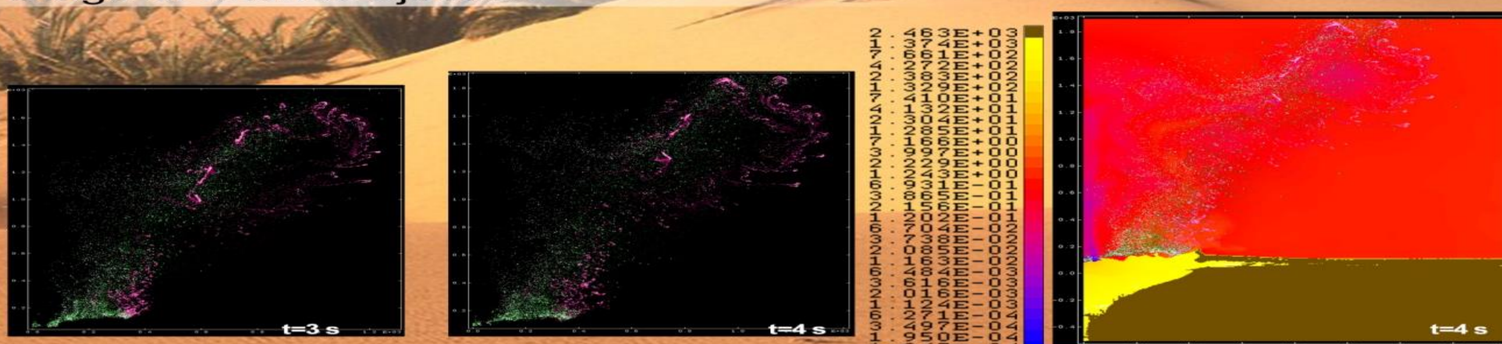
stone
(1.000E-03 - 1.974E-02)
(1.974E-02 - 3.898E-02)
(3.898E-02 - 7.696E-02)
(7.696E-02 - 1.519E-01)
(1.519E-01 - 3.000E-01)



Initial stage of the ejection



Stage of intense ejection



End of the ejection phase

Jet flow as one of the type of shear flows

POSSIBLE APPLICATIONS

- engines, fuel injectors

- burners and chemical reactions

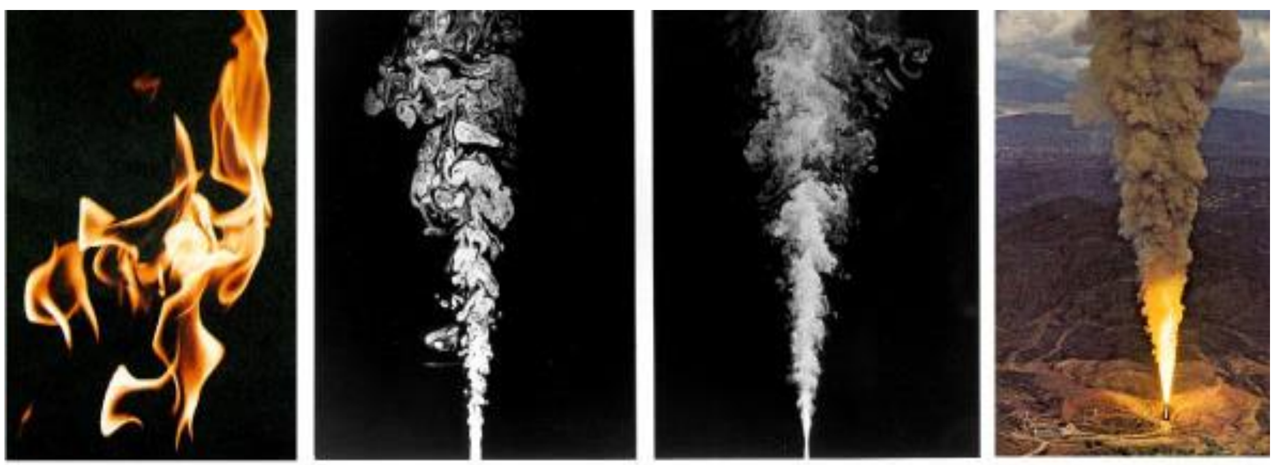
- heat exchangers

- gas and liquid cleaners

- pharmaceutical equipments

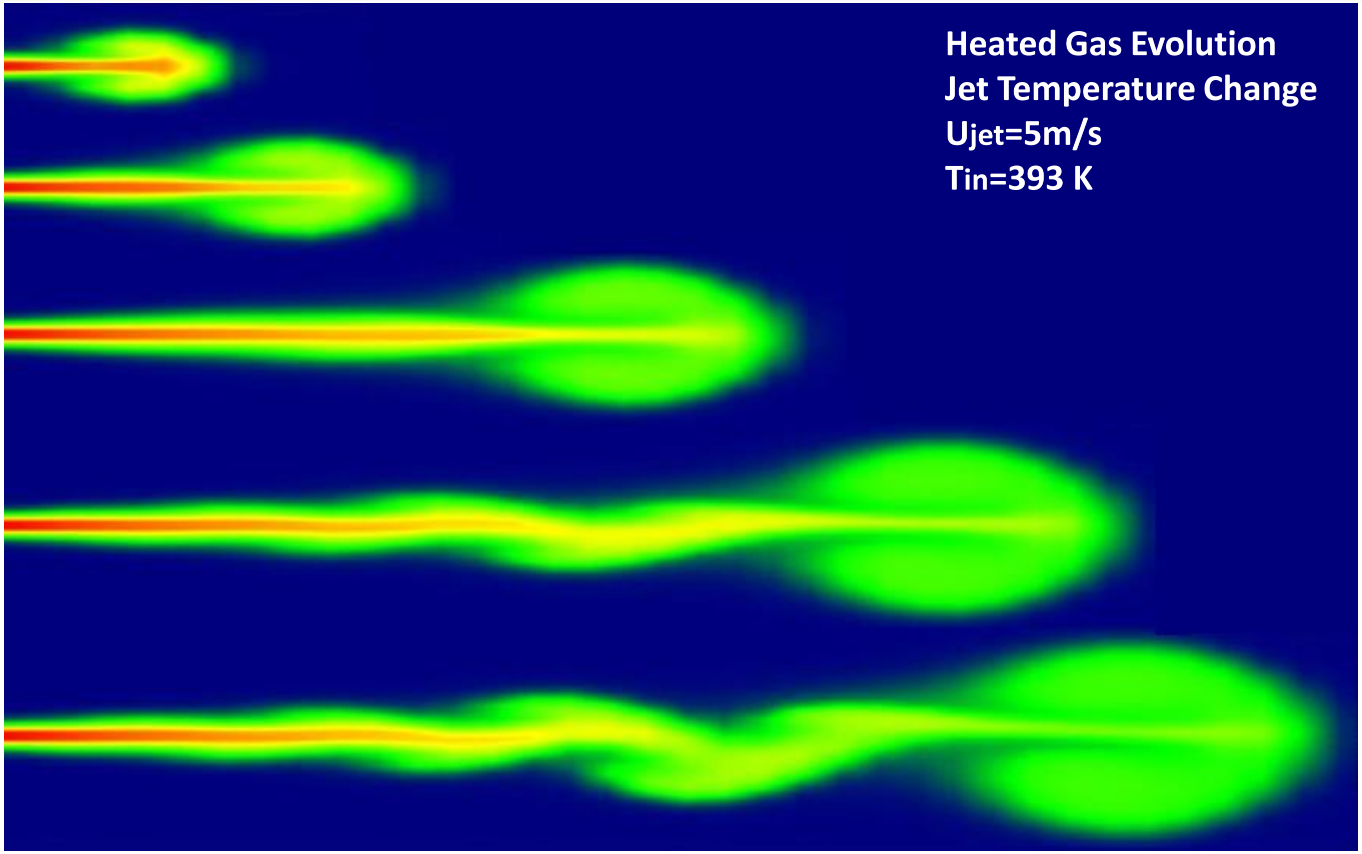
- flows in rivers, sea, oceans and atmosphere and etc.

Jet flow examples at different Reynolds number

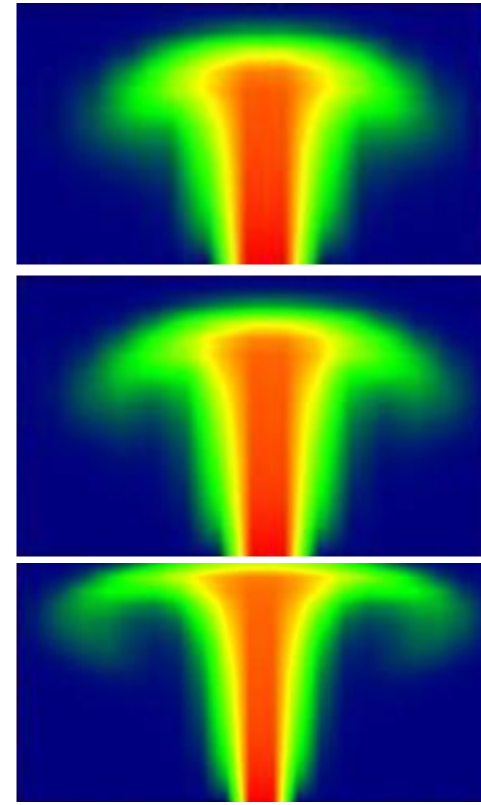


$Re \leq 10^3$ $Re \approx 2.5\times10^3$ $Re \approx 1.0\times10^4$ $Re > 10^8$

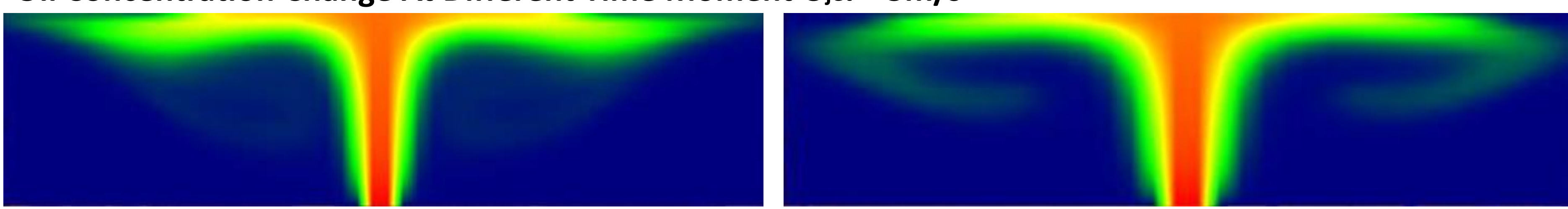
Turbulent Jet Simulation



Liquid Mixing Evolution



Oil Concentration Change At Different Time Moment U_{jet} = 5m/s

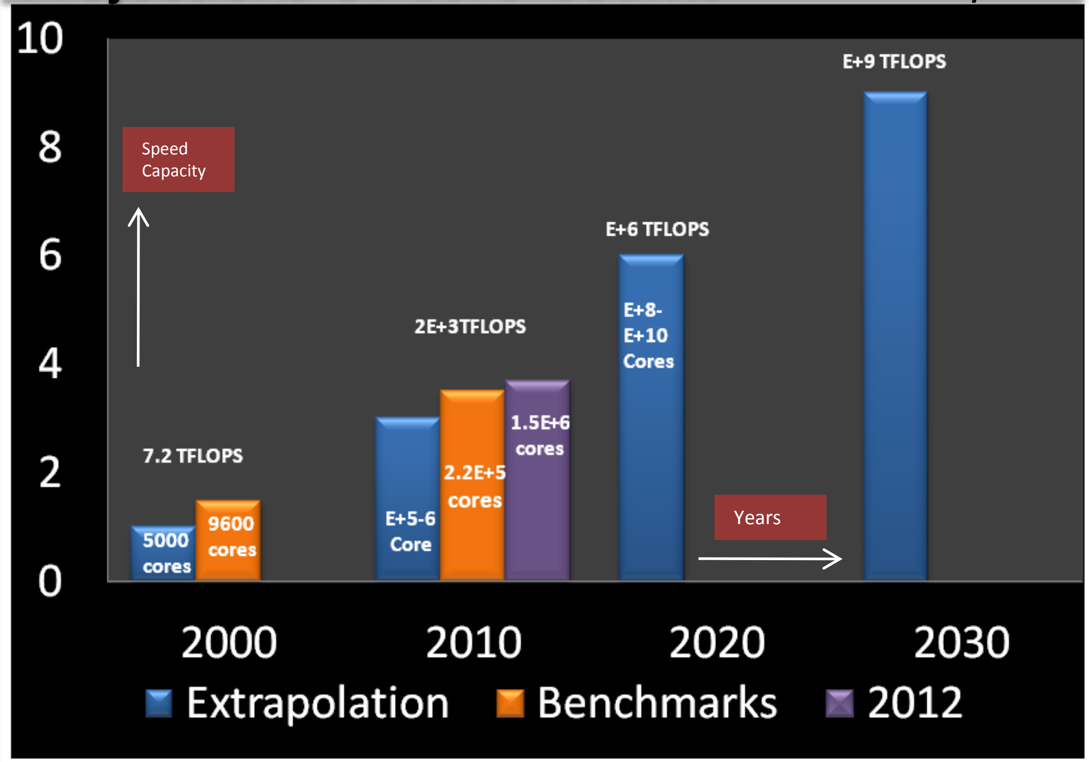


HPC Core Aspects

- **Size**: Many problems that are interesting to scientists and engineers can't be fitted on a regular machine due to the limitation of resources (CPU/RAM/Disk).
- **Speed:** Simulations require a lot of computing time: months or even years on a regular machine. But that only a few hours on a supercomputer.
- **Scale:** There are many questions for researchers on the scalability of the system such as can I make the run twice as fast with twice resources, Or, can I run twice workload with double resources within same time

Projections Of Core-Counts

Data Source: Metacomp



The future is bright for HPC's but challenges loom as we go from Peta-Flops to Exa-Flops even Zeta-Flops

How do we program for $10^{8\text{-}10}$ cores, especially if the cores are different?

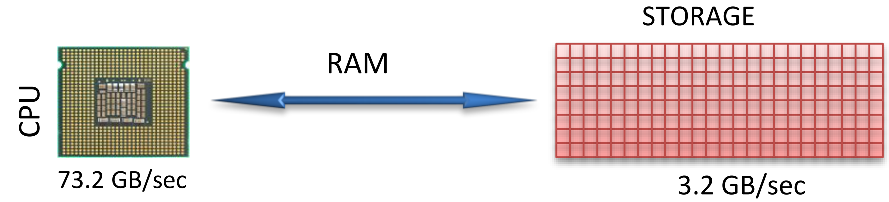
HPC Applications

1. **Simulation:** of physical phenomena,
   - ❑ Aerospace
   - ❑ Weather forecasting
   - ❑ Galaxy formation
   - ❑ Oil reservoir analyses
   - ❑ Multiphase flow
   - ❑ Bio analyses

2. **Data Mining :** fetching information from haystack of data,
   - ❑ Gene sequencing
   - ❑ Signal processing
   - ❑ Weather Forecasting

3. **Visualization:** representing a lot of data in graphical form that researchers can understand,
   - ❑ CFD
   - ❑ CAD
   - ❑ Mesh
   - ❑ Molecules

RELATION B/W MEMORY AND PROCESSOR



The speed of data transfer between Main Memory and the CPU is much slower than the speed of calculating, so the CPU spends most of its time waiting for data to come in or go out.

Data Source: oscer.ou.edu

1. Higher memory required for a given case depends on the numerical Schemes and the Model invoked, e.g. an algebraic multigrid scheme , multiphase flows etc.

2. Cases where you need more CPUs depends on the Number of equations and the model that is being invoked, which has a lot of computational overhead, e.g. the chemistry inversion in chemically reacting flows, solving a lot of equations on a large mesh size etc will take a lot of CPU time .

3. Some specific applications/numerical algorithms do not run well in multi-CPU HPC systems because they are not parallelized efficiently.

The Saudi Supercomputer “SANAM”

- King Abdualziz City for Science and Technology (KACST) in Riyadh, Saudi Arabia, along with Frankfurt Institute for Advanced Studies (FIAS), needed to develop a High Speed Cluster (HSC) solution based on GPGPU technology (General-Purpose computing on Graphics Processing Units) to support efforts in quantum chromodynamics and nanotechnology research.

- Adtech Global and AMD deliver a new standard in power-efficient supercomputing through high-end hardware integration, infiniband connectivity, and the AMD Fire Pro graphics card.

- SANAM is based on an enhanced technology of the Frankfurt supercomputer LOEWE-CSC, which was the most energy-efficient multipurpose supercomputer in Europe.

- In terms of computing speed, “SANAM” is about 40 percent faster than the German supercomputer LOEWE-CSC, but requires merely one third of the power per computing operation.

Source: *KACST, AMD , Adtech Global , Top500,Green500*

SANAM Technical Data

Technical Details

1. Built by KACST and German institutes in 2012, 421TFlops.
2. 3,360 CPU core, 840 AMD GPU cards, 26,880GB memory
3. AMD's 420 AMD FirePro™ S10000 dual-GPU server graphics cards.
4. A new standard in GPGPU-based, power-efficient supercomputing

Applications

Mainly Serve areas related to seismic, aerospace, bioinformatics, weather and numerical simulations etc.

Impact

The supercomputer redefines power-efficiency, securing the number four ranking on the global Green500™ List, as well as 52nd on the Top500 Super Computer List in June 2013, which evaluates computing based on total speed.

Source: *KACST, AMD , Adtech Global , Top500,Green500*

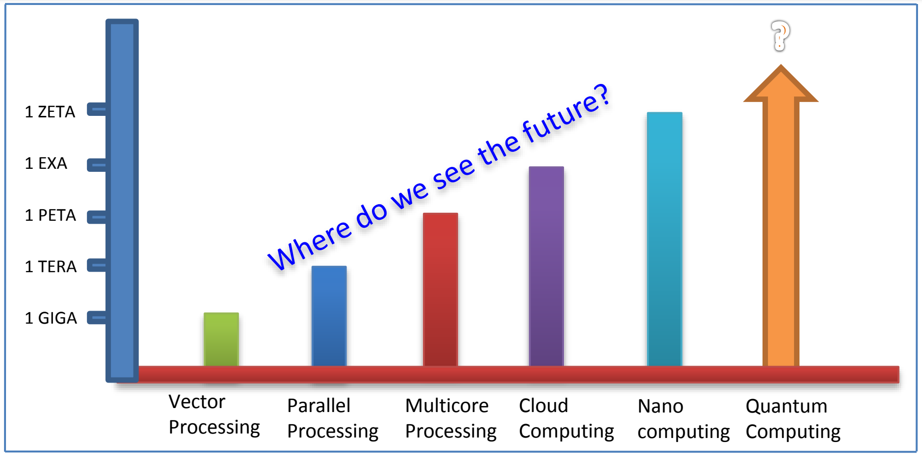
Closing Thoughts

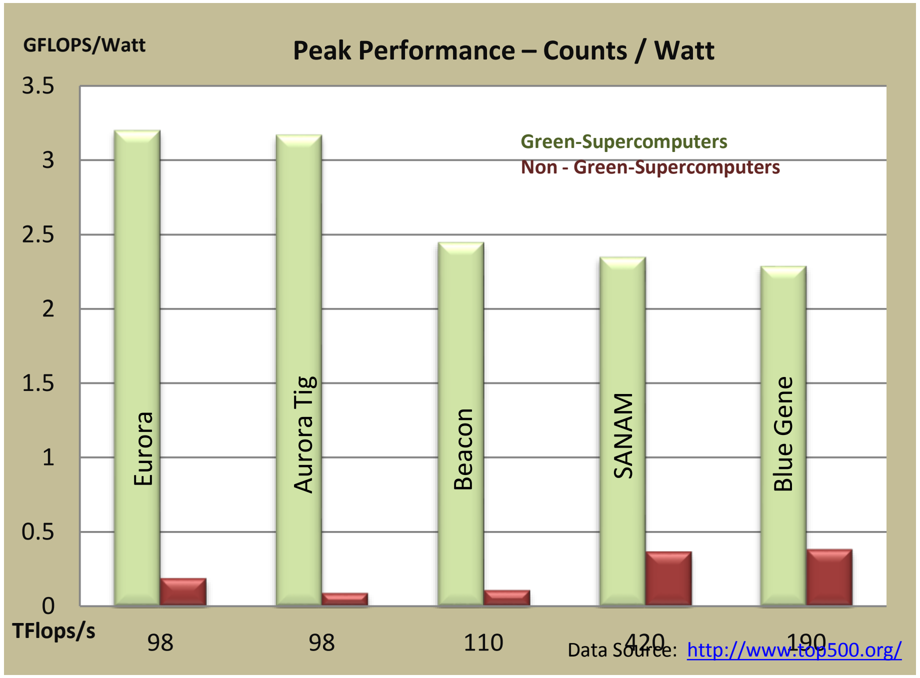
- ❑ **HPC is evolving with passage of time.**
- ❑ **Future is towards Extreme Scale Computing.**
- ❑ **Benefits of the problems solved at petascale.**

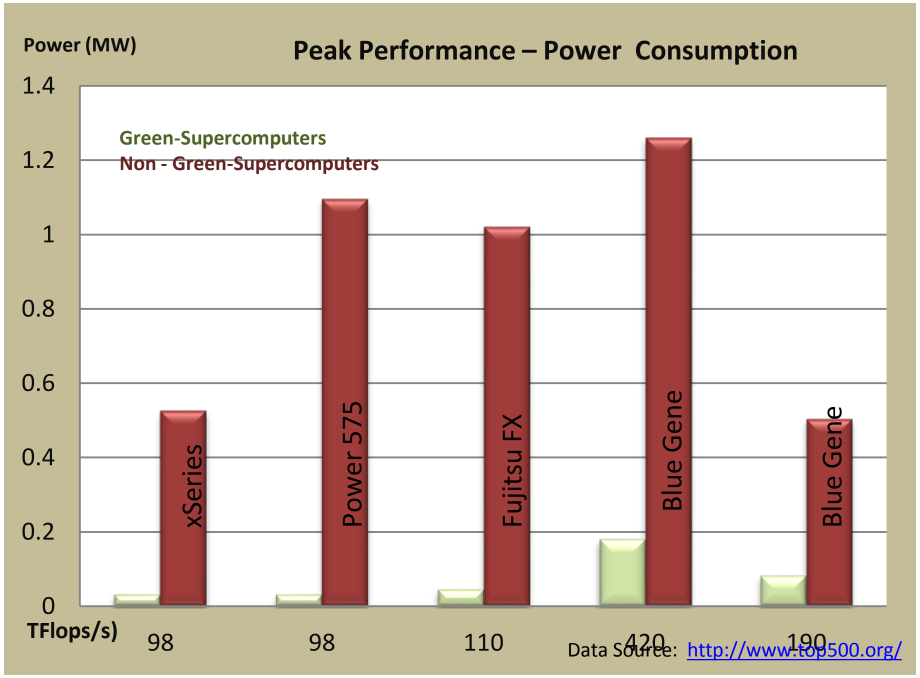
It is estimated that 20 percent of world energy consumption is traceable by turbulent flow analysis and the energy it dissipates. [Source : ICES, University of Texas]

- ❑ **Eco-Efficient Computers.**

Why burn more power ,when same speed is achievable with less? (SANAM)







Thank You For Your Kind Attention