

# **BIG DATA:**

**Computational Fluid Dynamics (CFD):  
Basic Science and Engineering Applications  
(Cinvestav-Abacus & ININ Projects)**

**Cinvestav-Abacus: Centre for Applied  
Mathematics and High Performance Computing**

**ININ: National Institute for Nuclear Research**

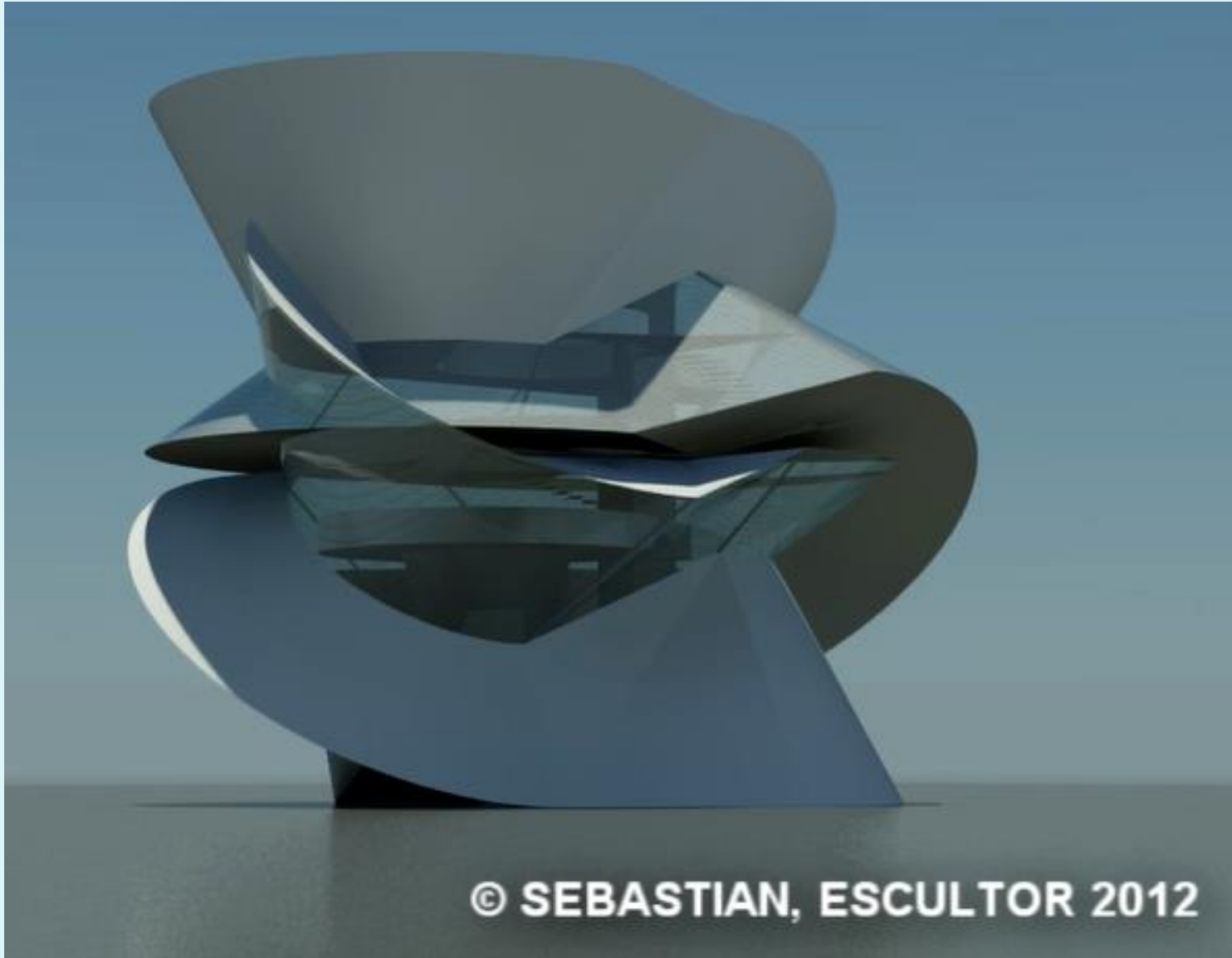
**Jaime Klapp**

**Cinvestav-Abacus e ININ**

# National Institute for Nuclear Research



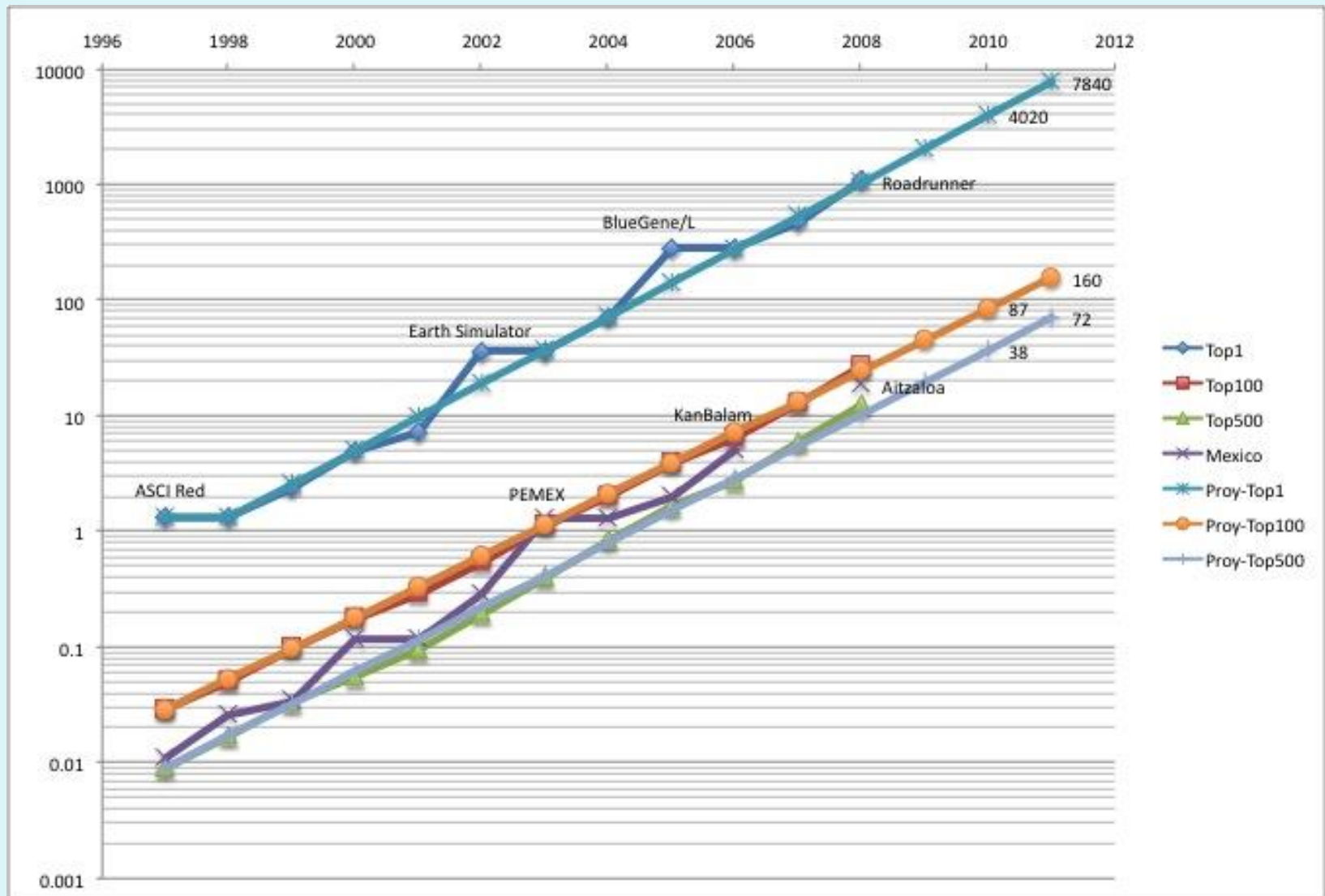
# Cinvestav-Abacus



# Abacus Centre for Applied Mathematics and High Performance Computing (supercomputer will start operation by mid may 2015, this is in 3 weeks!!)

- Campus in Km 38.5 México-Toluca highway
- 15 mins from Santa Fe (Mexico City) and Toluca, 5 mins from ININ.
- **Computer with: (430 Tflops)**
- 9,000 Haswell Intel cores 2.6 Ghz
- 4 GB RAM per core (36,000 GB)
- 1,500 TB HD
- 100 GPUs Kepler K40 (200,000 cores)
- Water cooled

# Evolution of the largest Supercomputers in Mexico





# Abacus–ININ Wide Band connection



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## Estudio de Factibilidad para el Desarrollo de la Red NIBA Urbana en el Estado de México

Coordinación de la Sociedad de la Información y el Conocimiento  
“e-México”

Secretaría de Comunicaciones y Transportes

Solicitante:

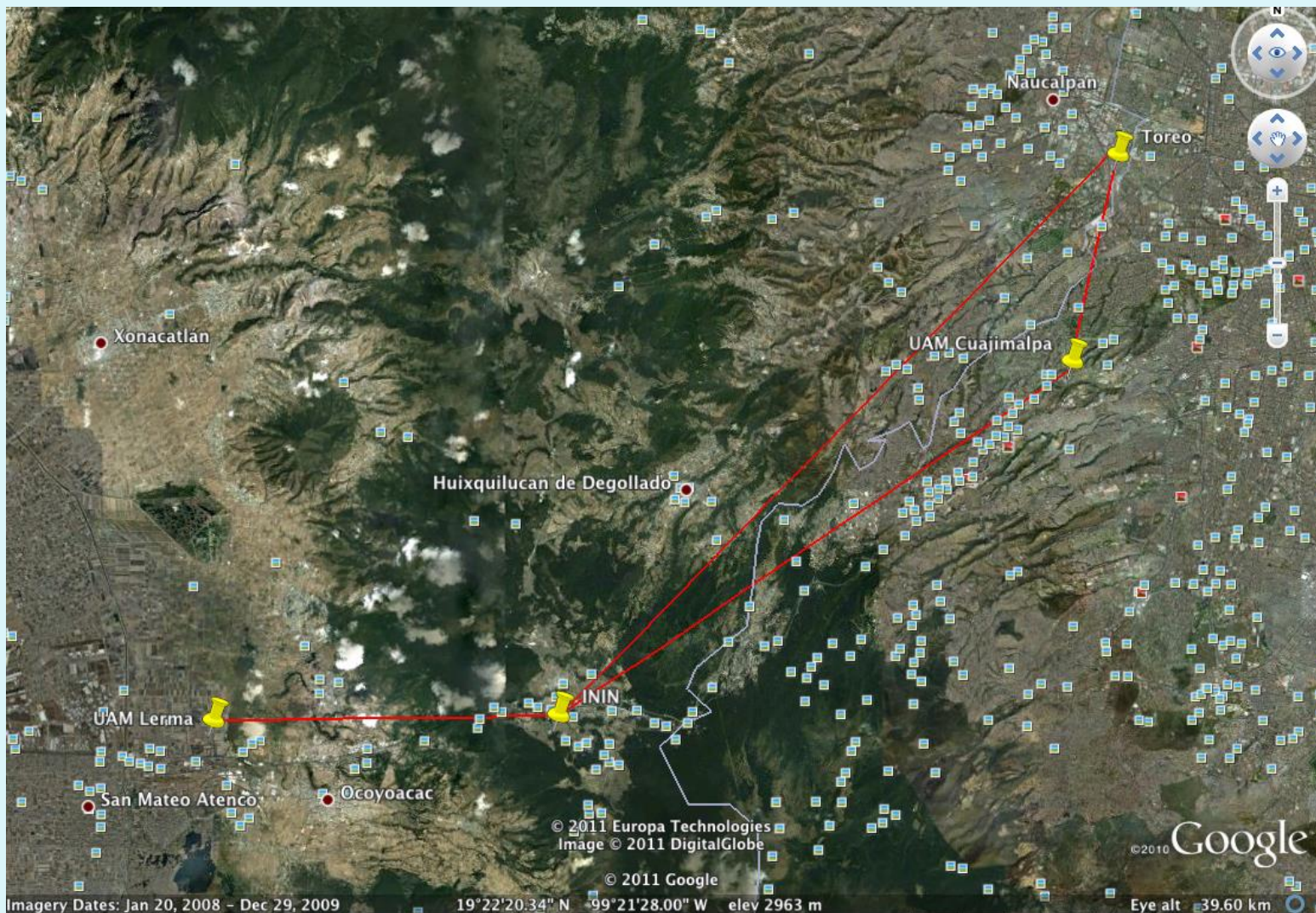
**Mtra. Mónica Aspe Bernal**  
Coordinadora

### ***Responsables Globales del Proyecto***

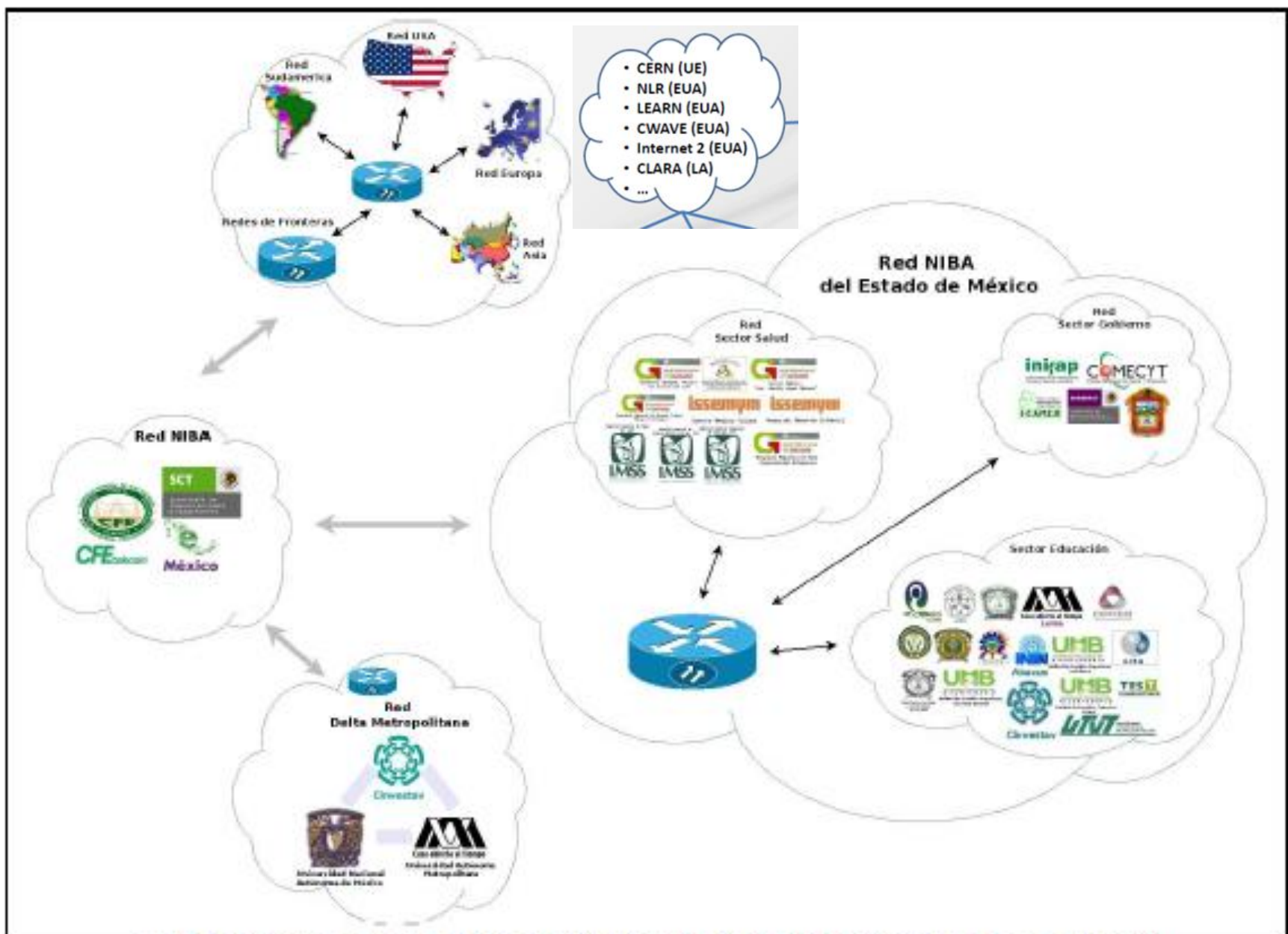
Cinvestav  
Institución Responsable del Proyecto de Conectividad en el Estado de México  
**Dr. José Pablo René Asomoza**  
Director General

Responsable del Proyecto de Conectividad  
**Dr. Jaime Lazaro Klapp Escribano**  
Cinvestav-Abacus e ININ

# Abacus and ININ location: we have Red Niba 10 GBs







Red Institucional del Estado de México, Red NIBA, Delta Metropolitana y Otras Redes de Clase Mundial

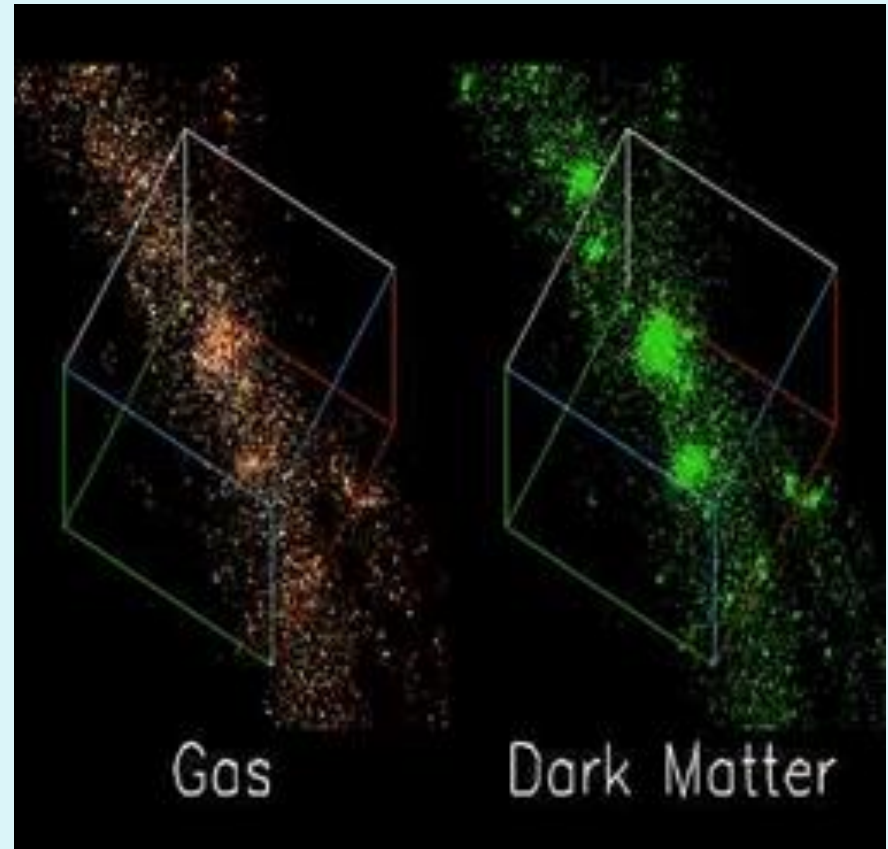


# What is a fluid?

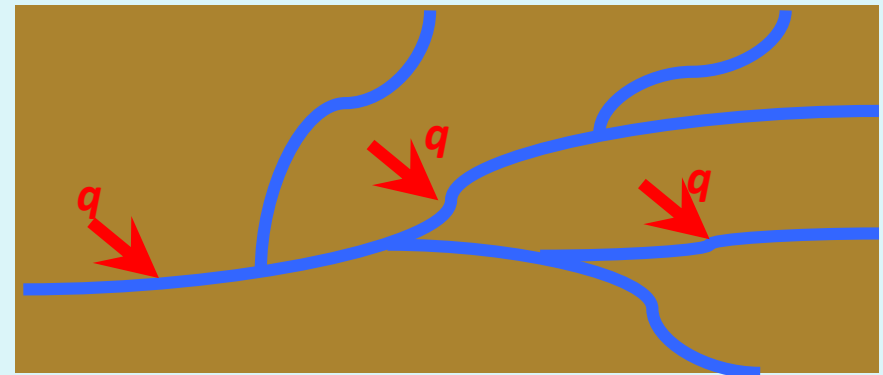
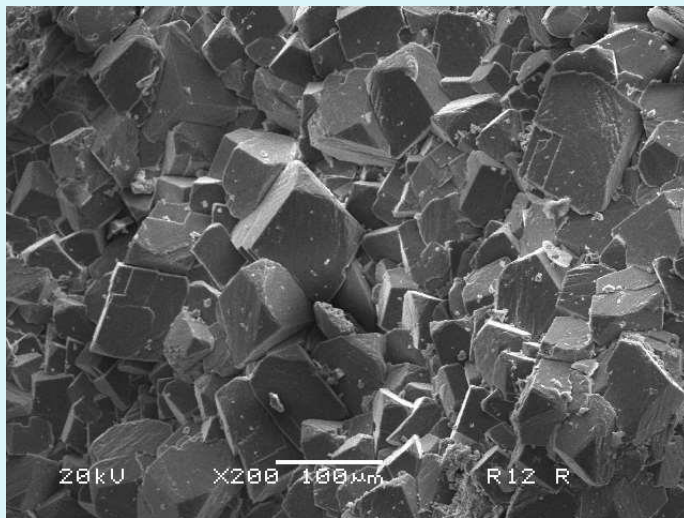
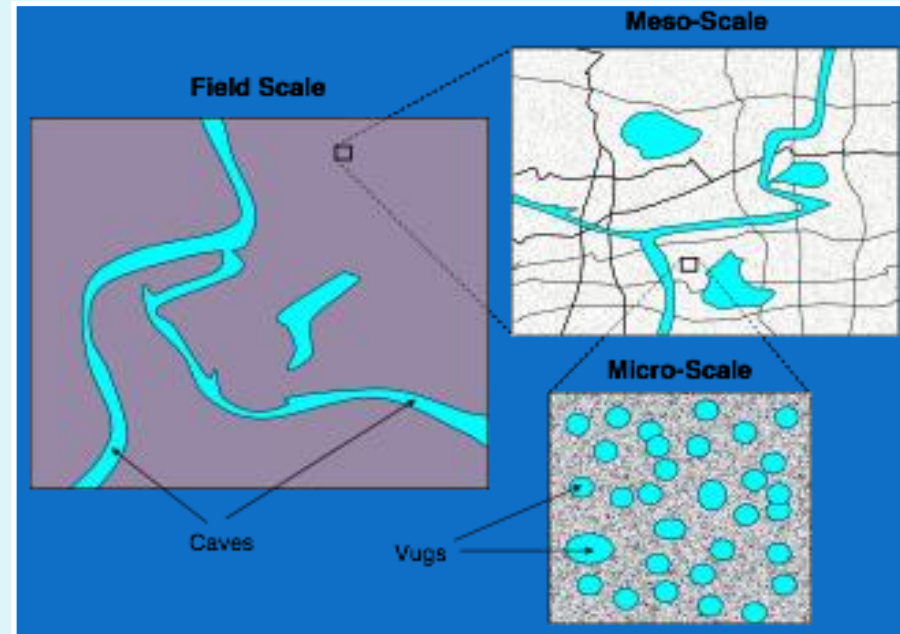
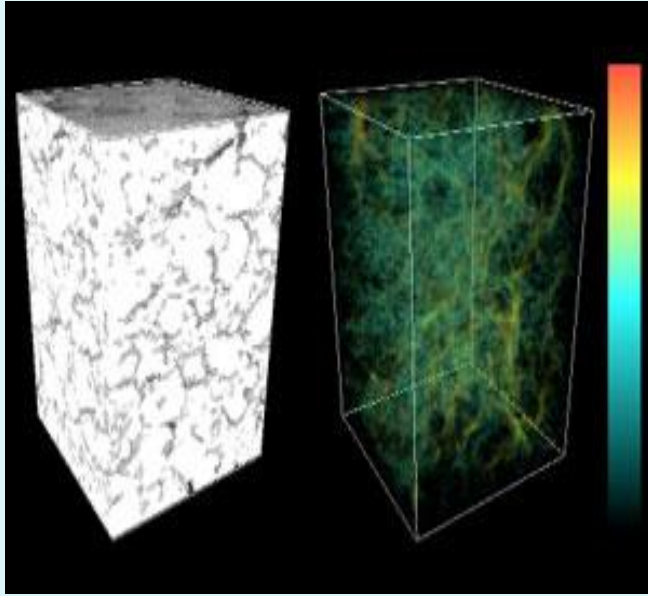
- Universe, galaxies, stars, etc.
- Atmosphere
- Ocean, tides and rivers
- Blood flow
- Car flow in cities and highways
- Electric energy flow
- Electron flow in a metal
- Population migration
- Oil through a fractured porous media
- Large amount of systems found in science, engineering and many human activities

# Why supercomputing?

- Consider a computational 3D region divided in  $1000 \times 1000 \times 1000 = 10^9$  cells.
- If we have 10 equations, we have 10 variables that we have to solve at each point, this is  $10^{10}$  variables or equations to solve at each time. A time evolution could require to solve the system  $10^{4-5}$  times.

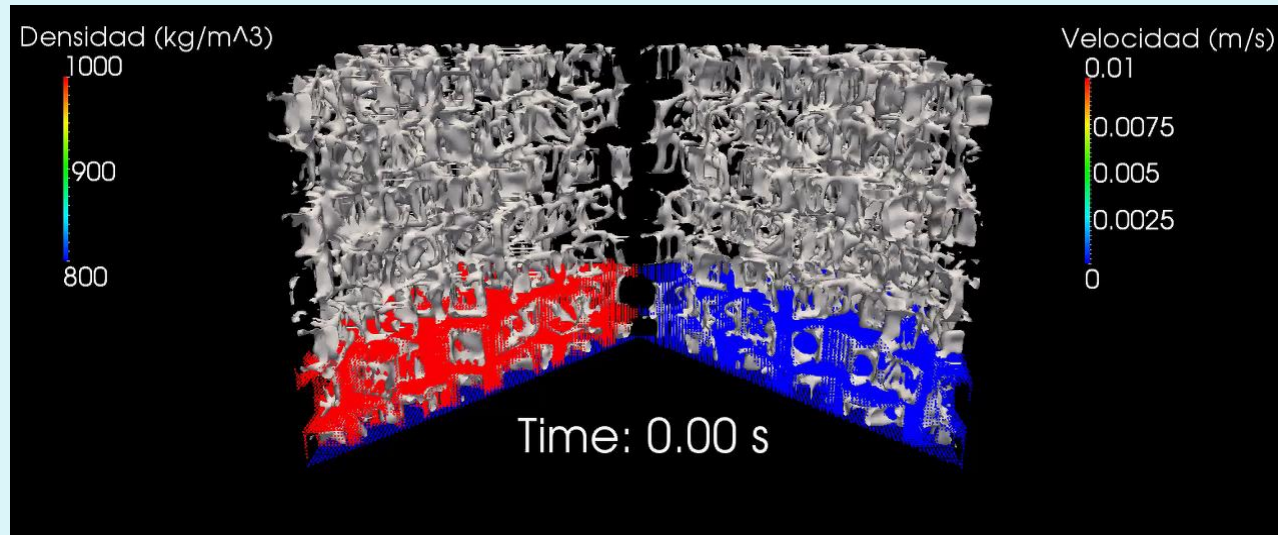
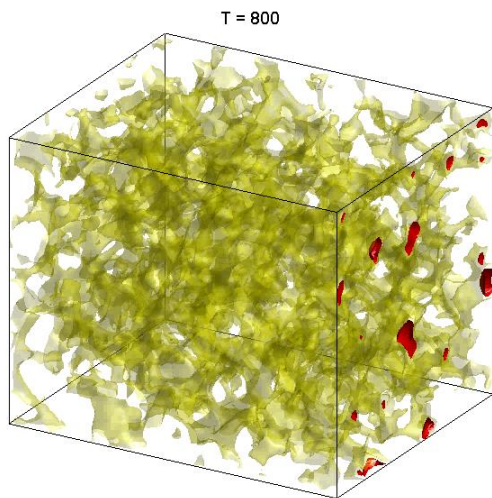
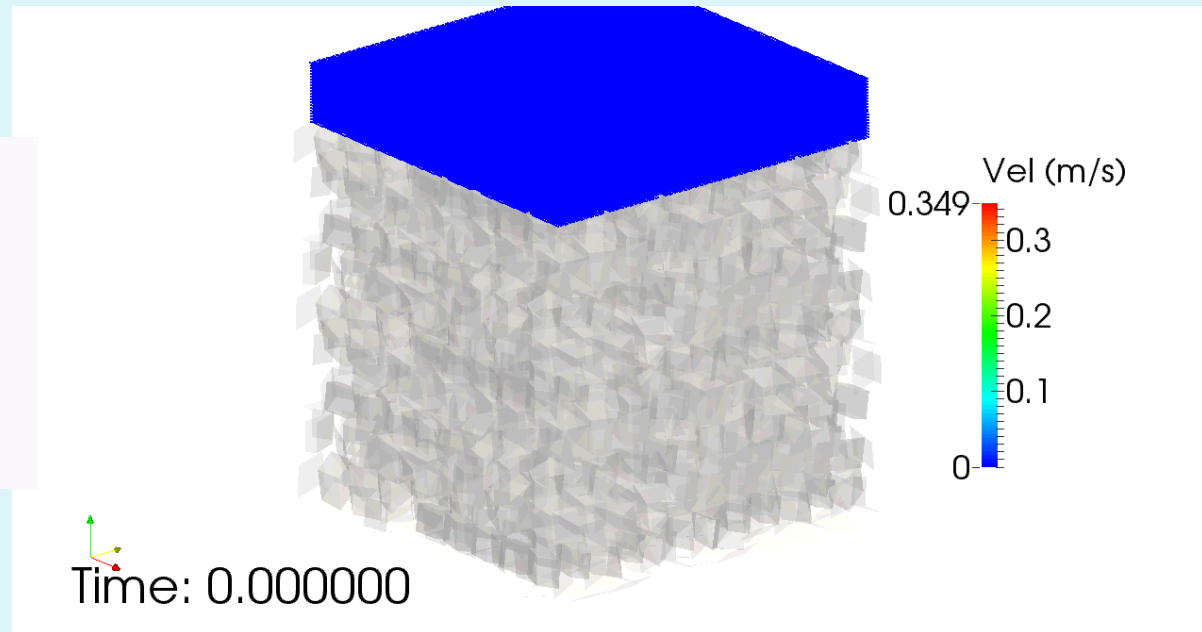
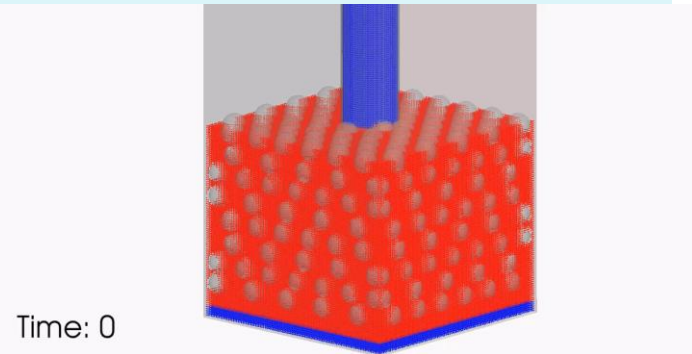


# An example of our calculations: simulation of fractured oil reservoirs





# An example of our calculations



# More examples: climate change, global warming and brain simulations



# Example of Big Data: Sloan Digital Sky Survey



The Data Volume of Data  
**Release 12** is about **116 TB**:

[http://www.sdss.org/dr12/data\\_access/volume/](http://www.sdss.org/dr12/data_access/volume/)



Another example:

# The High-Altitude Water Cherenkov Gamma-Ray Observatory



- The HAWC Observatory was officially inaugurated on Mar. 20, 2015, Sierra Negra volcano near Puebla, Mexico
- HAWC will produce massive amounts of data – upwards of **10 Terabytes per day (3,650 TB per year)**

(<http://www.rh.gatech.edu/news/390961/hawc-captures-evidence-powerful-cosmic-visitors>)

- <http://www.hawc-observatory.org/>

# Example (Abacus): Large CFD calculation with 500-1000 million particles

1 model (calculation): 10-100 TB

For a paper we require, say 5 runs: 50-500 TB.

For example, if in Abacus we produce 10 papers like this per year, we require 500-5000 TB per year. I estimate we will produce 1-5 PB per year. **Similar to HAWC.**

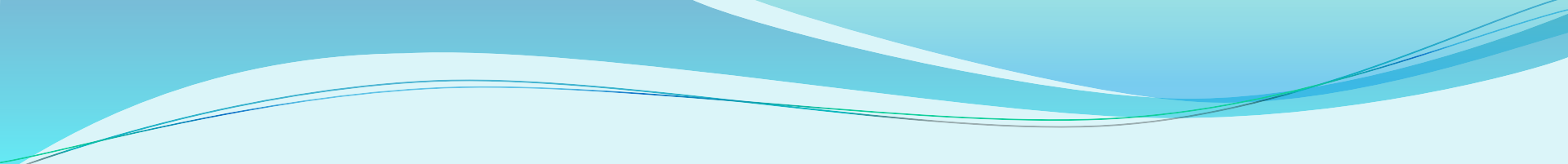
**In 1-2 years we will run out of space (only 1500 TB), or get the data out of the computer to the final users. A large portion of our data can be erased or cleaned after some time.**

Solution:

Leave all the data in the supercomputer, plot and visualize in the same machine, **only transfer images or videos. Many users want to analyze the data locally.**

Problem: Supercomputers usually ask users to move the data out from the machine in 2 weeks to few months.

**We have to solve the data problem.**



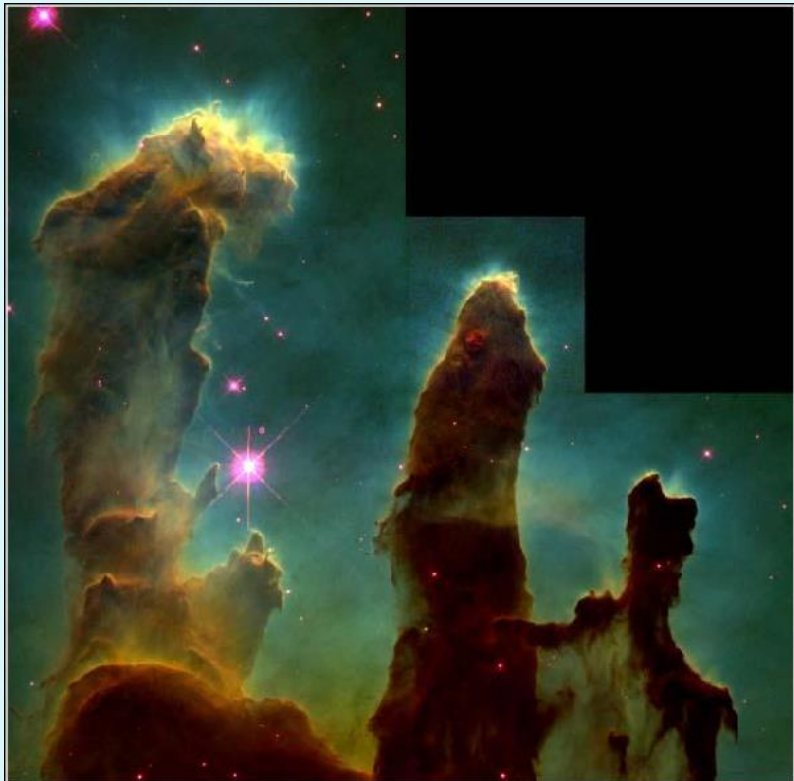
CFD projects applied to Science and  
Engineering in Cinvestav-Abacus  
and ININ.



# Astrophysics and Cosmology

- Stellar evolution
- Galaxy collisions
- Cosmology

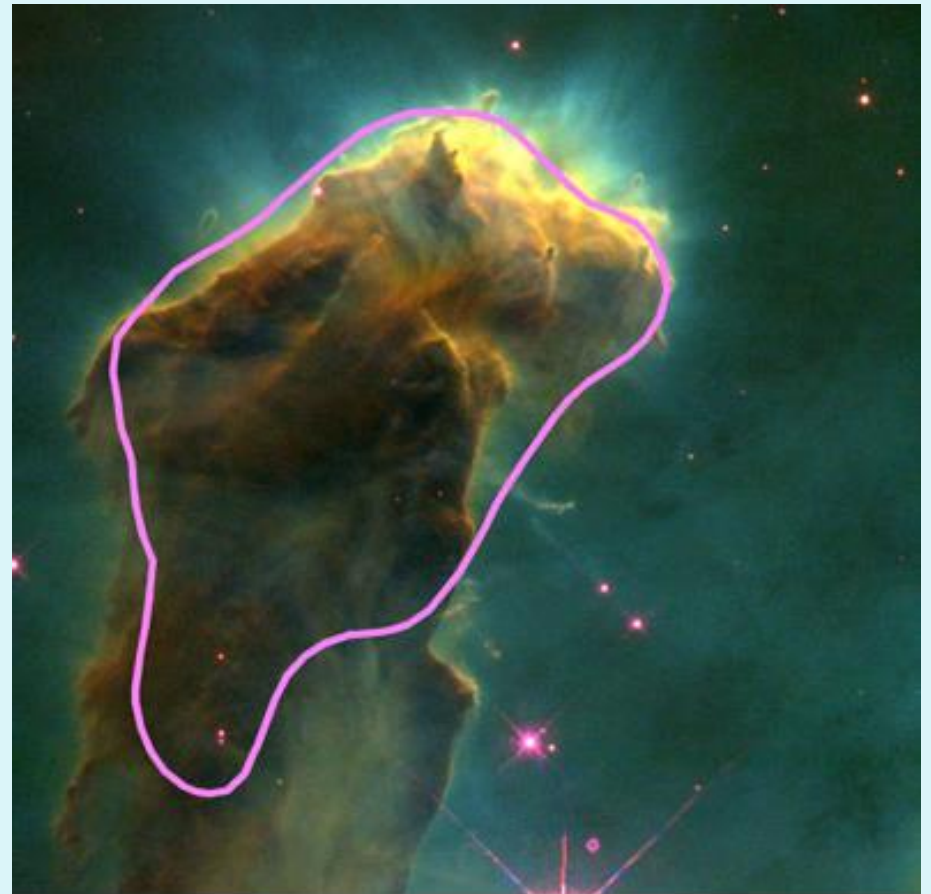
# Star formation: molecular clouds



**Gaseous Pillars · M16**

HST · WFPC2

PRC95-44a · ST ScI OPO · November 2, 1995  
J. Hester and P. Scowen (AZ State Univ), NASA

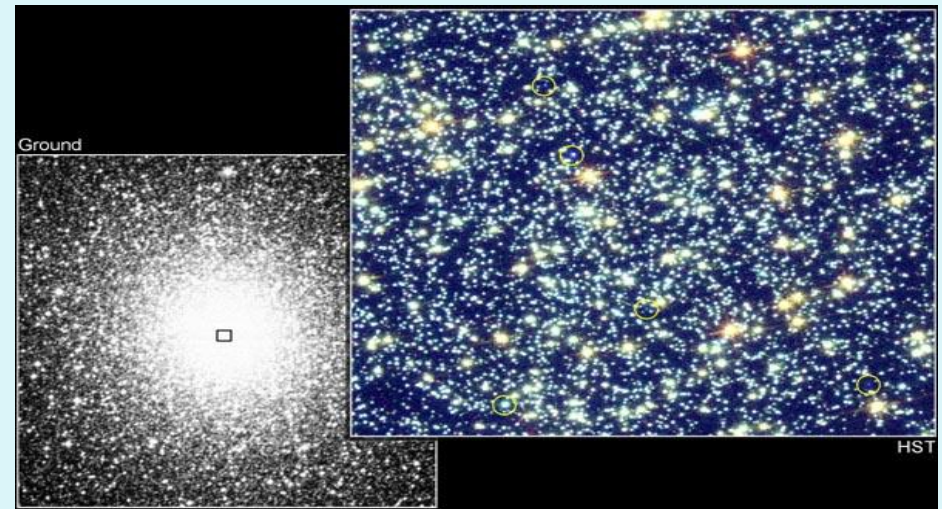
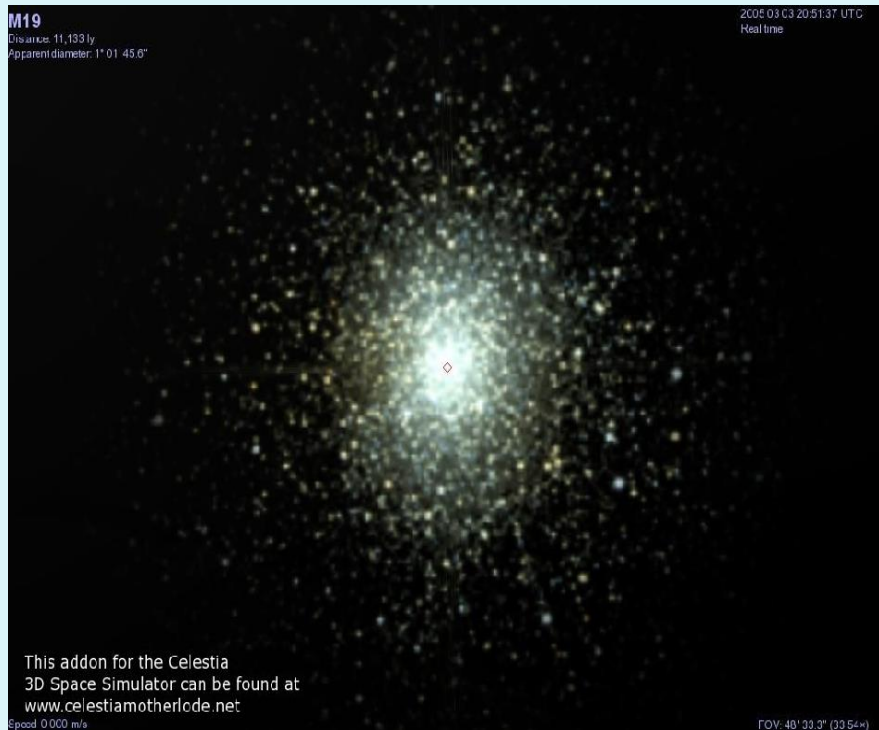


## New solar systems forming in Orion



Hubble Space Telescope photographs of proto-planetary disks in the star-forming nebula of Orion. <http://hubblesite.org>

# Molecular clouds $\rightarrow$ stellar clusters

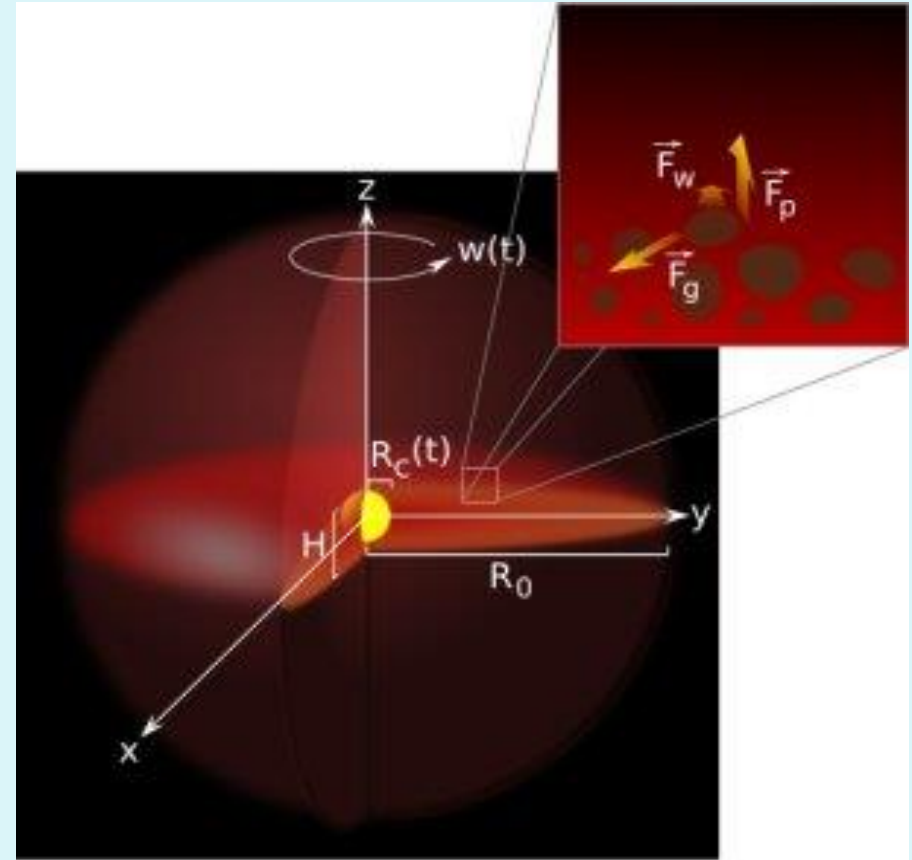
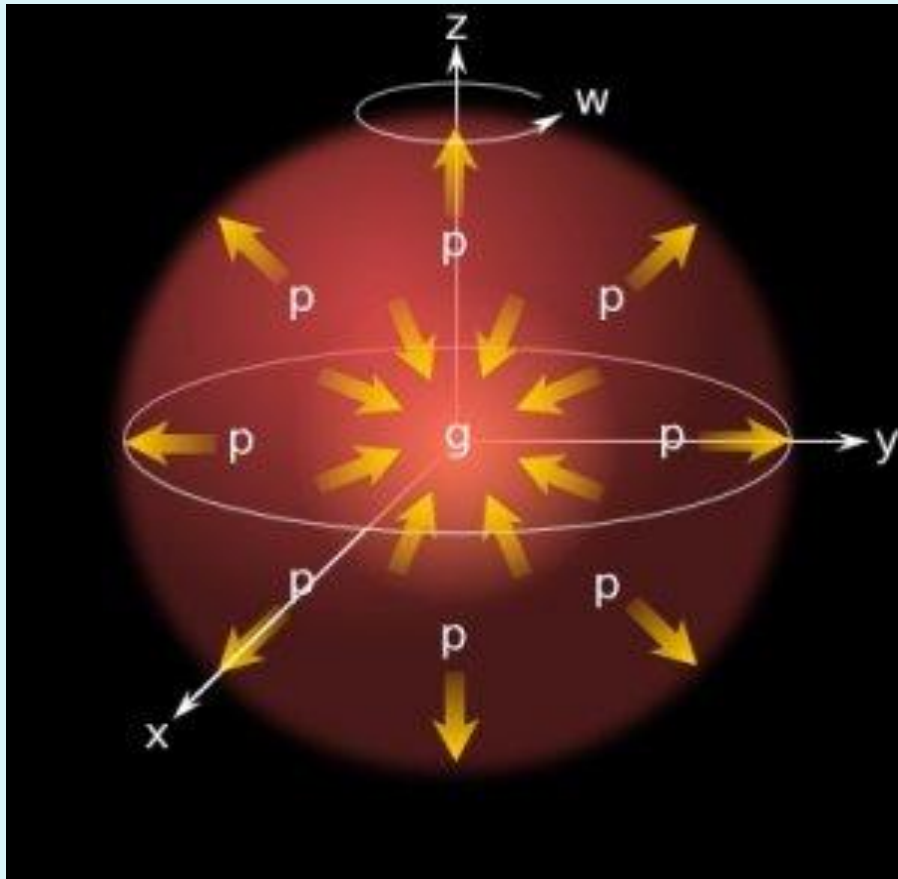




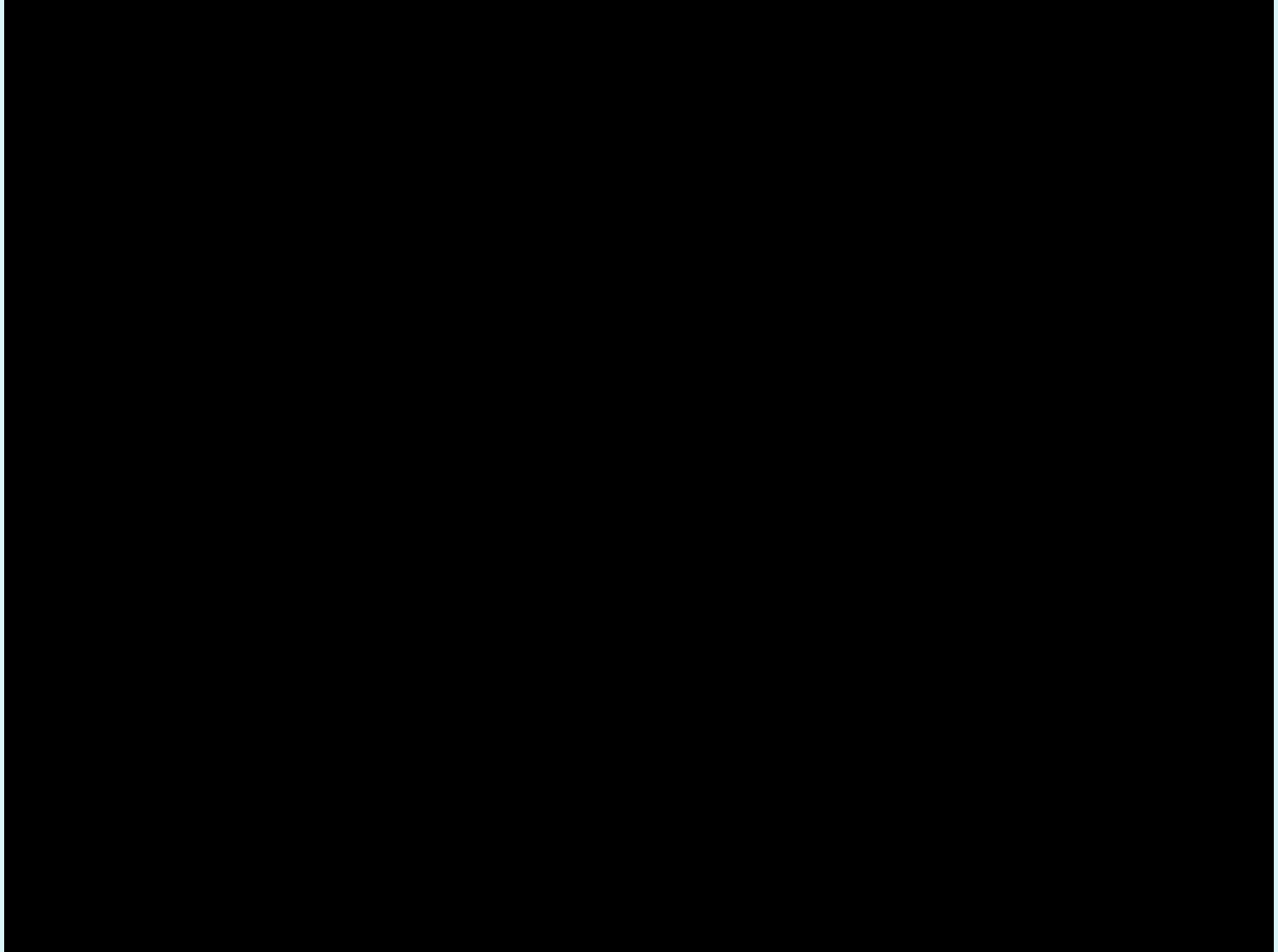
# Open clusters



**Gravitational collapse that leads to fragmentation (star formation) occurs if gravity is more intense than pressure and other forces (magnetic)**



# Collapse and fragmentation of protostellar clouds



# Galaxy collisions

- Galaxy collision simulations and comparison with observational data.

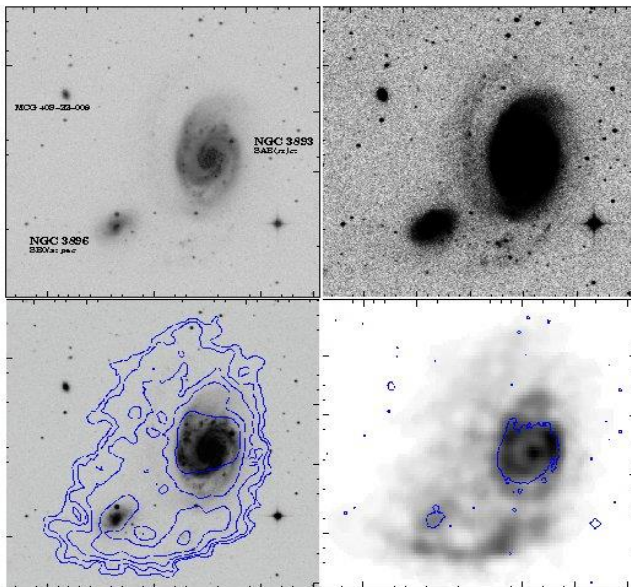
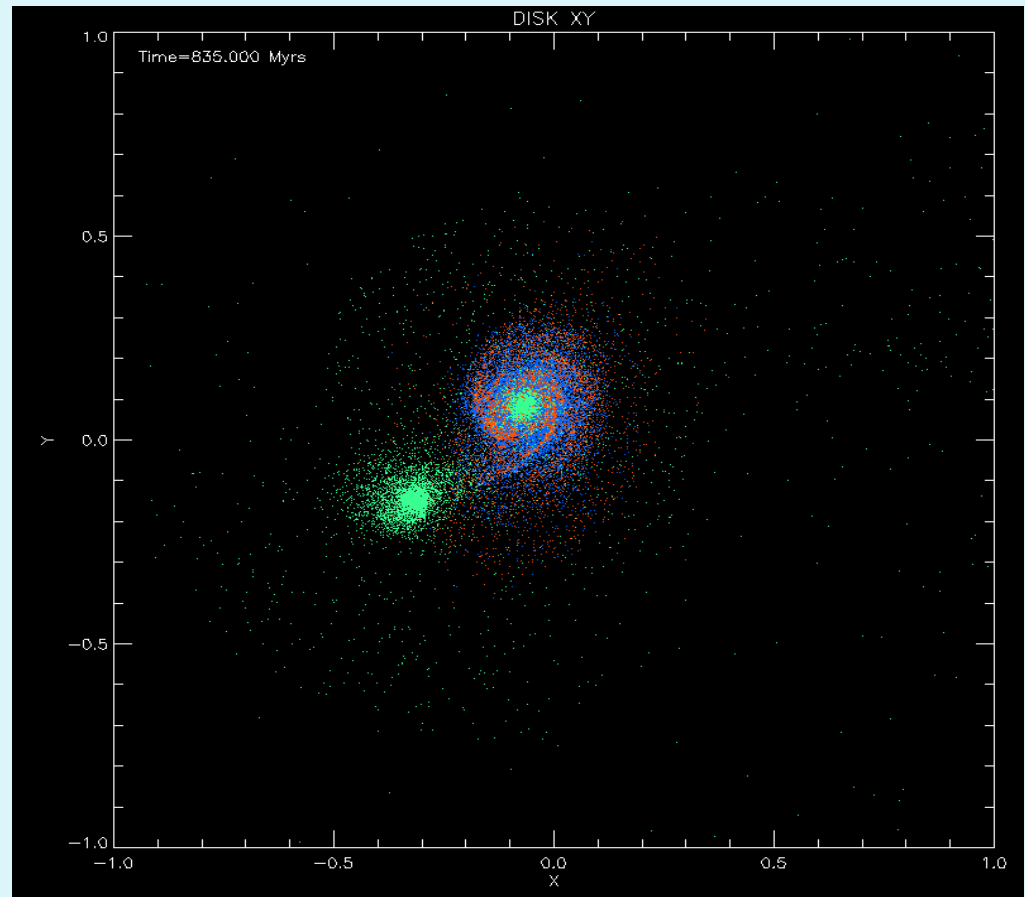
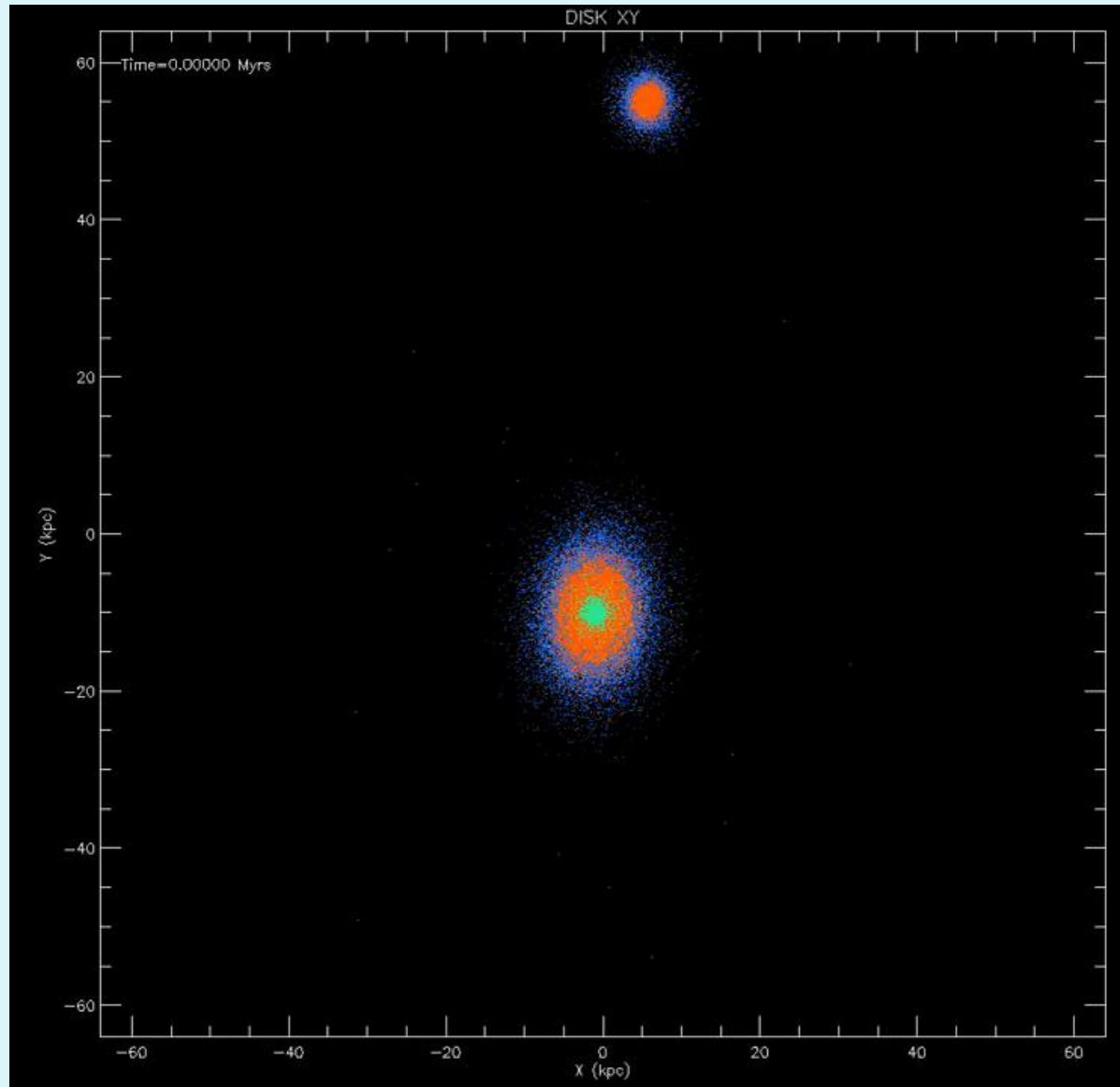


Figure 1. The NGC 3893/6 System.  
H: WISE, 30" resolution, contours= $1 \times 10^{20} \text{ cm}^{-2} \times 2''$ .  
Optical: DSS, FOV= $10' \times 10'$ .  
Notes: Member of the Ursa Major Cluster. See also Fig. ??.  
Reference: Verheijen, M. A. W., & Sancisi, R. 2001, A&A, 370, 765.

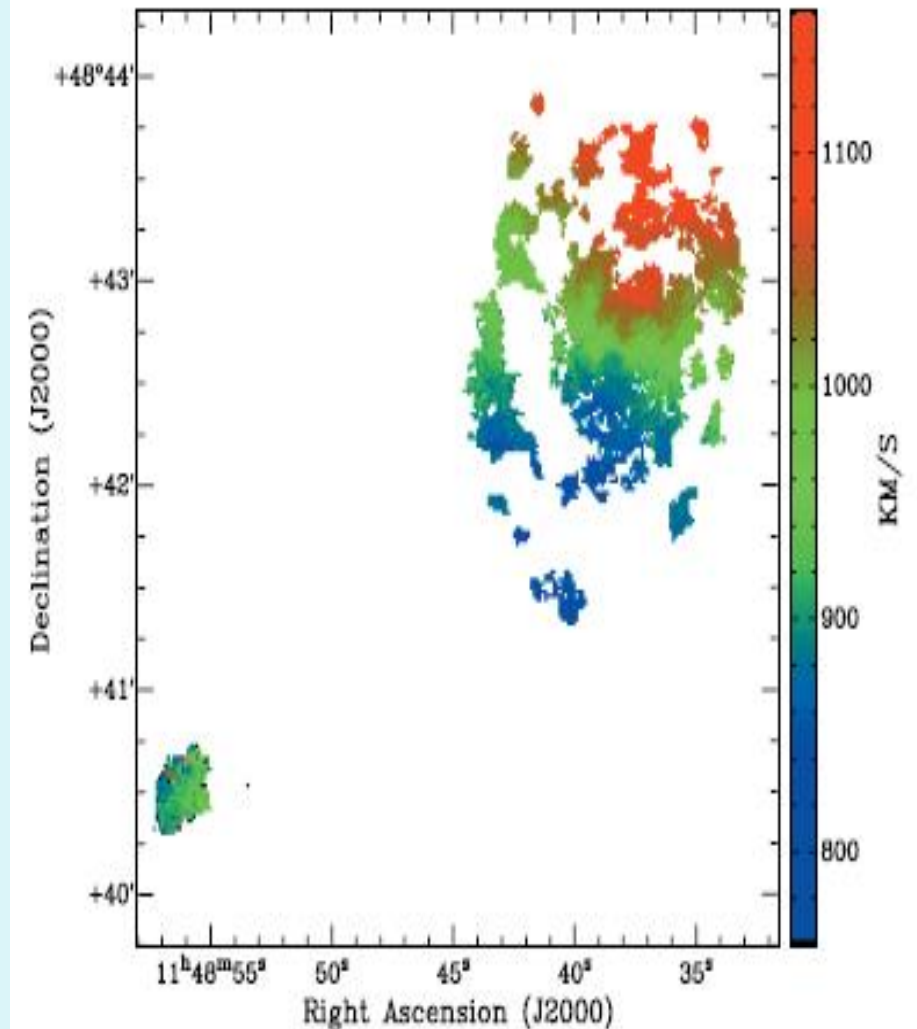
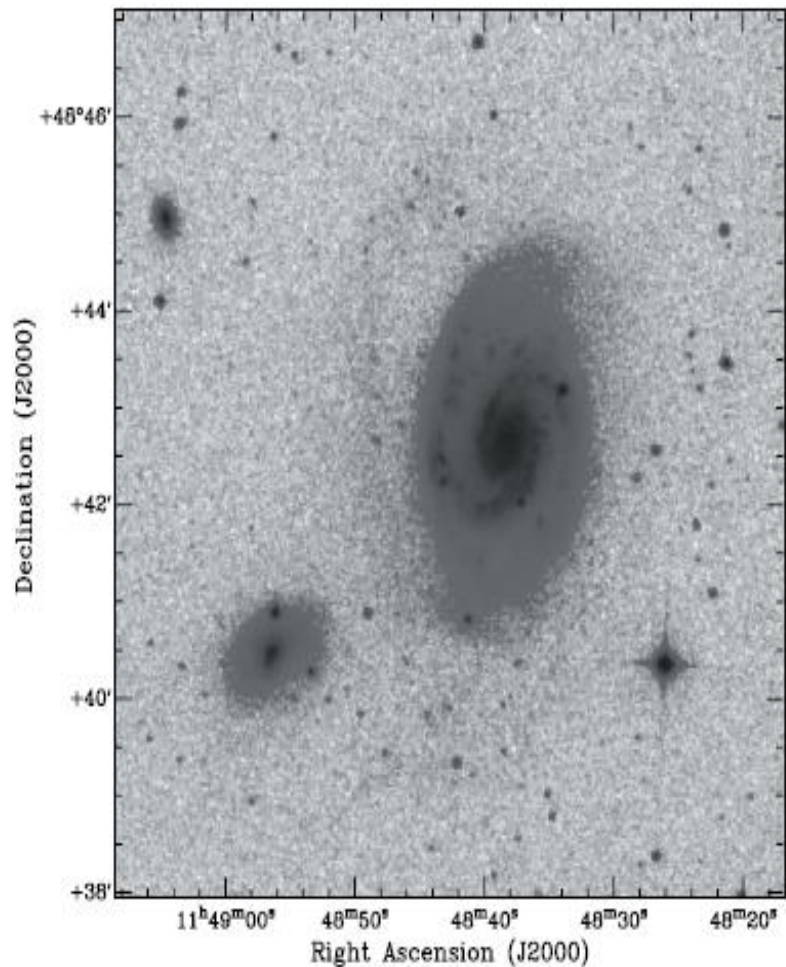




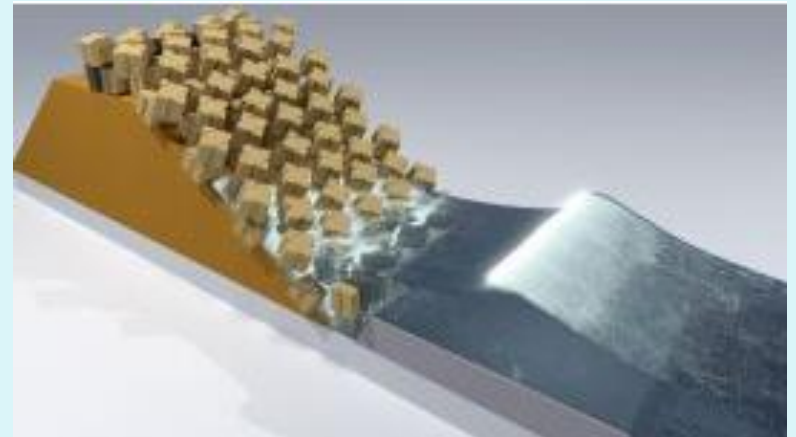
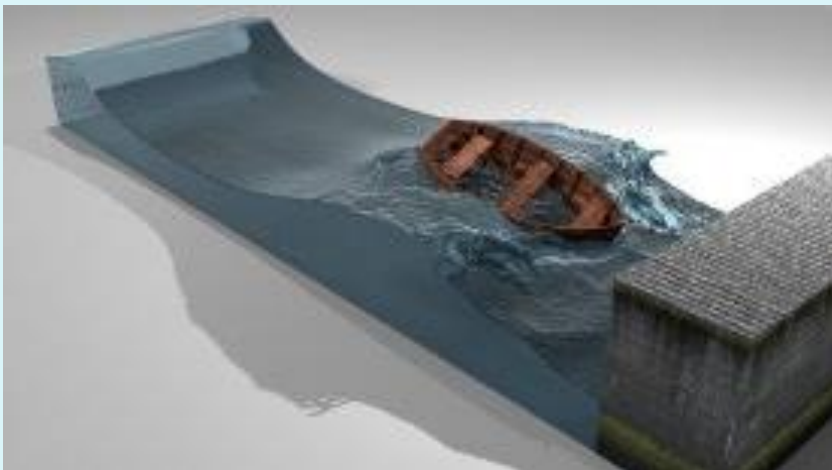
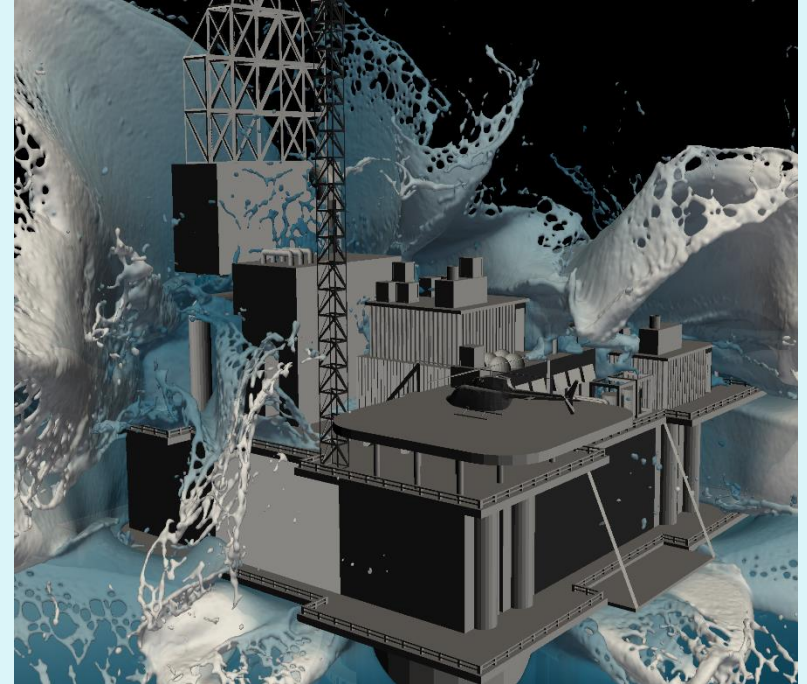
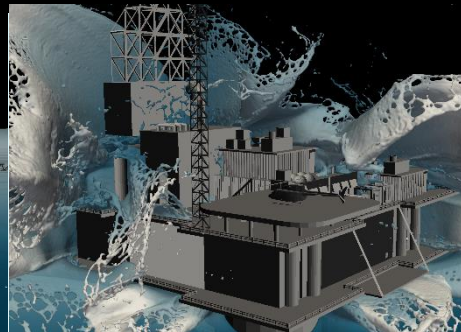
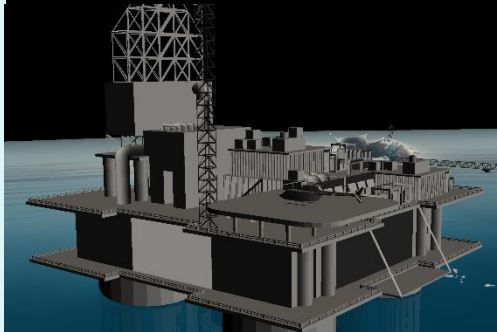
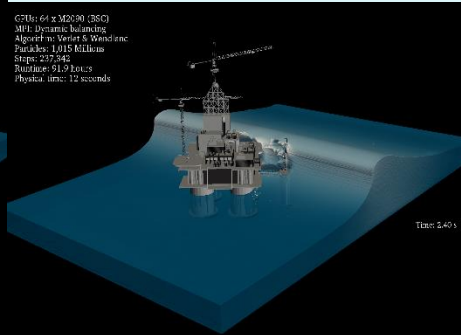
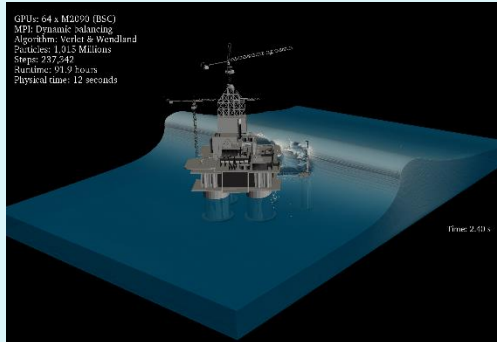
# Numerical simulations of a galaxy collision that produced the Galaxy pair KPG 302.



***Image of the Galaxy pair KPG 302 (left) and numerical simulation of the interaction (right).***



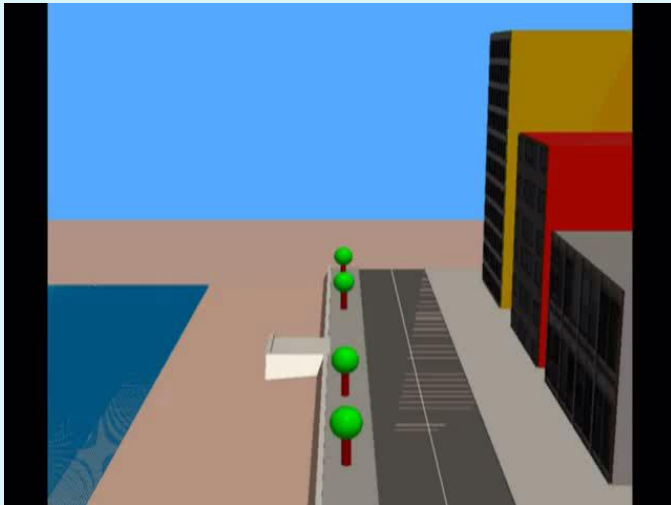
# Examples of simulations



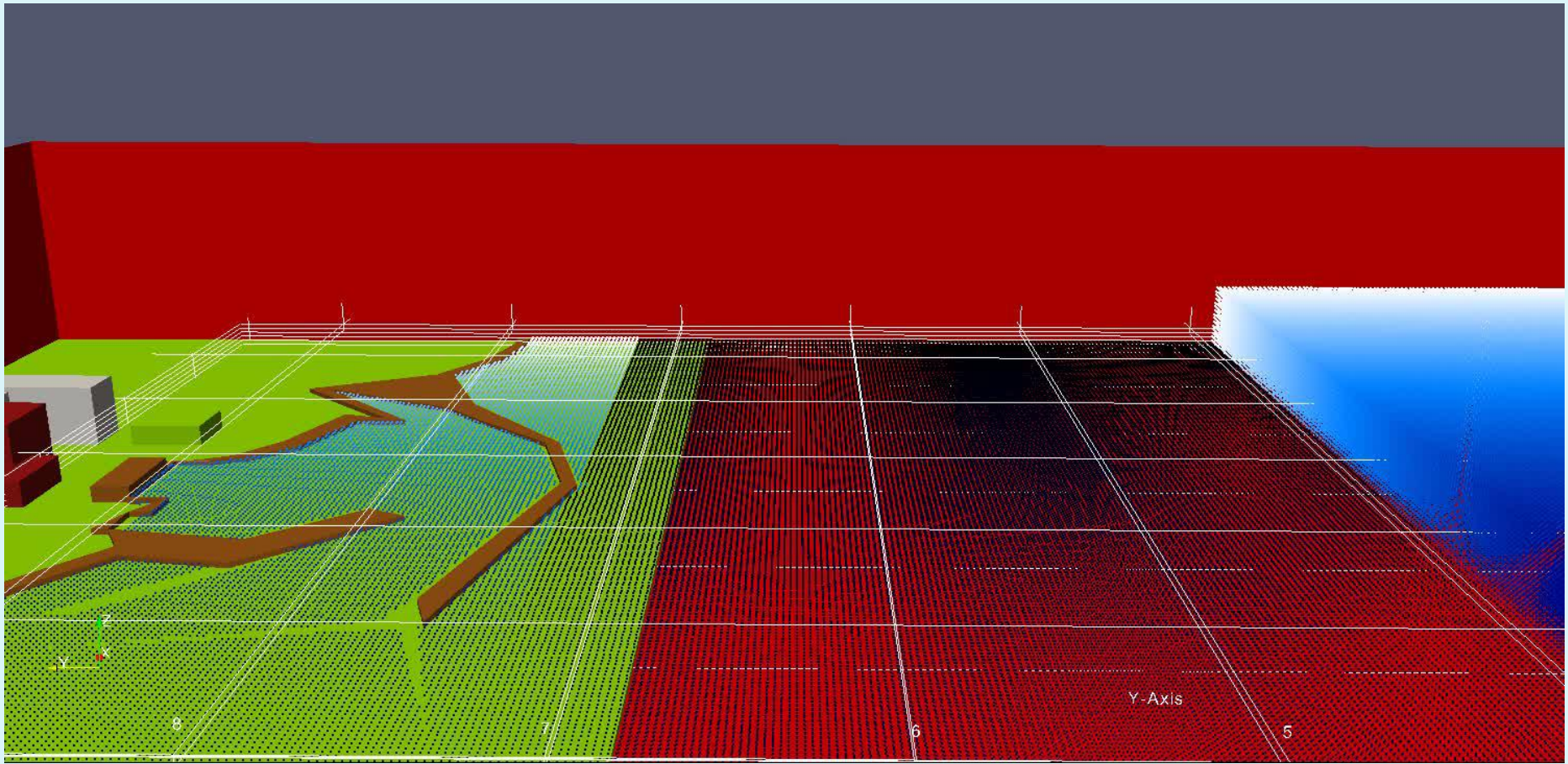


# SPH simulations with GPUs of tsunamis (or large waves) vs the Mexican Laguna Verde nuclear plant in Veracruz.

Code: collaboration with U. Vigo and U. Manchester

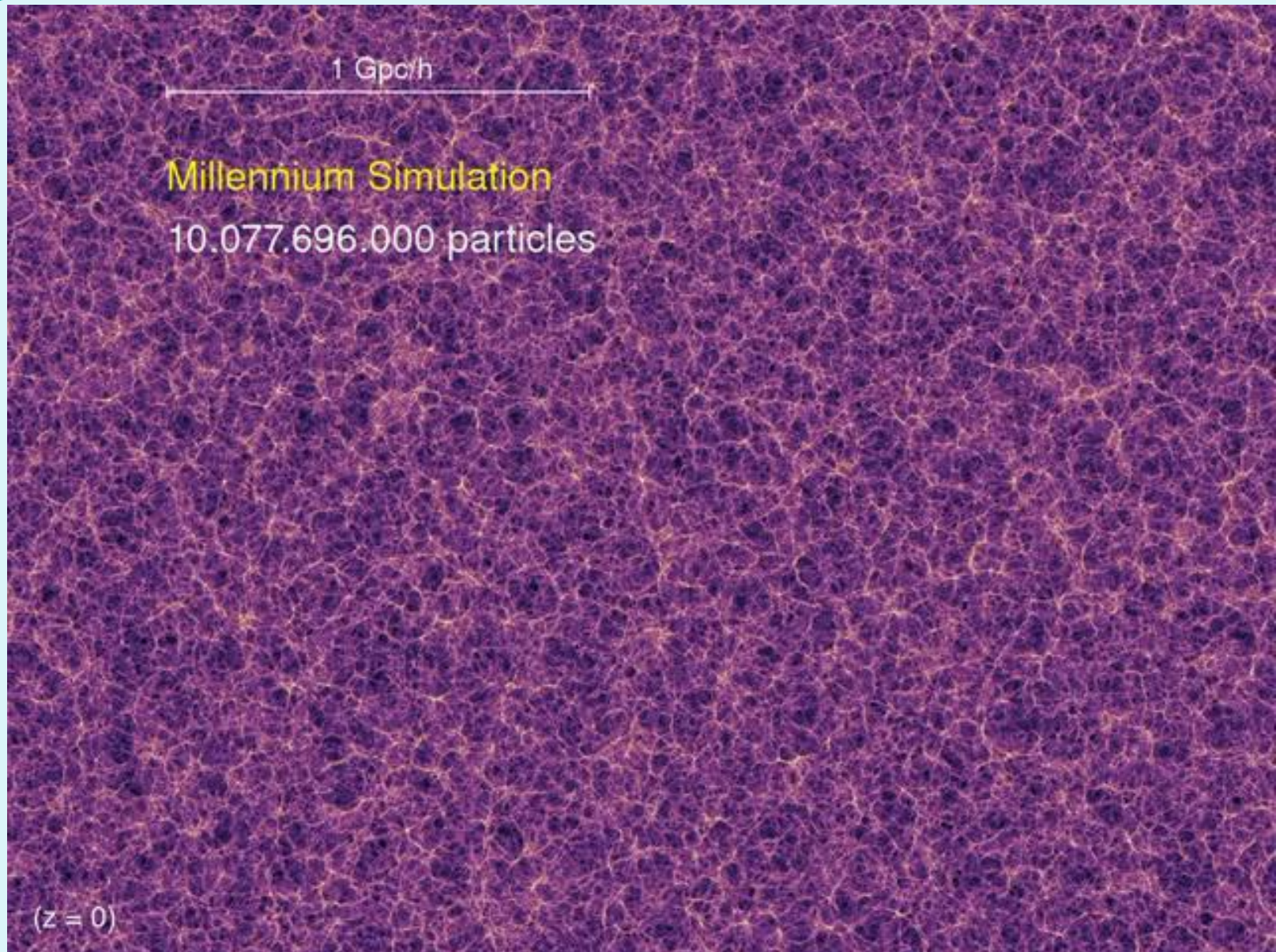








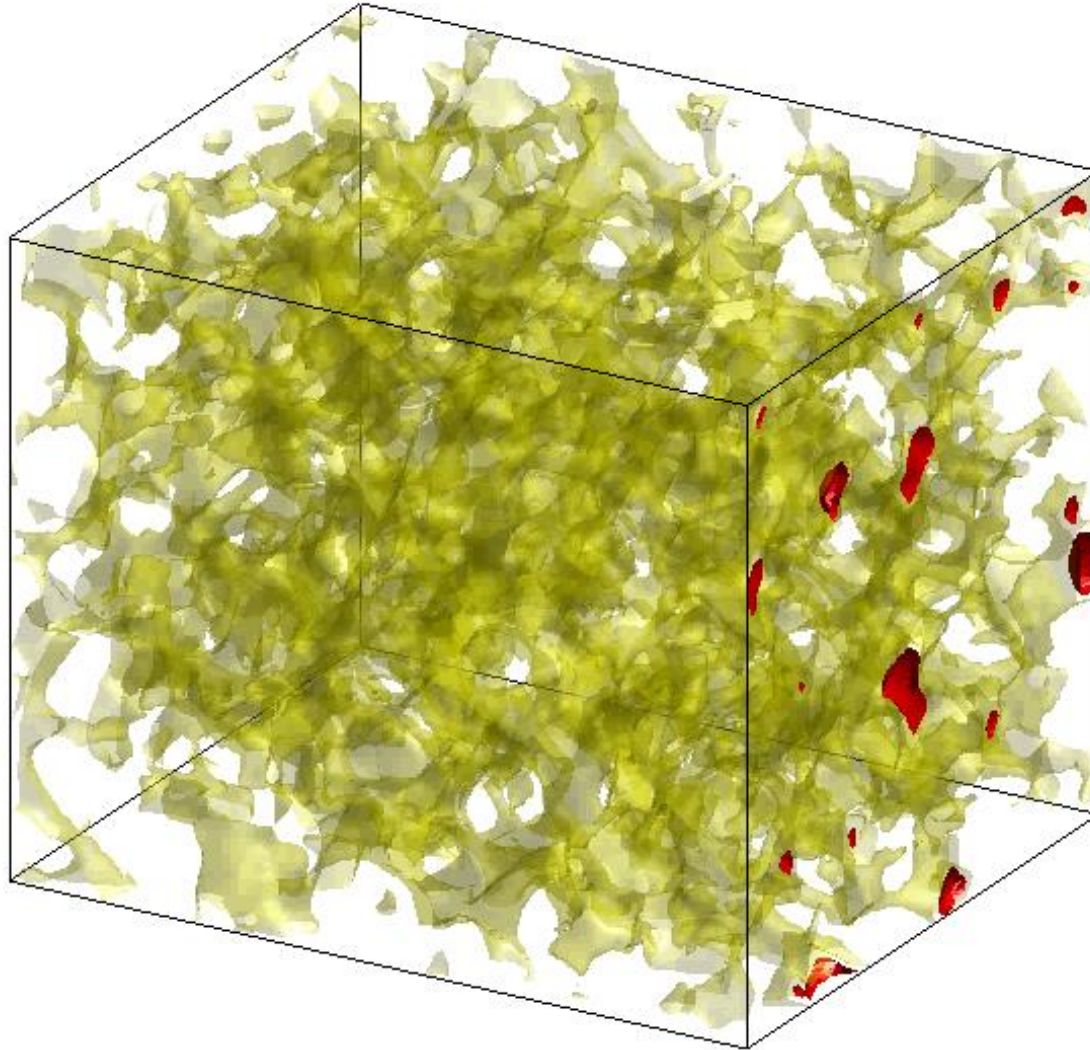
# Cosmology



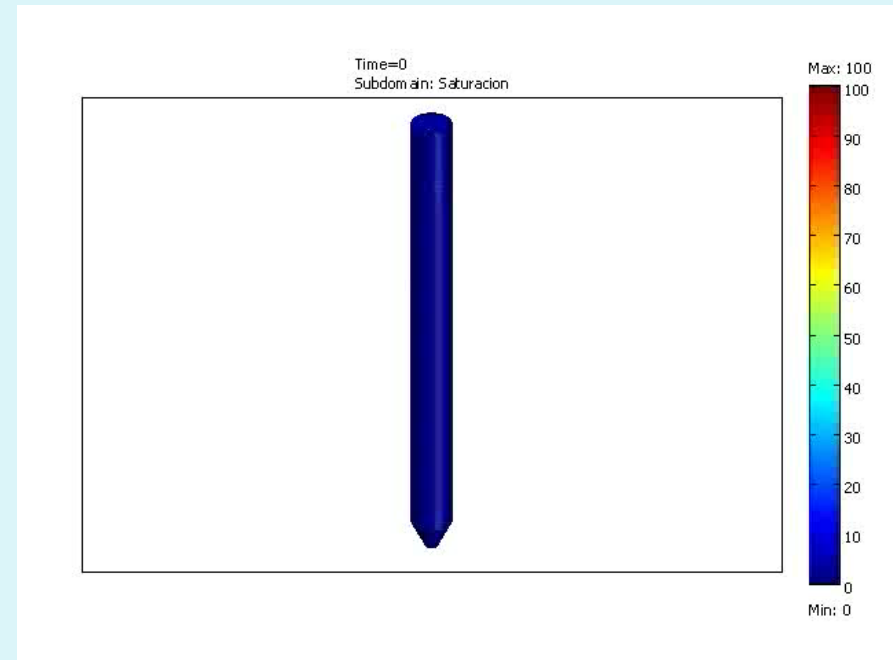
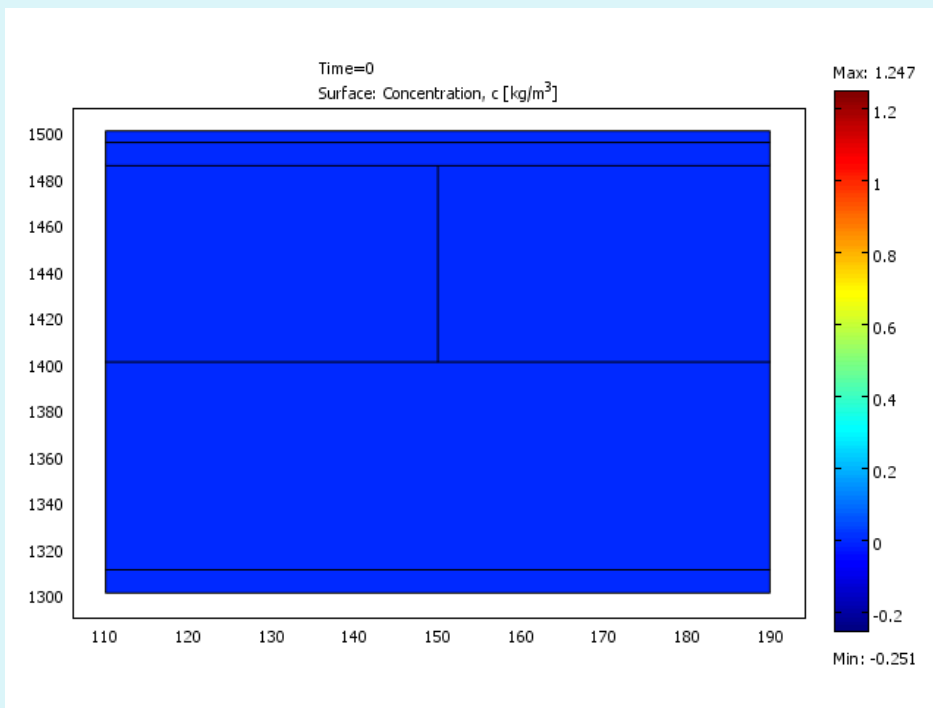


# Digital petrochemistry

$T = 800$



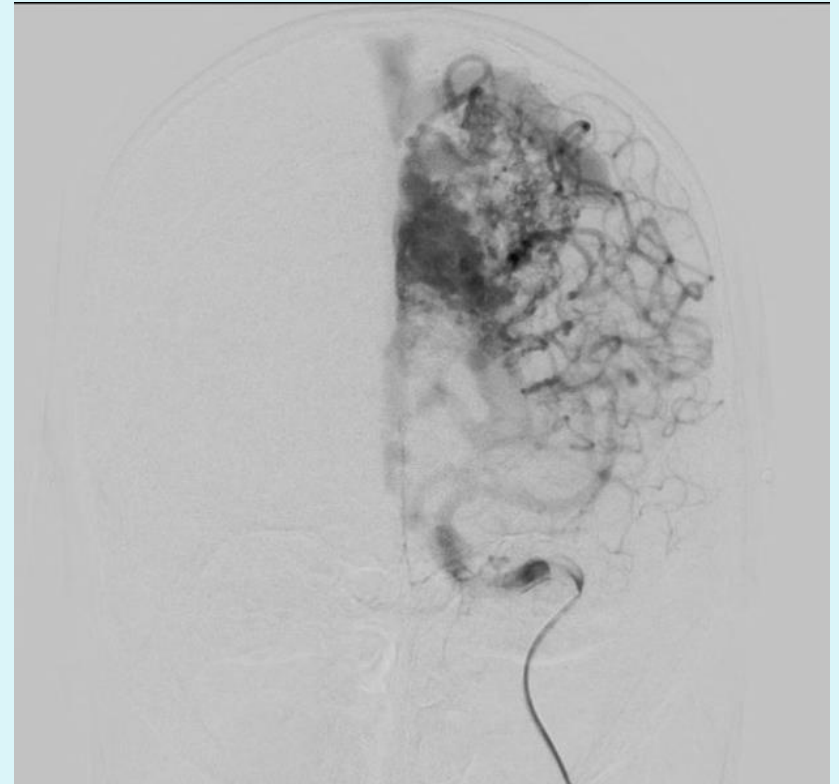
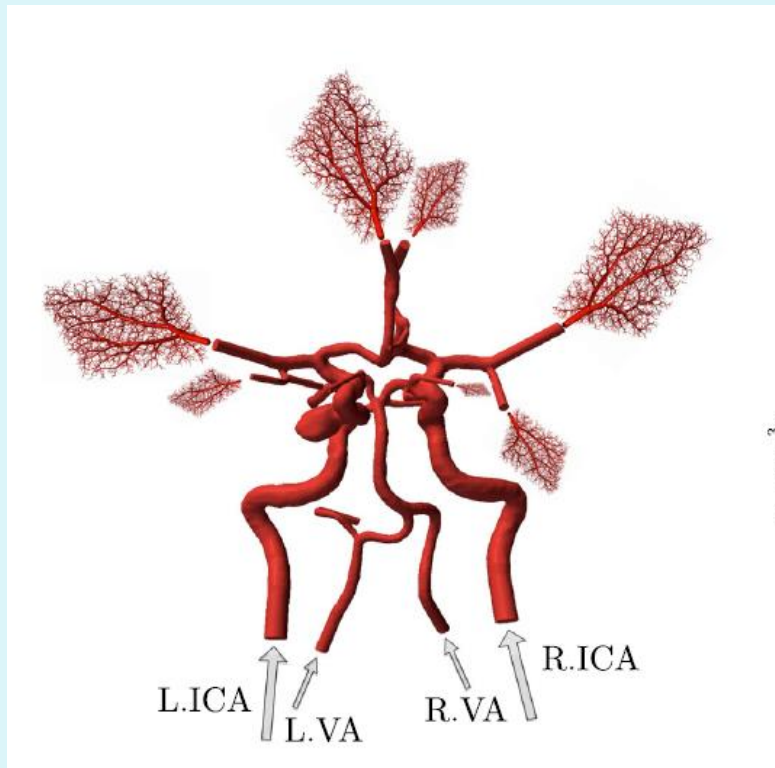
# Multiplase flow through a porous media: Radioactive material (left) and Absorption of Arsenic and Selenium by biomass (right). Codes: COMSOL and Alya.







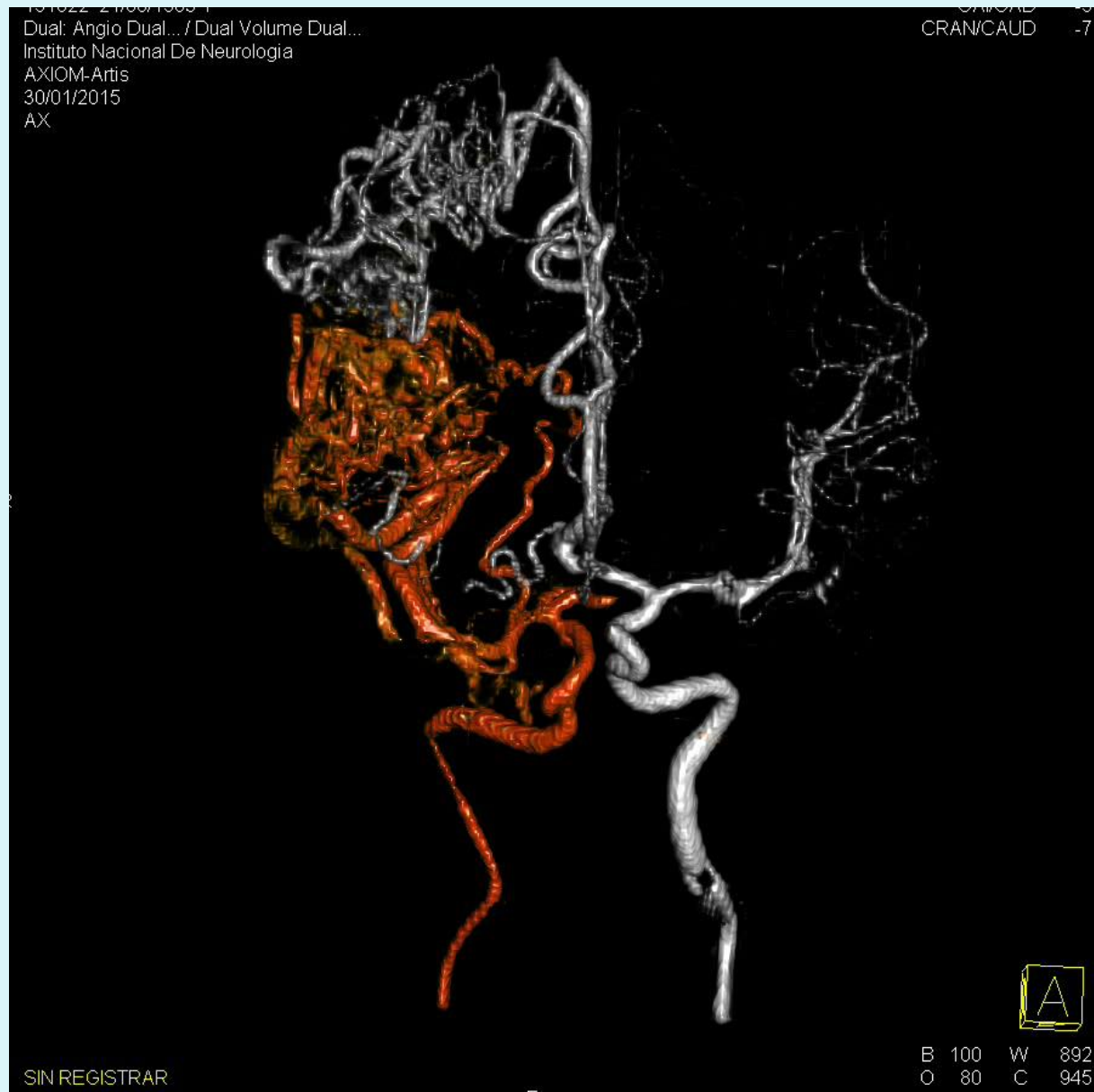
**Project: Hemodynamic simulations of brain malformations (MAVS), pre-treatment and comparison of patient variables. (Aid for helping surgeons in the treatment of Mavs, calculate risks for specific patients, better understanding the patient problem before surgery).**



# Brain arteries and arterioles system

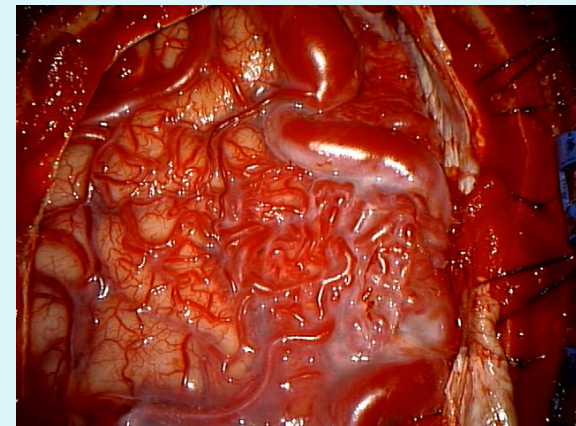
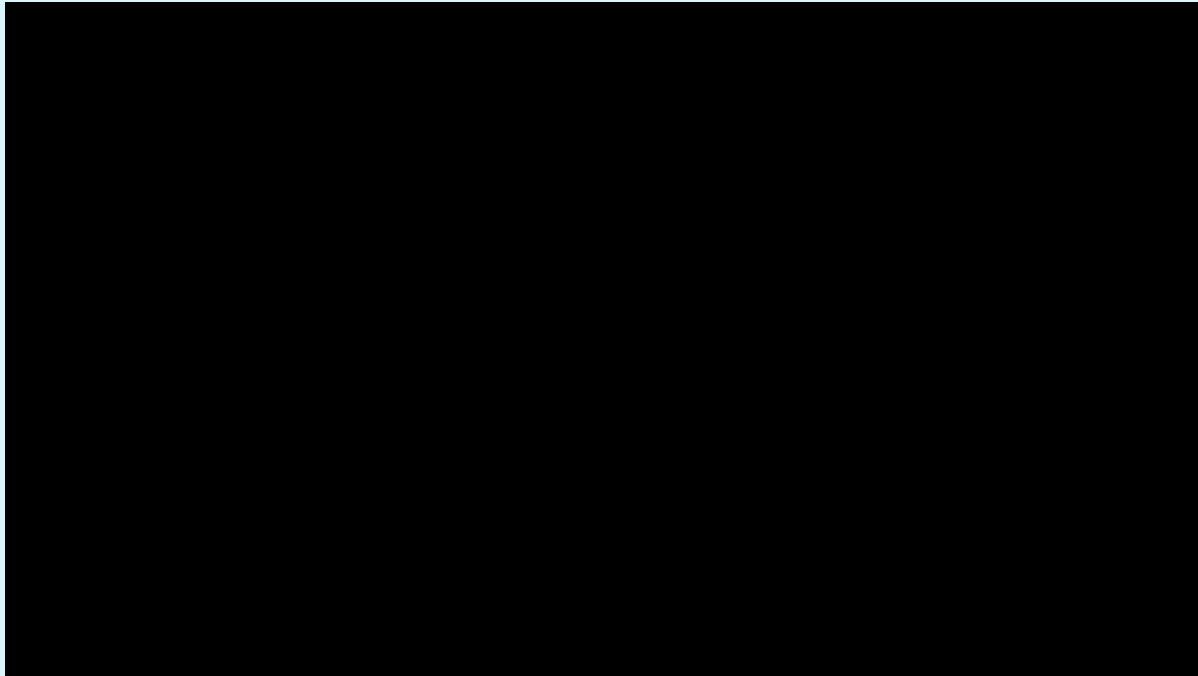
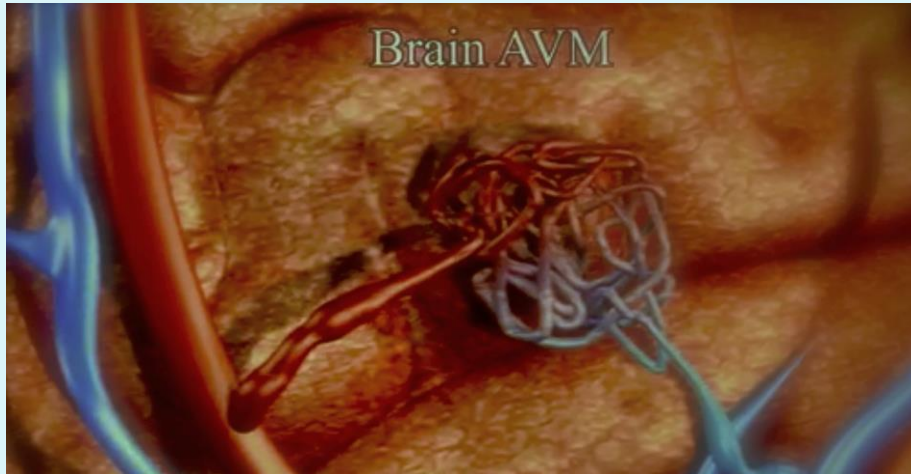


# Brain arteries and arterioles system

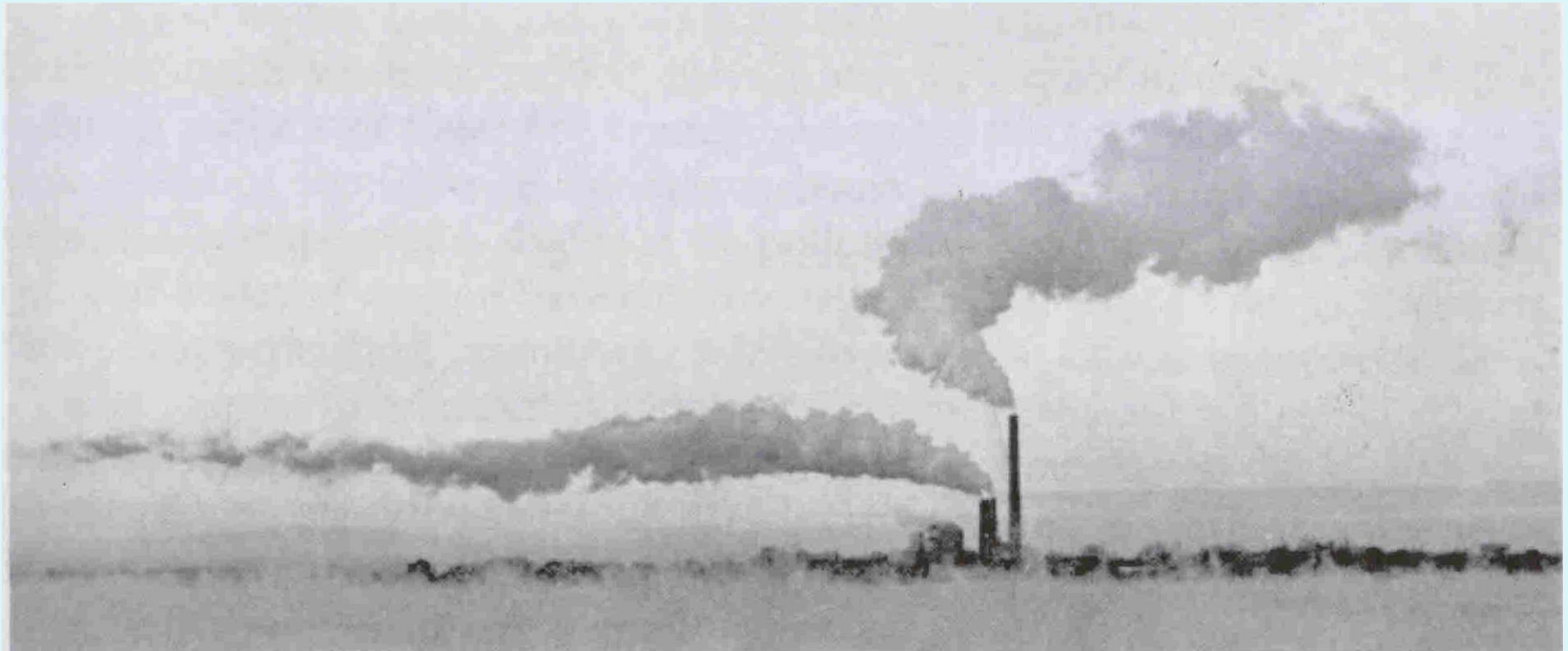


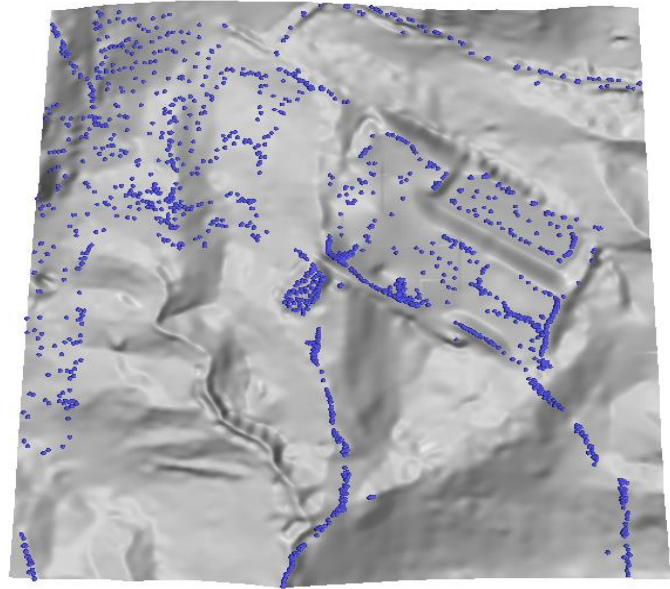
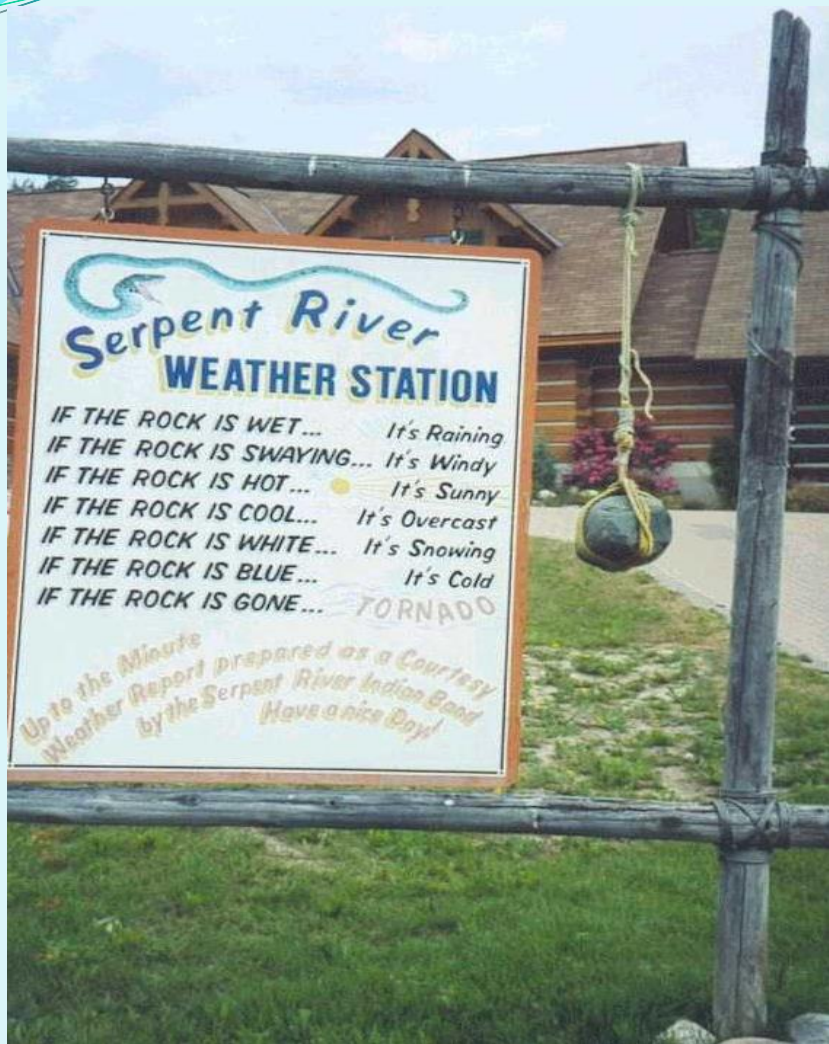


# Brain malformation (MAVS)

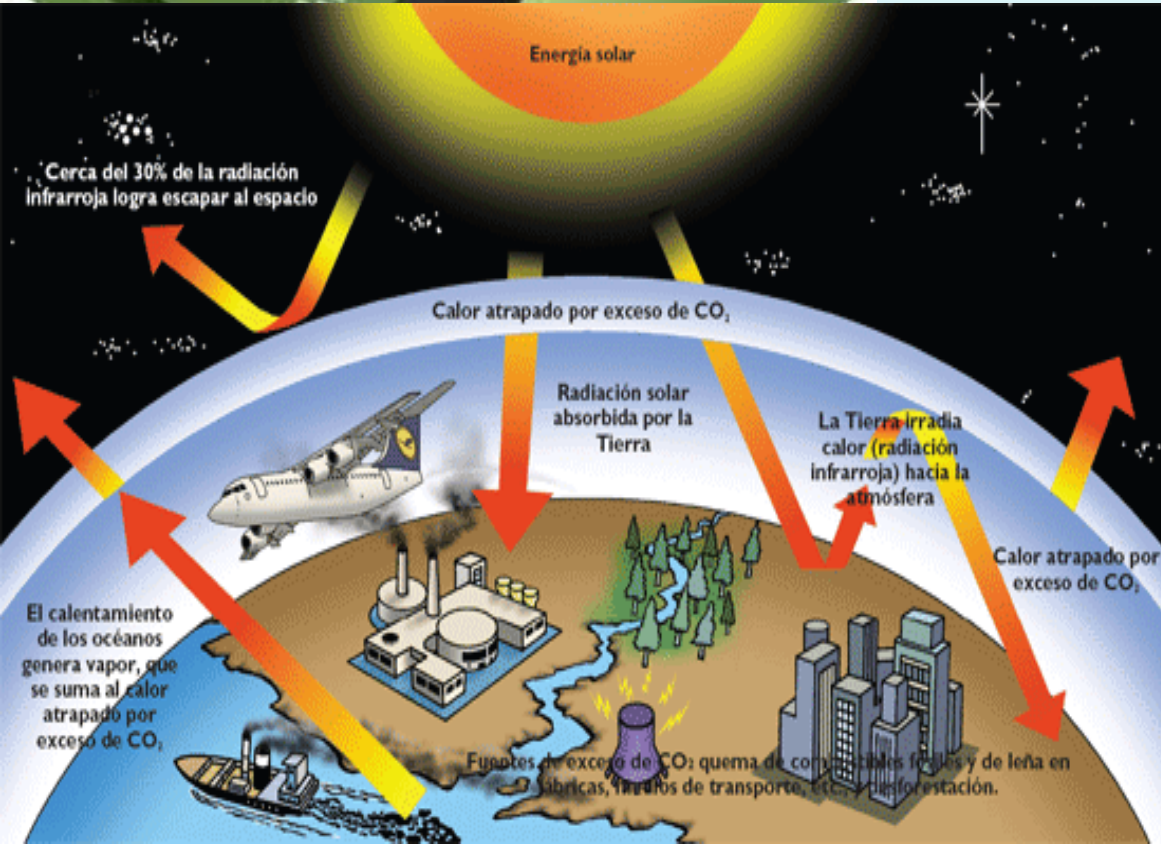
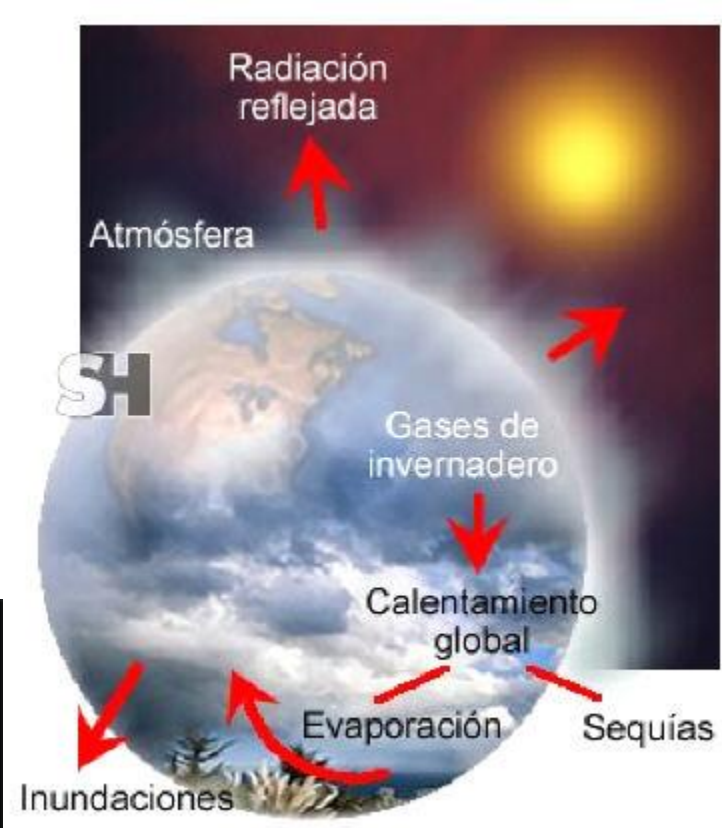


# Climate change, global warming, air quality and dispersion of contaminants in air (WRF)









*Atmospheric modelling is very complicate and computationally very expensive*



# Abacus forecast system

Weather Research and Forecast Model(WRF) para Mexico

[Características](#) [Acerca de](#)

## Fecha

📅 03/03/2012 (Sábado)

🕒 00:00 UTC [Local 18:00]



## Parametros de pronostico

Dominio:

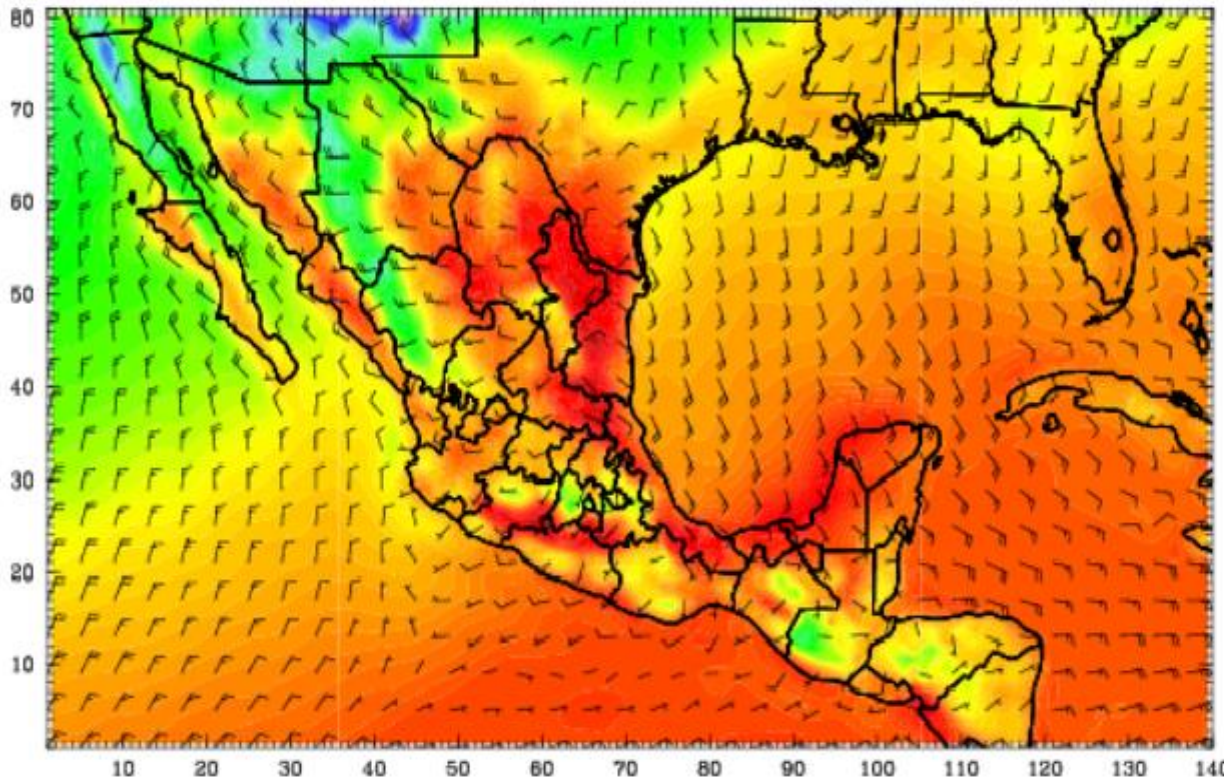
Region 1

Tipo:

Mapa

Variable:

Temperatura



# Intelligent cities







**IBM**

Welcome to  
TheSmarterCity™



Watch the Documentary

Smarter Industries ▶



Transportation  
Airports & Rail



Public Safety



Social Services



Education



Healthcare



Economic  
Development



Transportation  
Traffic



Energy & Utilities



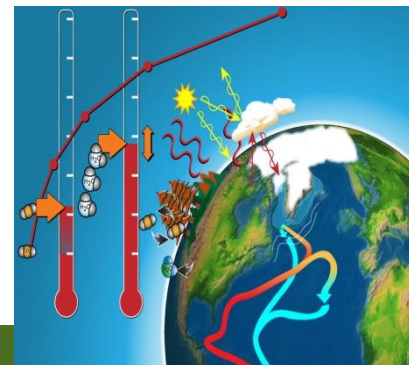
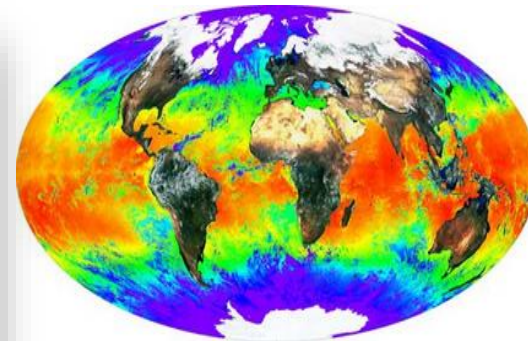
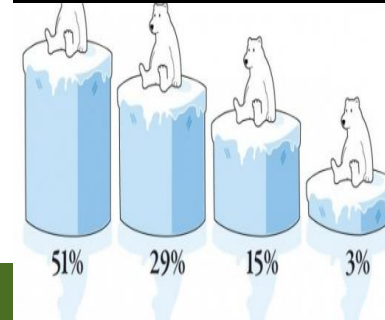




**EDOMEX PROJECT:** GLOBAL WARMING STUDY IN THE STATE OF MEXICO FOR UNDERSTANDING THE FOREST IMPACT ON GLOBAL WARMING AND TO HELP THE GOVERNMENT TO TAKE SPECIFIC MEASURES TO REDUCE GLOBAL WARMING  
(PROJECT WITH CONAFOR: NATIONAL FOREST COMMISSION)



**Forests** play a role of great importance to mitigating climate change, since they have the ability to attach and absorb the carbon dioxide (CO<sub>2</sub>), one of the main greenhouse gases, in a natural way and thereby regulate the climate.



*Devaluation of the ecological functions of forests: by not having clear and precise information of the percentages of greenhouse gas removals.*



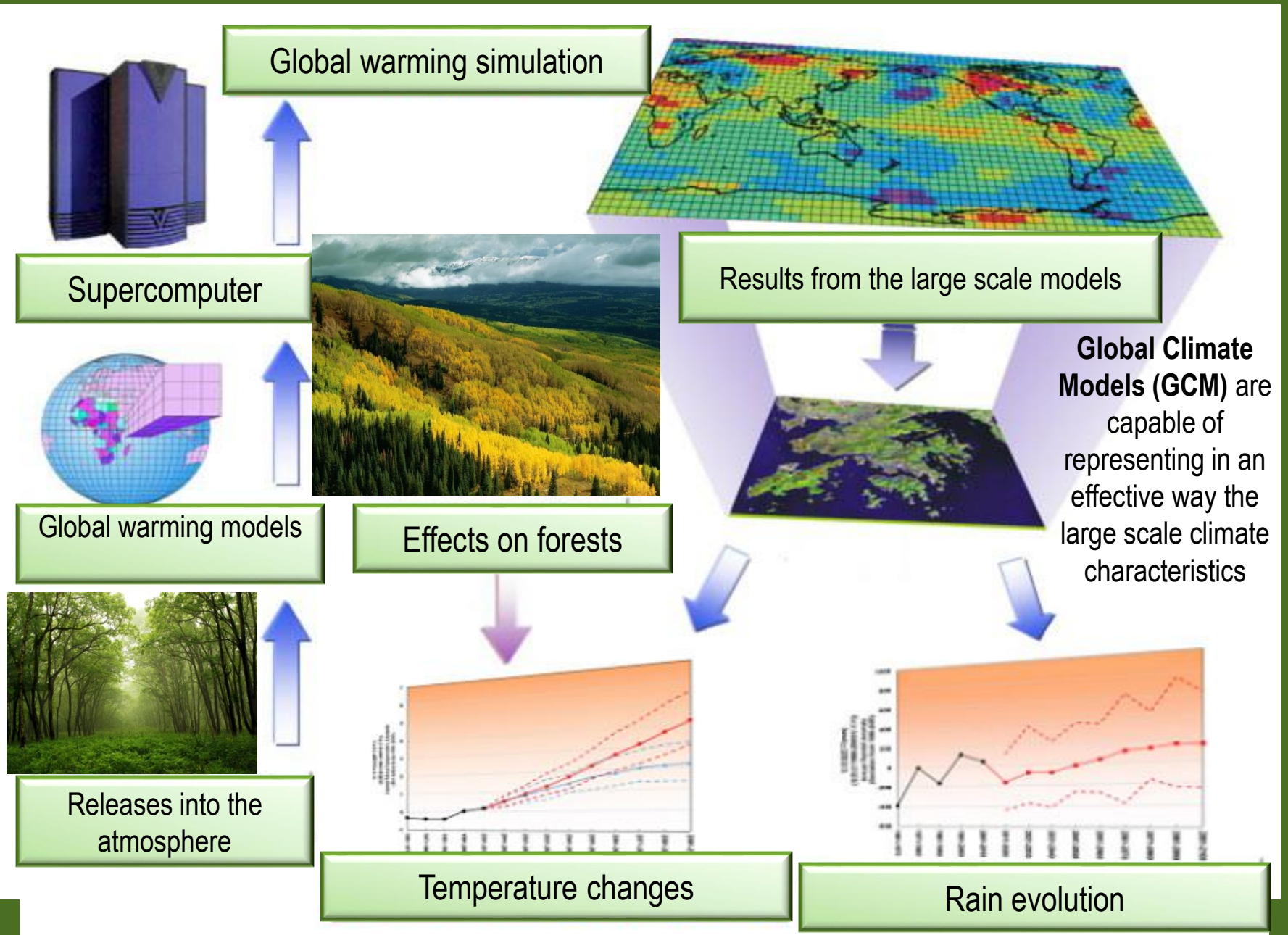
## **Preliminary proposal of domain definition over the state of Mexico for climate change simulations:**

**resolution 30 km, 360x160 cells**

**Domain 2: resolution 10 km, 226x148 cells . Both centered in 21°N,-99°W**



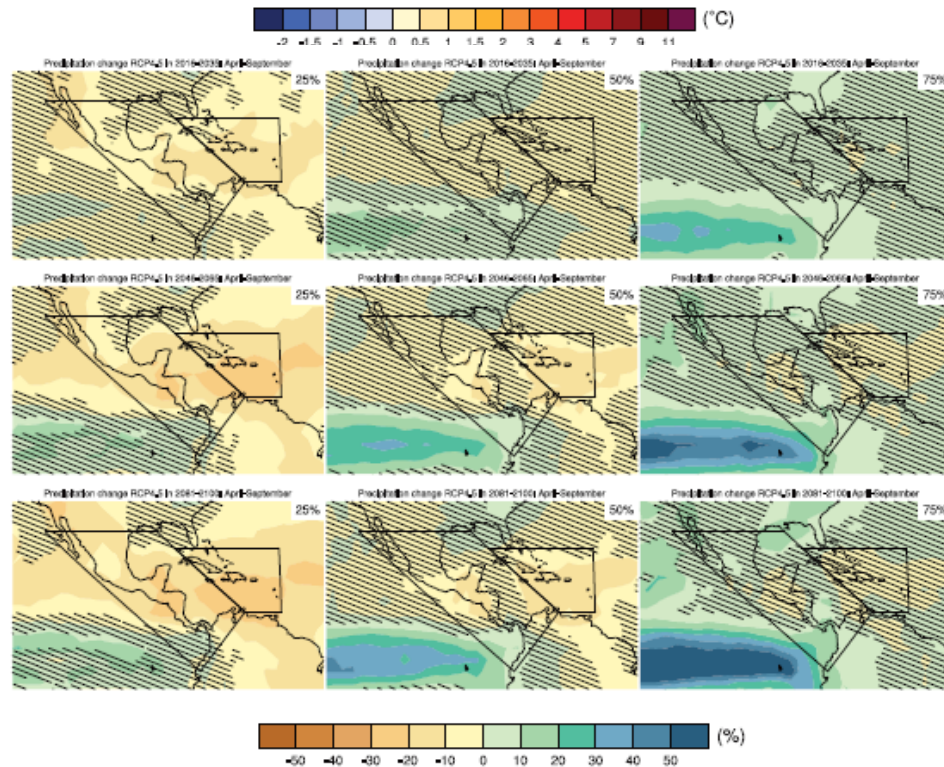
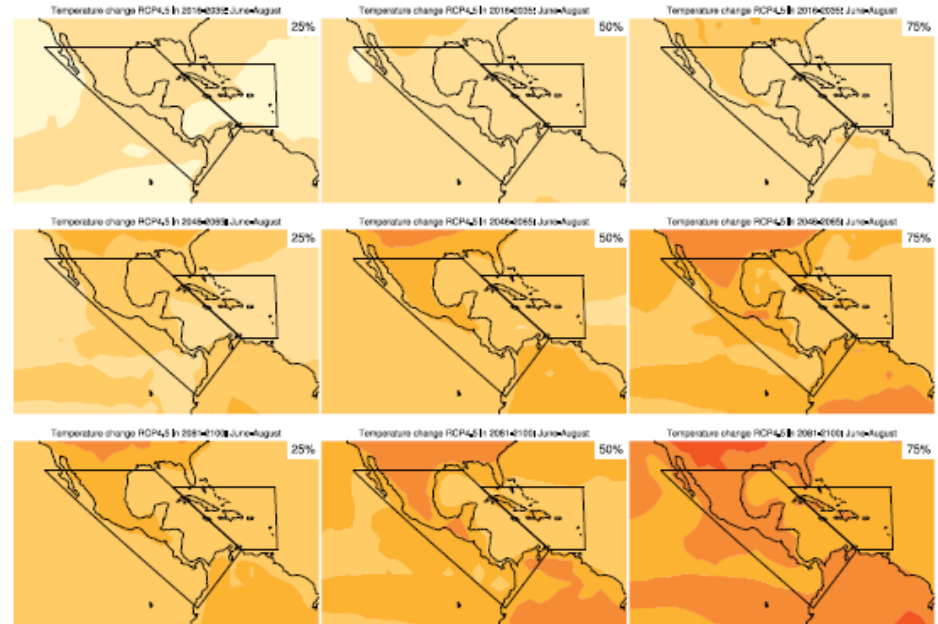
# Simulation of the control period using GCM data



# Projections of regional climate for Central America (IPCC, 2013)

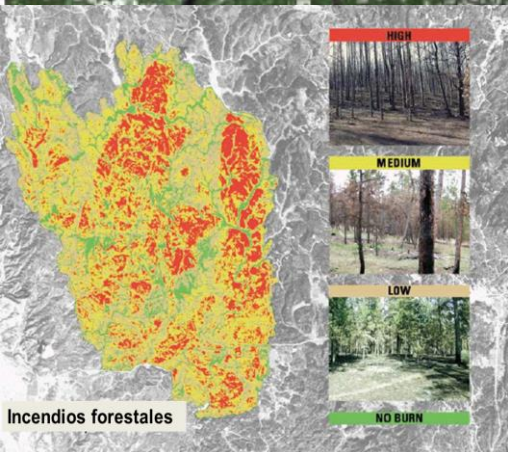
*IPCC Intergovernmental Panel on Climate Change*

Projected changes in temperature (June to August) and precipitation (April to September) in different future periods (2016-2035 and 2046-2065, 2081-2100) regarding the current conditions (1986-2005), according to forecasts by the RCP4.5

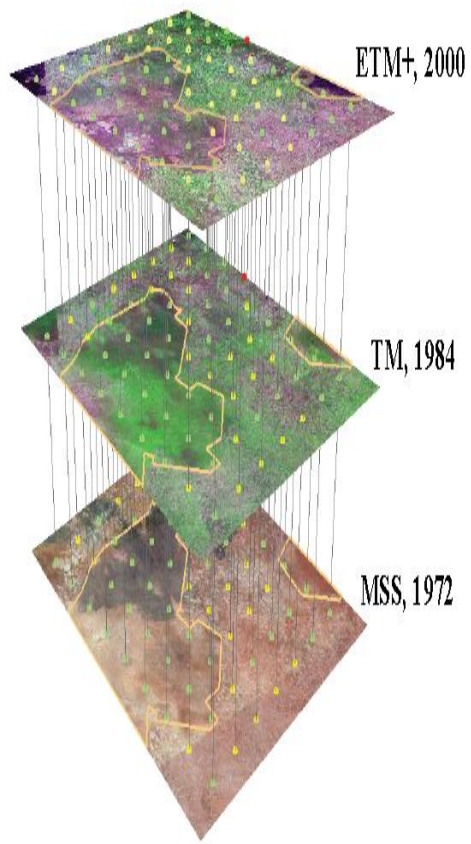
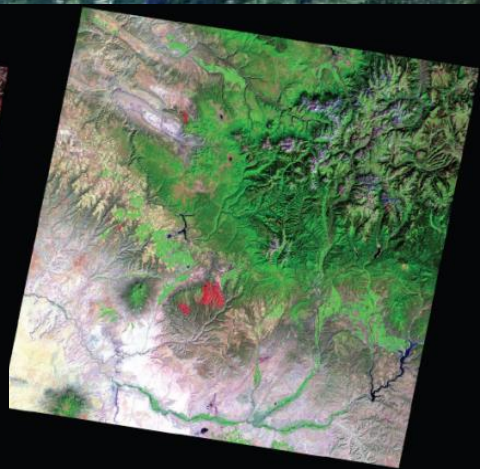
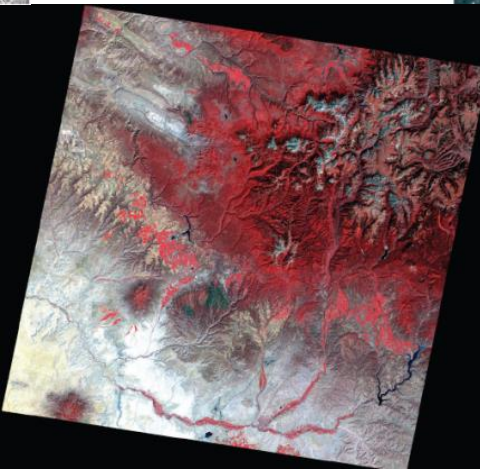
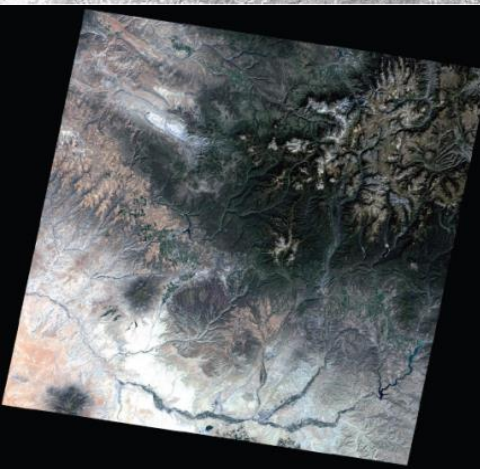
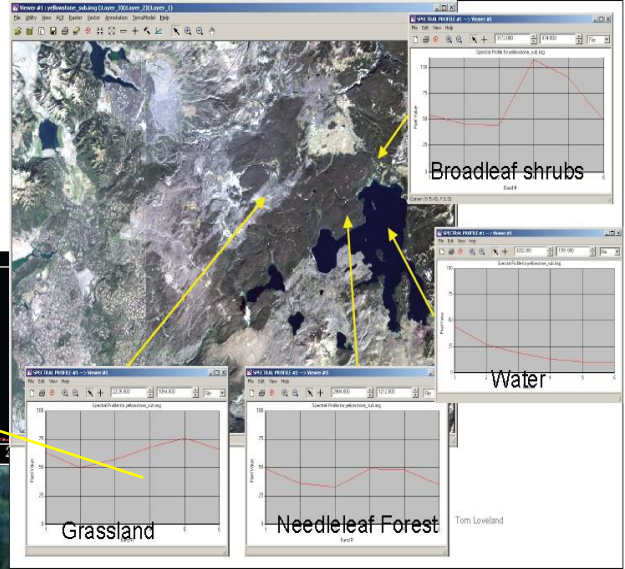
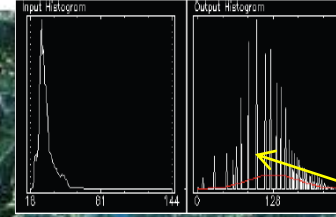




# Vegetation cover change detection



ERDAS, ENVI, IDRISI, ILWIS,  
MULTISPEC, GVSIG, ARCGIS





**Stage 4**

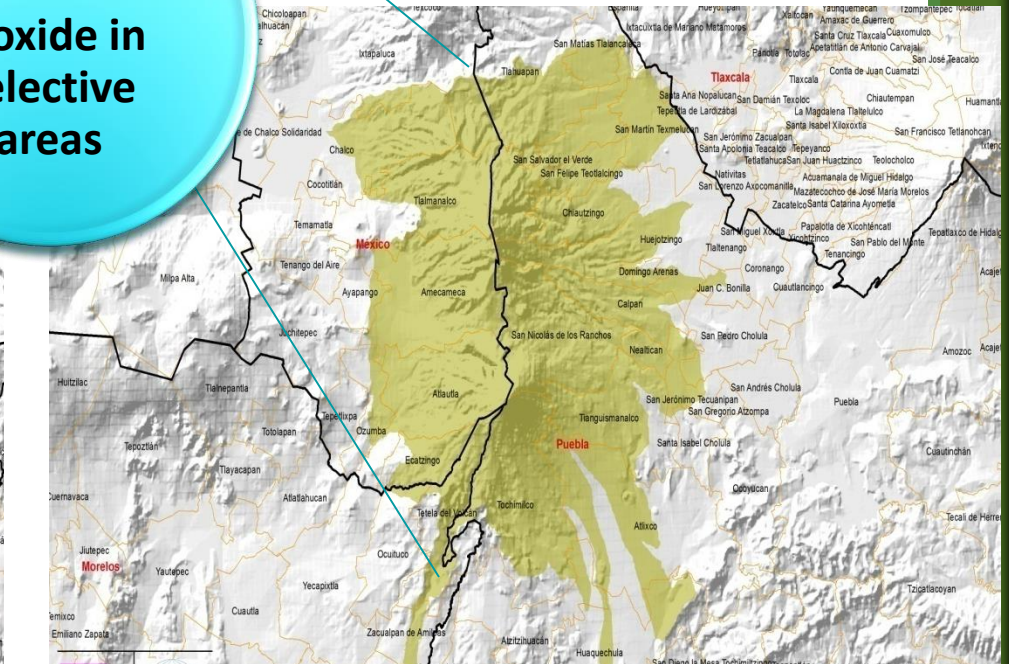
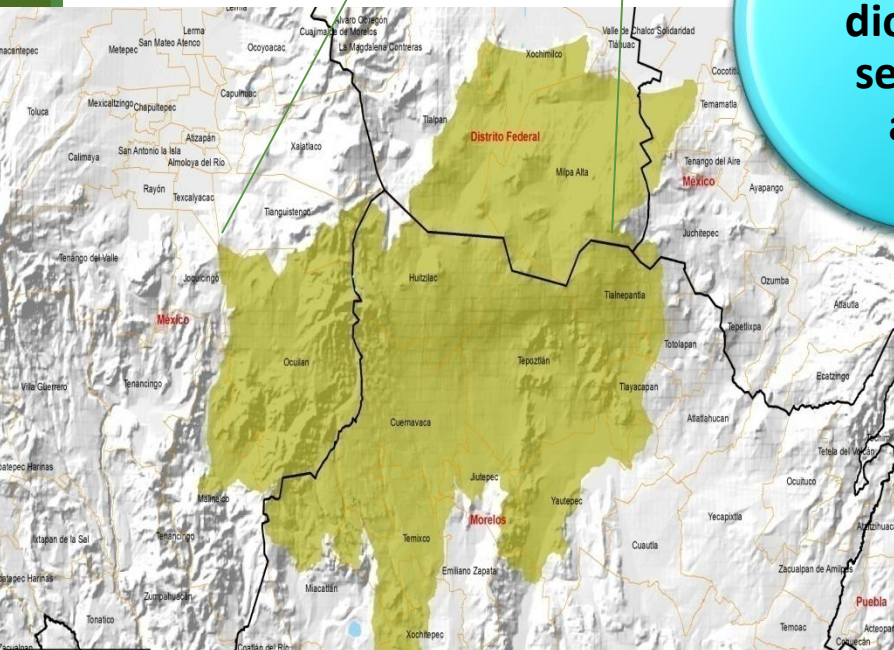
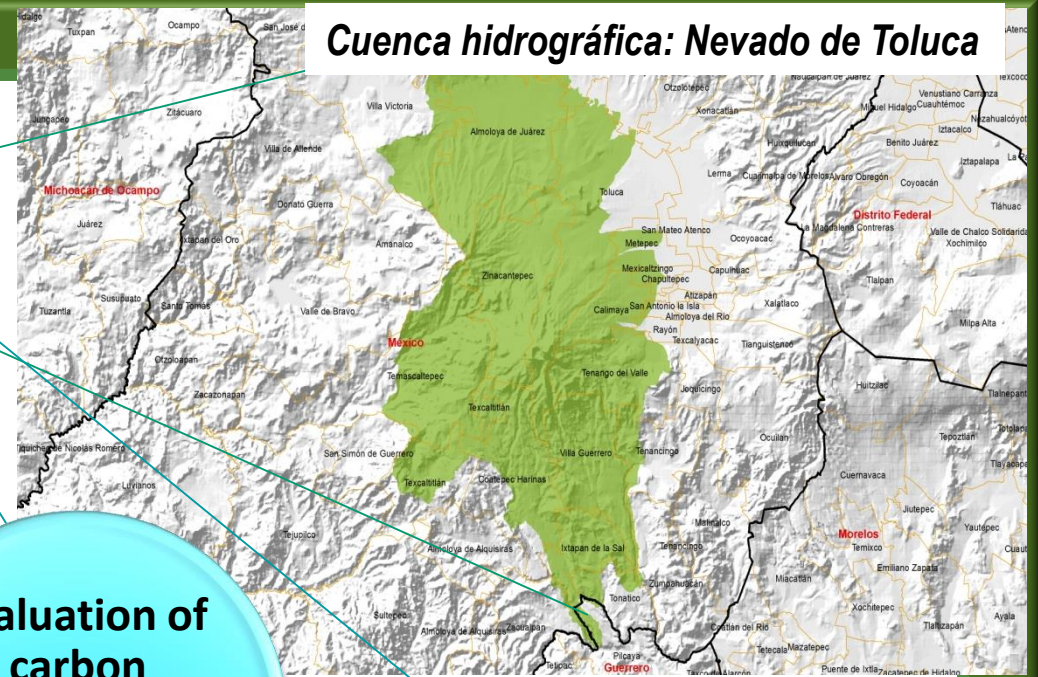
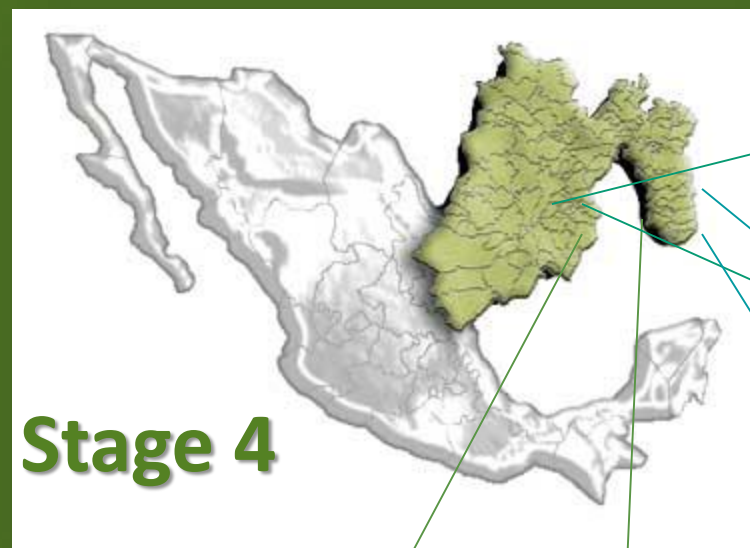
**CONAFOR**

**Evaluation of carbon dioxide in selective areas**

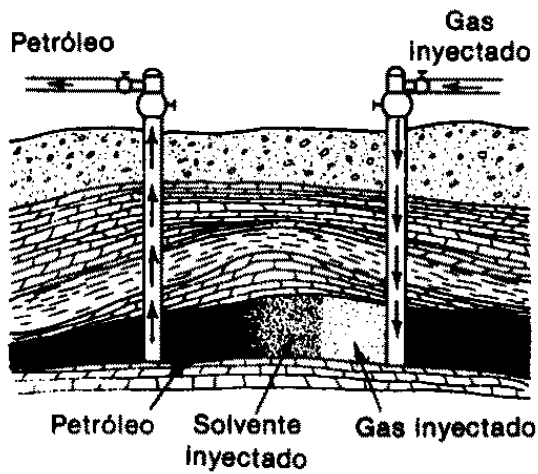
**Cuenca hidrográfica: Nevado de Toluca**

**Cuenca hidrográfica: Chichinautzin**

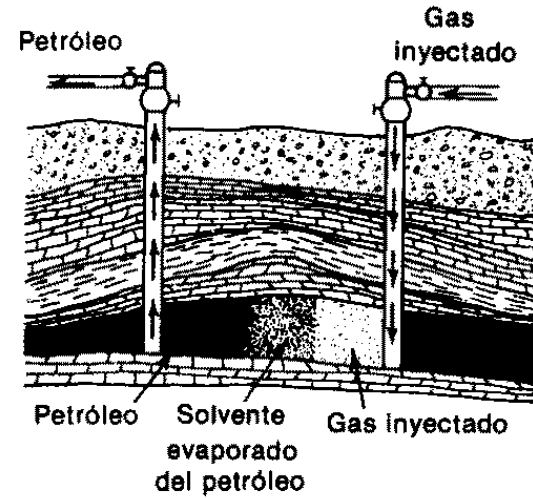
**Cuenca hidrográfica: Iztaccíhuatl–Popocatépetl**



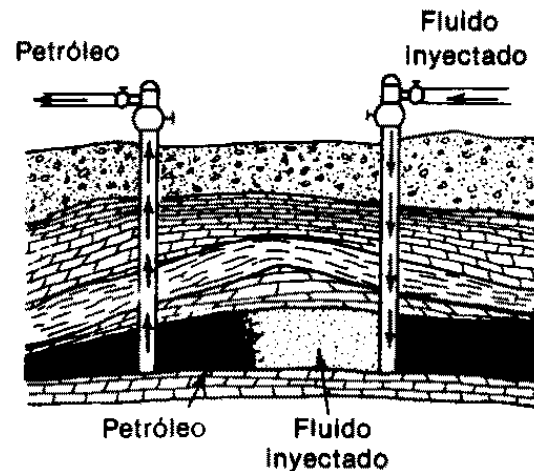
# Simulator of naturally fractured reservoirs



(a)



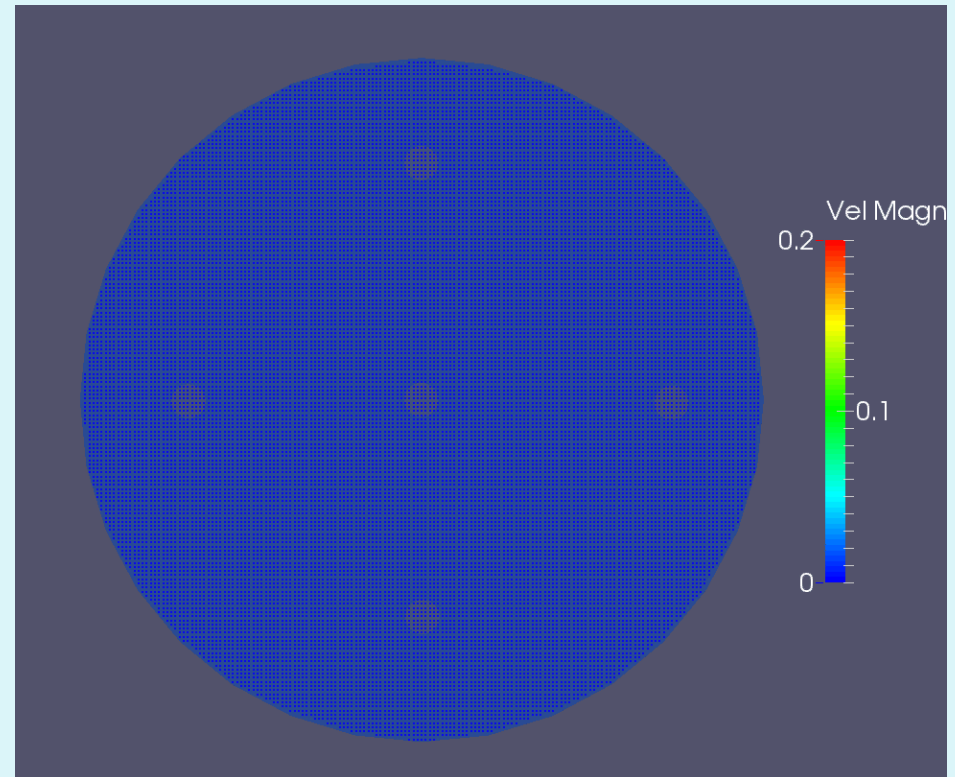
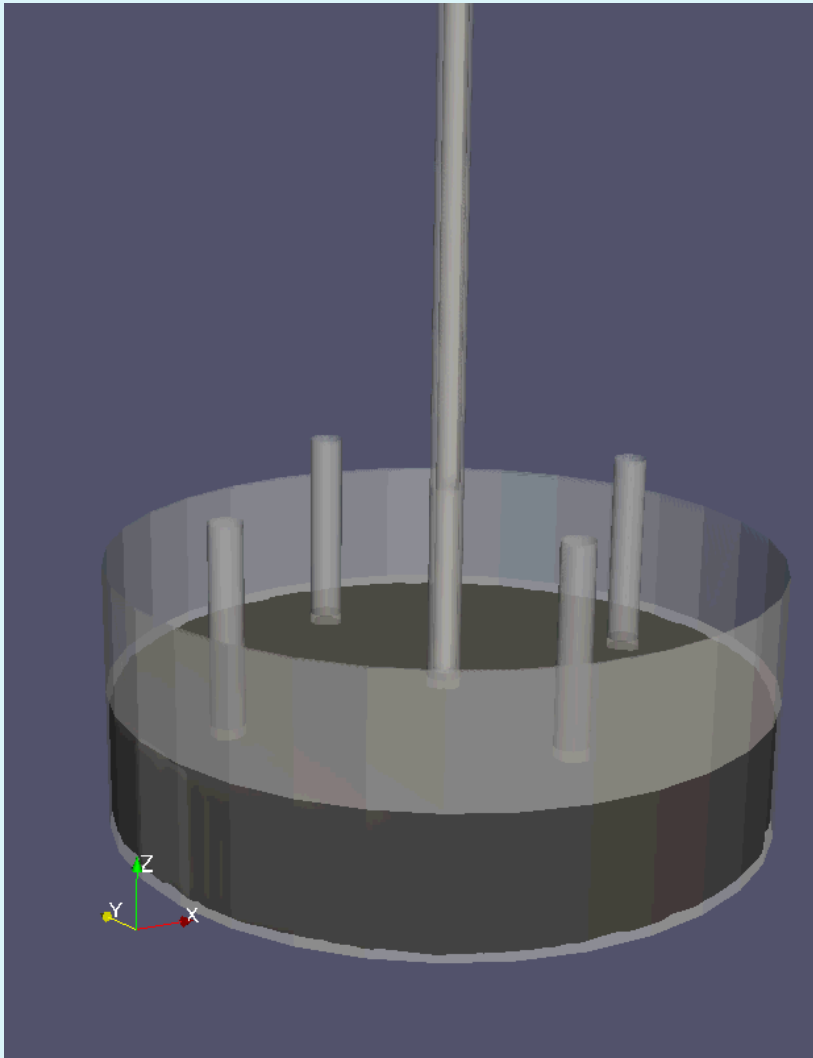
(b)



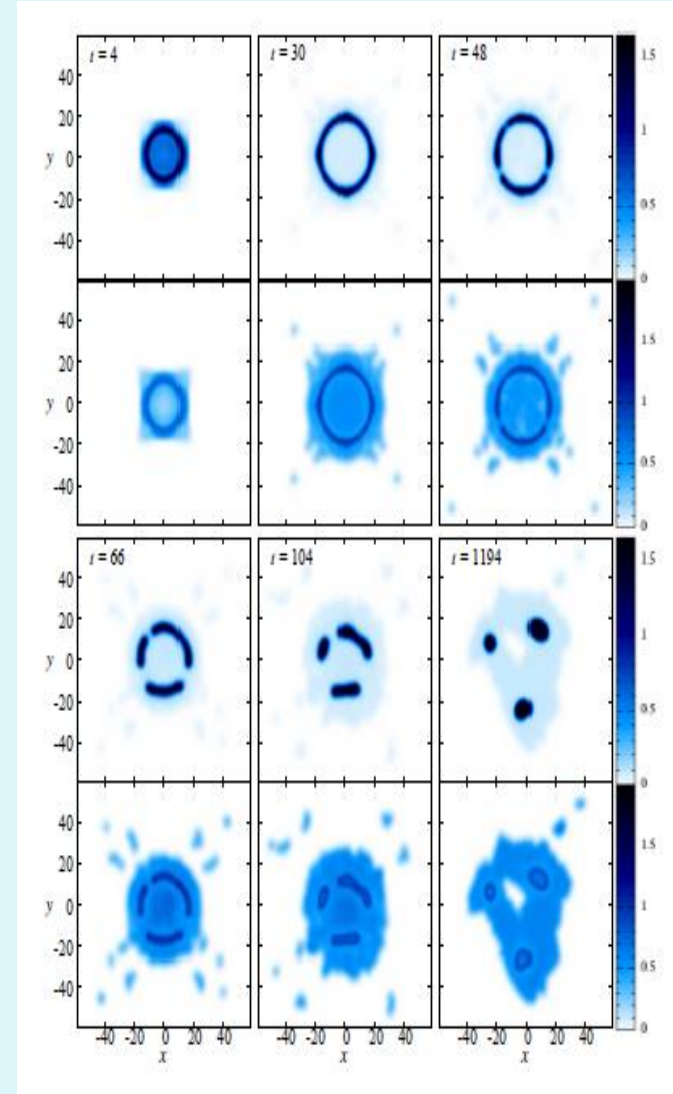
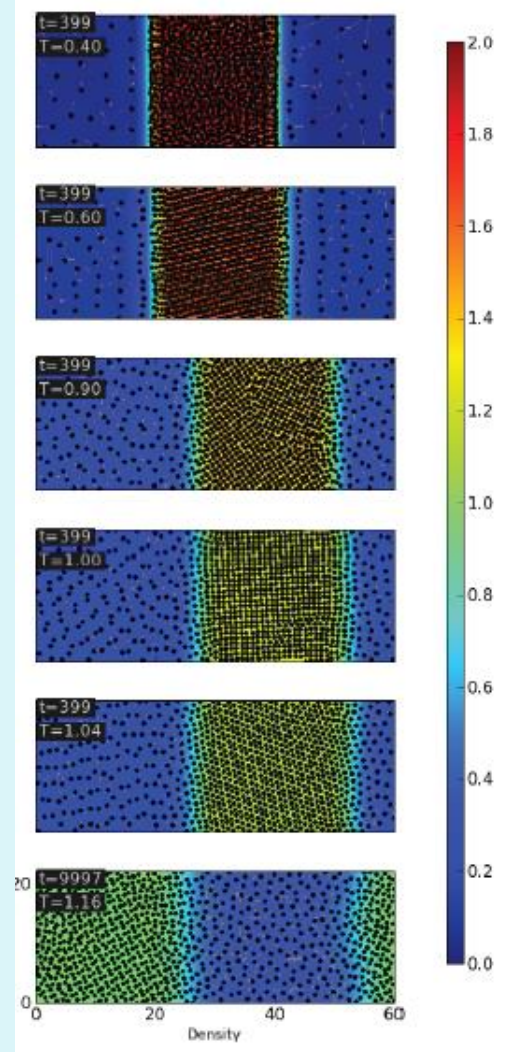
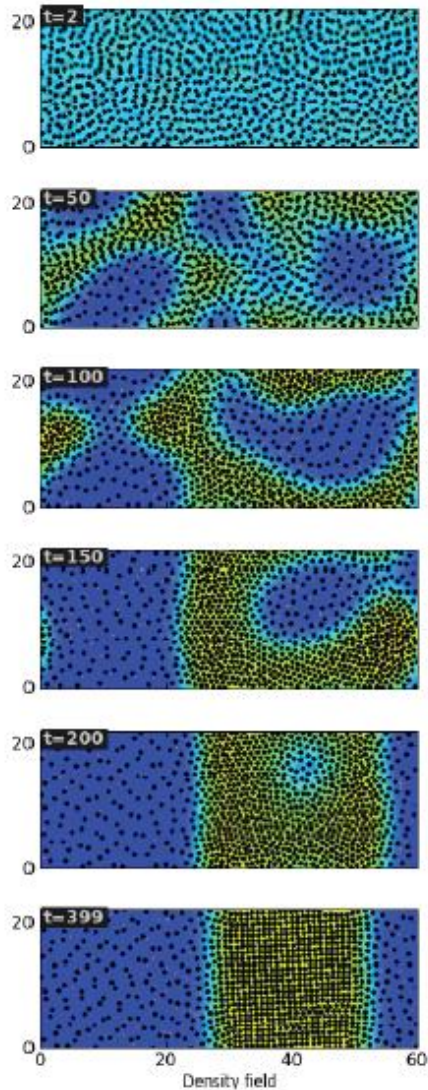
(c)

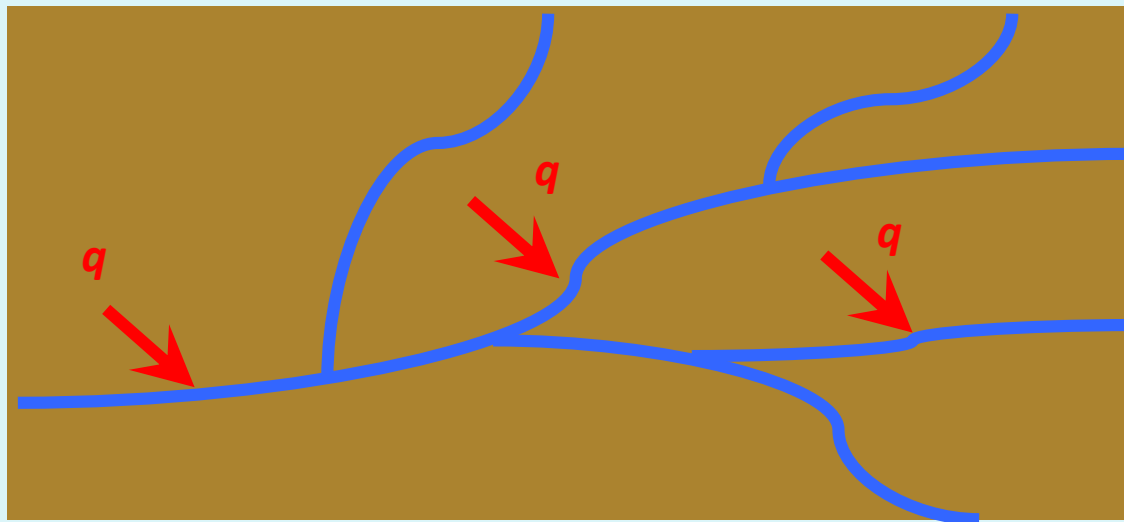
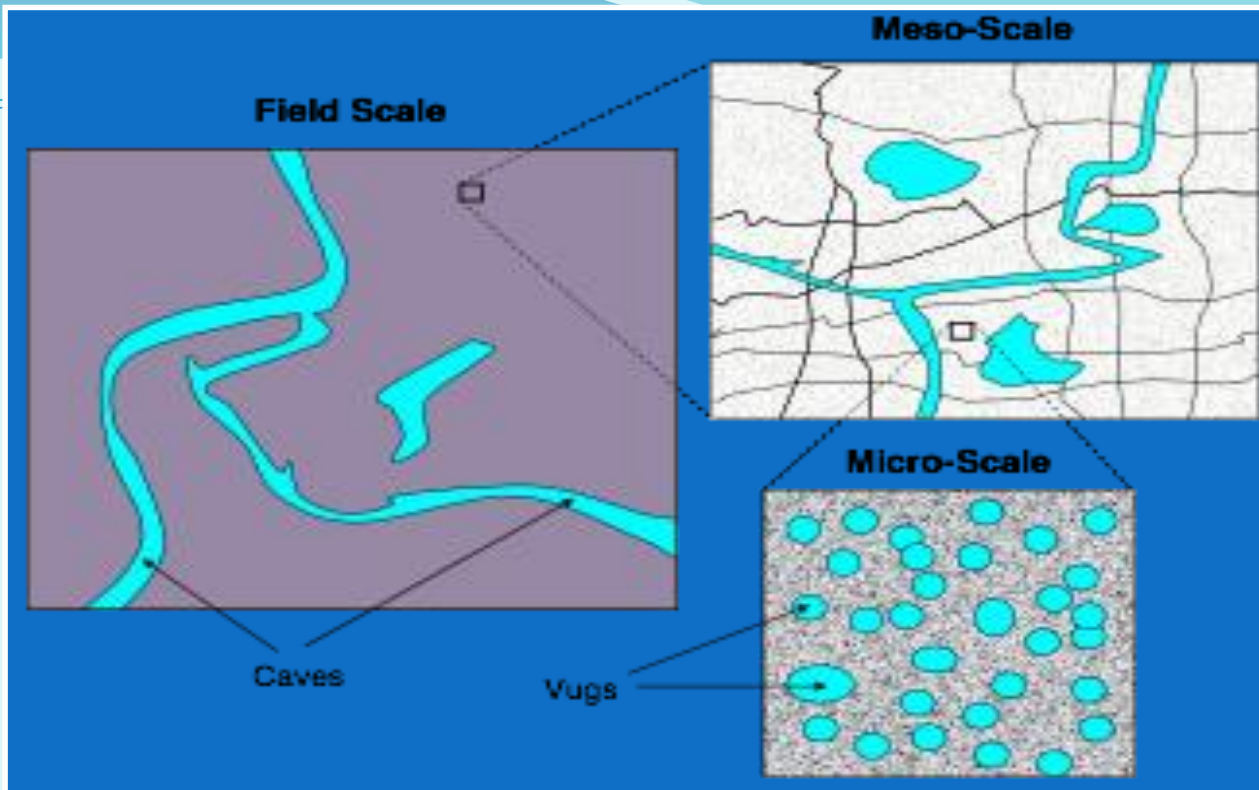


# Injection of gas and liquids for oil extraction



# Modeling of 2-phase coexistence, surface tension, capillarity and porosity.







# Conclusions

We have presented some of our Computational Fluid Dynamics Projects.

The Abacus Project will produce a large amount of data, perhaps 1 PB per year.

We have to solve the problem of moving the data to the final user.

I have only described the Computational Fluid Dynamic applications in Abacus, we have many more applications: biology, chemistry, energy, medicine, engineering, economy, health, etc.