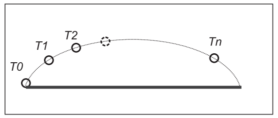
Lecture 1

source

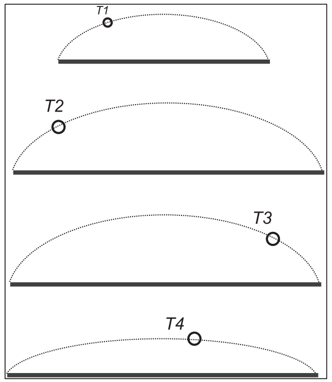
www.tevza.org/home/course/modelling-II_2011

Why model?



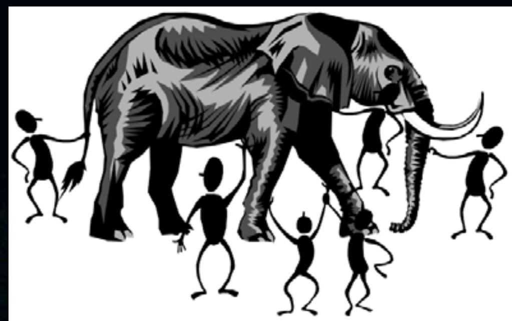
Consequent data

Inconsequent data:



Modelling Elephant

How good is the model?

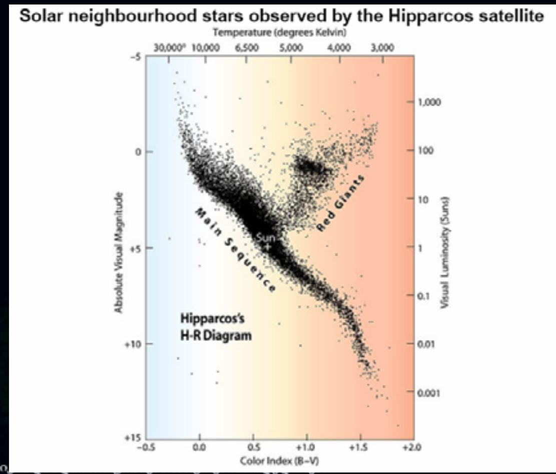


Astrophysical simulations

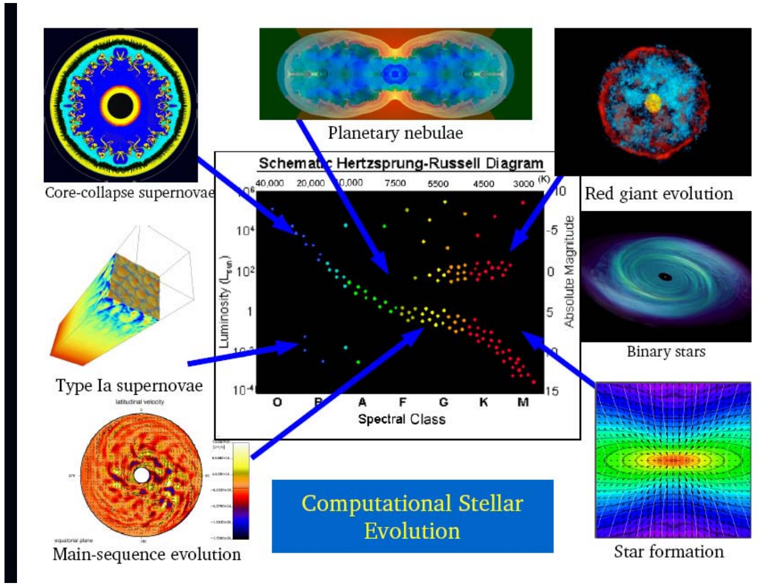
Different physics:

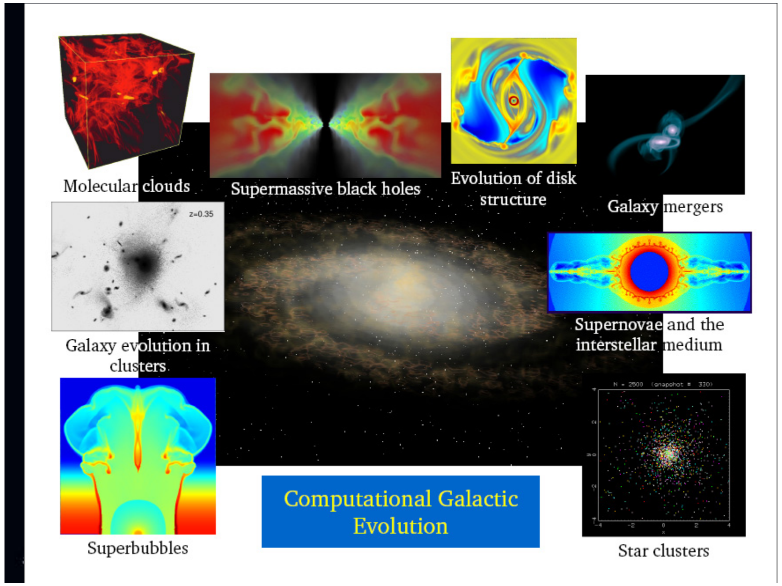
- Different classes
- Different stages of the evolution
- Different scales

Hertzsprung-Russell diagram



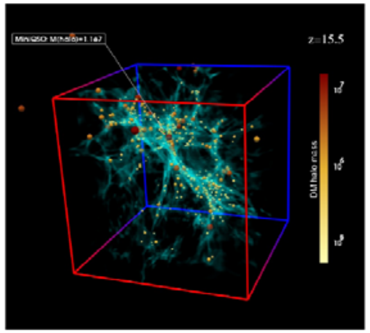
ასტროფიზი ... ალ. თევზაძე (2011)



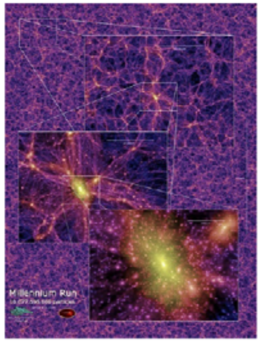


Computation on the Cosmological Scale...

- On the scale of the Universe, the cosmological scale factor is evolved.
- Self-gravity dominates the evolution



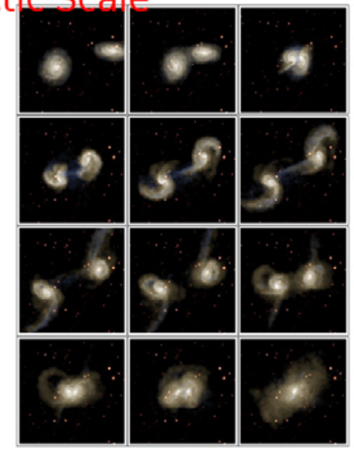
The first mini quasar effects on the surrounding IGM (Kuhlen et al.)



Simulating the growth of structure and the formation of galaxies. (Springel et al. 2005)

...the Galactic Scale

We can understand how galaxies interact and merge. It takes 100s of million years to play out in nature—we can see the evolution at a much accelerated pace.

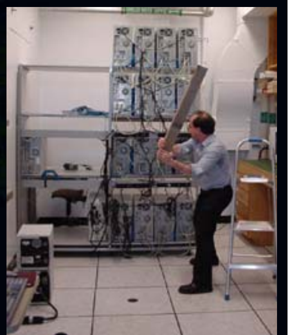


Colliding and merging galaxies
Springel & White (1999)

Simulations

Major aspects:

Physics
↓
Code
↑ ↓
Hardware



Some publicly available simulation codes

Code	Type	Physics	Parallel	Reference
Cactus	Eulerian/Nested	Gas, gravity (GR)	MPI	Allen et al 99
Enzo	AMR/PM	Gas, particles, gravity, cosmology	MPI	Norman & Bryan 98; O'Shea et al 04
FLASH	AMR/PM	Gas, particles, gravity, cosmology, nuclear, MHD	MPI	Fryxell et al 00
GADGET	P3M; TPM (v.2); SPH	Gas, particles, gravity, cosmology	MPI	Springel et al 01
Hydra	AP3M/SPH	Gas, particles, gravity, cosmology	No	Couchman 91
MLAPM	AMR/PM	Particles, gravity	No	Knebe et al 01
PMcode	PM	Particles, gravity	No	Klypin & Holtzmann 97
TITAN	1D AMR	Gas, radiation	No	Gehmeyr & Mihalas
VH-1	Eulerian	Gas	No	Blondin et al 91
Zeus-MP	Eulerian	Gas, gravity, MHD	MPI	Stone & Norman 92

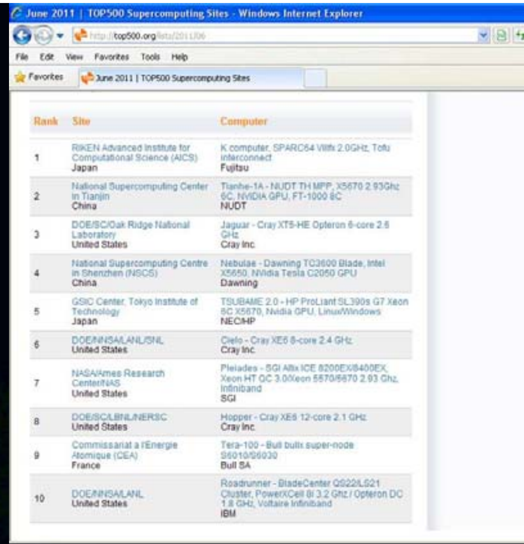
http://www.cactuscode.org
http://cosmos.ucsd.edu
http://flash.uchicago.edu
http://www.mpa-garching.mpg.de/gadget
http://hydra.mcmaster.ca/hydra
http://www.aip.de/People/AKnebe/MLAPM
http://astro.nmsu.edu/~aklypin/pm.htm
http://wonka.physics.ncsu.edu/pub/VH-1

Parallel Computers

Symmetric Multi-Processor (SMP)
- Processors share bus to main memory and I/O
- Processors may share cache memory
- Operating system distributes load
- Example: sipapu (workstation)

Distributed Shared Memory
- Processors have separate local memories
- Special bus connects memories
- Nonlocal memory appears "local" but is somewhat slower
- Operating system distributes load
- Example: copper (IBM p690)

Distributed Multi-Processor (Cluster)
- Processors have separate local memories, separate I/O
- Interprocessor communication over proprietary or commodity network (much slower than memory)
- Applications distribute load
- Example: tungsten (Dell Linux cluster)



June 2011 | TOP500 Supercomputing Sites - Windows Internet Explorer

Rank	Site	Computer
1	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu
2	National Supercomputing Center in Tianjin China	Tianhe-1A - NUDT TH MPP, X5670 2.93Ghz 6C, NVIDIA GPU, FT-1000 8C NUDT
3	DOE/SC/Oak Ridge National Laboratory United States	Jaguar - Cray XT5-HE Opteron 6-core 2.6 GHz Cray Inc.
4	National Supercomputing Centre in Shenzhen (NSCS) China	Nebulae - Dawning TC3600 Blade, Intel X5650, NVidia Tesla C2050 GPU Dawning
5	GSIC Center, Tokyo Institute of Technology Japan	TSUBAME 2.0 - HP ProLiant SL390s G7 Xeon 6C X5670, Nvidia GPU, Linux/Windows NEC/HP
6	DOE/NNSA/LANL/SNL United States	Cielo - Cray XE6 8-core 2.4 GHz Cray Inc.
7	NASA/Ames Research Center/NAS United States	Pleiades - SGI Altix ICE 8200EX/8400EX, Xeon HT QC 3.0/Xeon 5570/5670 2.93 Ghz, Infiniband SGI
8	DOE/SC/LBNL/NERSC United States	Hopper - Cray XE6 12-core 2.1 GHz Cray Inc.
9	Commissariat a l'Energie Atomique (CEA) France	Tera-100 - Bull bullx super-node S6010/S6030 Bull SA
10	DOE/NNSA/LANL United States	Roadrunner - BladeCenter QS22/LS21 Cluster, PowerXCell 8i 3.2 Ghz / Opteron DC 1.8 GHz, Voltaire Infiniband IBM

ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდელირება   ალ. თევზაძე (2011)

Overview of Simulation in Astrophysics

NASA

NASA/Ames Columbia machine—a 10240 processor SGI Altix system.

NCCS

The NCCS/ORNL jaguar machine—currently there are 11,000 compute nodes, each with a 2.6 GHz dual-core AMD Opteron processor and 4 GB of memory

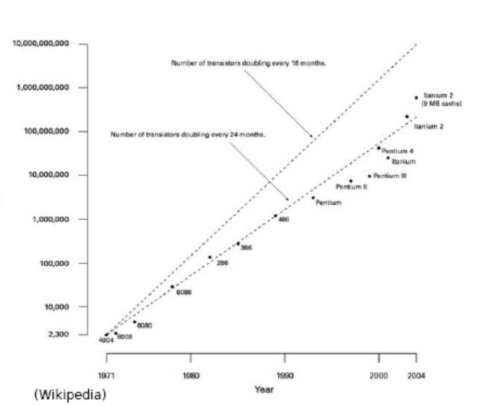
Beowulf cluster

ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდ

Perspective

Moor’s law

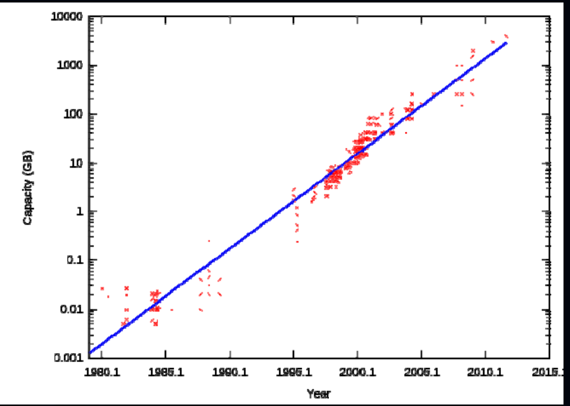
Doubling of the number of transistors on integrated circuits (1.5-2 years)



Perspective

Kryder’s law

Doubling of the magnetic disk areal storage density (1 year)



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BASIC CONCEPTS

ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდელირება ალ. თევზაძე (2011)

Method

- Continuum -> Discrete
- Physical Model -> Numerical Model

(Vx,Vy,Vz, Rho, P)
(Px, Py, Pz, E, M)

Where to introduce numerical errors:
Discretization, Subgrid, interpolation, etc.

Error propagation science

ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდელირება ალ. თევზაძე (2011)

Workflow

Configuration
- Initial conditions
- Boundary conditions

Calculus
- Compilation
- Run

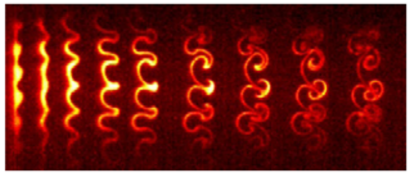
Data analysis
- Post processing
- Visualization

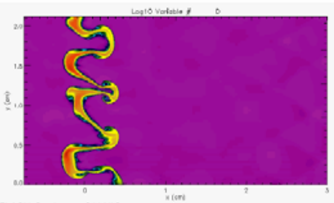
Are my results correct?

Indicators:

- Exact Analytic Solutions
- Different Numerical Methods
- Code Validation

Code Validation





(FLASH Center and LLNL)

Catastrophic cancellation

Calculate the equation with ***a=77617*** and ***b=33096***

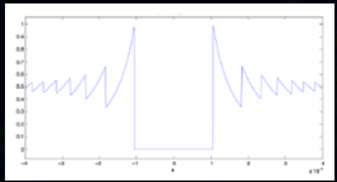
$$y = 333.75b^6 + a^2(11a^2b^2 - b^6 - 121b^4 - 2) + 5.5b^8 + \frac{a}{2b}$$

answer depends of the compiler
(C, Fortran, Matlab) processor type!

$$\stackrel{?}{=} 5.76461\ldots \times 10^{17}$$
$$\stackrel{?}{=} 6.33825\ldots \times 10^{29}$$
$$\stackrel{?}{=} 1.1726\ldots$$
$$\stackrel{?}{=} -0.827396\ldots$$

Catastrophic cancellation

Plot function: $f(x) = \frac{1 - \cos x}{x^2}$ $-4 \cdot 10^{-8} \leq x \leq 4 \cdot 10^{-8}$.



cos(x) = 0.99999999999999988897769753748434595763683319091796875.

Catastrophic cancellation. Devastating loss of precision when small numbers are computed from large numbers, which themselves are subject to roundoff error.

Numerical catastrophes

Ariane 5 rocket. [June 4, 1996]

10 year, $7 billion ESA project exploded after launch.

64-bit float converted to 16 bit signed int.

Unanticipated overflow.

Vancouver stock exchange. [November, 1983]

Index undervalued by 44%.

Recalculated index after each trade by adding change in price.

22 months of accumulated truncation error.

Patriot missile accident. [February 25, 1991]

Failed to track scud; hit Army barracks, killed 28.

Inaccuracy in measuring time in 1/20 of a second since using 24 bit binary floating point.

ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდელირება ალ. თევზაძე (2011)

Courant-Friedrichs-Lewy condition

CFL number: numerical stability

$$CFL = \frac{u\Delta t}{\Delta x}$$

CFL < 1

2D:

$$\frac{u_x \Delta t}{\Delta x} + \frac{u_y \Delta t}{\Delta y} = C[2D]$$

$$\Delta t = Min[CFL * u_{ij} \Delta x_{ij}]$$

ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდელირება ალ. თევზაძე (2011)

Properties of Numerical Models

A robust simulation has the following properties:

(J.H. Ferziger and M. Peric, Computational Methods for Fluid Dynamics, Springer, 1999)

- **Consistency** (regular, statistical)
- **Stability**
- **Convergence** (analytic solution, ?)
- **Conservation**
- **Boundedness**
- **Realizability**
- **Accuracy**

ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდელირება ალ. თევზაძე (2011)

Stability Theory

- Lyapunov stability
- Asymptotic stability
- Exponential stability

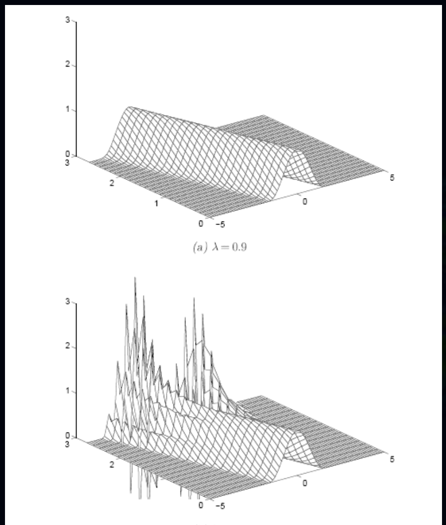
1. The origin of the above system is said to be **Lyapunov stable**, if, for every $\varepsilon > 0$, there exists a $\delta = \delta(\varepsilon) > 0$ such that, if $\|x(0)\| < \delta$, then $\|x(t)\| < \epsilon$, for every $t \geq 0$.
2. The origin of the above system is said to be **asymptotically stable** if it is Lyapunov stable and if there exists $\delta > 0$ such that if $\|x(0)\| < \delta$, then $\lim_{t\to\infty} x(t) = 0$.
3. The origin of the above system is said to be **exponentially stable** if it is asymptotically stable and if there exist $\alpha, \beta, \delta > 0$ such that if $\|x(0)\| < \delta$, then $\|x(t)\| \leq \alpha \|x(0)\| e^{-\beta t}$, for $t \geq 0$.

Numerical Stability

An algorithm is stable if the numerical solution at a fixed time remains bounded as the step size goes to zero

- Numerical diffusion
- CFL number (0.4 .. 0.6)

Numerical Instability


(a) $\lambda = 0.9$

(b) $\lambda = 1.1$

Numerical Methodology

DNS (Finite difference, finite volume, split, unsplit, etc.)

Spectral Methods (Fourier, Chebishev)

Pseudo-Spectral

N-body

Mesh

Static grids

- Uniform grid
- Linearly nonuniform grid
- Complex nonuniformity (Chebishev, etc)
- Non-Cartesian grids

Dynamical grids

- Adaptive Mesh Refinement (AMR)

Algorithms

Spatial Integration:

Temporal Integration:

Time step determination: CFL condition

Parallelization

Hardware

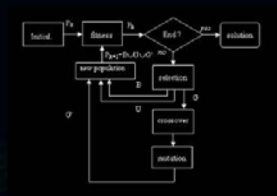
PC, Beowulf, HPC,

Software

- MPI
- PVM
- OpenMP

Pseudocode

Algorithm development



Pseudocode:

Code intended for human reading rather then the machine reading

- *no variable definitions;*
- *no memory management;*
- *no subroutines;*
- *no system-specific code;*

Pseudocode language choice: Matlab

- Avoid Matlab specific functions and simulink

Pseudocode

Pseudocode is intended to be rewritten in low level programming language later

Pseudocode	Java implementation

Pseudocode:

```
{
  //IF robot has no obstacle in
  front THEN
      // Call Move robot
      // Add the move command to
         the command history
      // RETURN true
  //ELSE
      // RETURN false without
         moving the robot
  //END IF
}
```

Java implementation:

```
{
   if (aRobot.isFrontClear())
   {
       aRobot.move();
       cmdHistory.add(RobotAction.MOVE);
       return true;
   }
   else
   {
        return false;
}
```


PDE classification

Linear second order Partial Differential Equation

$$a\frac{\partial^2}{\partial x^2}\Psi + b\frac{\partial^2}{\partial x\partial y}\Psi + c\frac{\partial^2}{\partial y^2}\Psi + d\frac{\partial}{\partial x}\Psi + e\frac{\partial}{\partial y}\Psi + f\Psi = g$$

Elliptic: $b^2 - 4\,a\,c < 0$

Parabolic: $b^2 - 4\,a\,c = 0$

Hyperbolic: $b^2 - 4\,a\,c > 0$

PDE classification

Elliptic equation: *Poisson equation*

Parabollic equation: *Diffusion equation*

Hyperbolic equation: *Wave equation*

EXAMPLES

Numerical methods: individual treatment

Conservation laws

Modelling conservation laws:

Method - rewrite set of equations in the form of the general set of conservation laws (analytically)

Conserved quantities: volume integrals

Differential form of continuity eq.: $\frac{\partial\rho}{\partial t} + \nabla(\rho V) = 0$

Mass conservation in total volume: $M = \int_V \rho dV = const.$

Conservation laws

Generalized form of conservation laws:

$$\frac{\partial \Phi}{\partial t} + \nabla(J) = 0$$

Φ – numerical variable

J – numerical flux of the variable **Φ**

ρ, P, V (physical variables): primitive variables

Task: *reducing existing system of hyperbolic PDE to the conserving form*

EXAMPLES

end