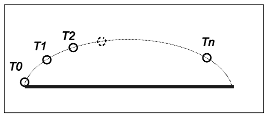
ივანე ჯავახიშვილის სახელობის
თბილისის სახელმწიფო უნივერსიტეტი

ლექცია 1

source

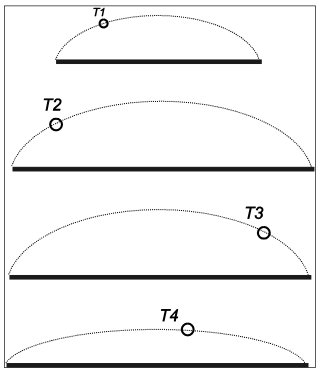
www.tevza.org/home/course/modelling-II_2016/

Why model?



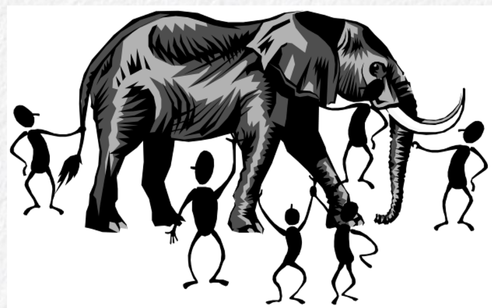
Consequent data

Inconsequent data:



Modelling Elephant

How good is the model?

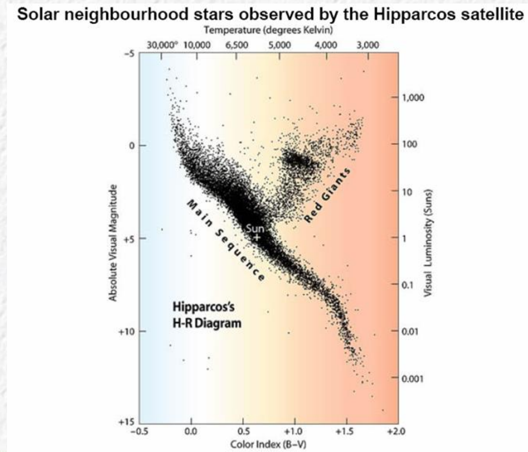


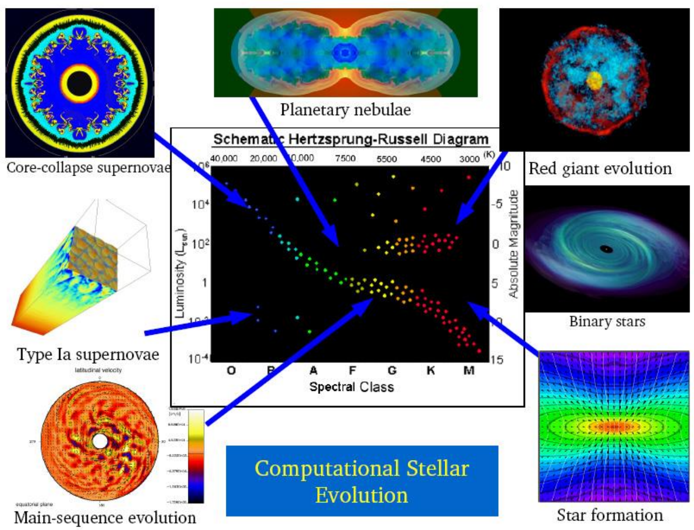
Astrophysical simulations

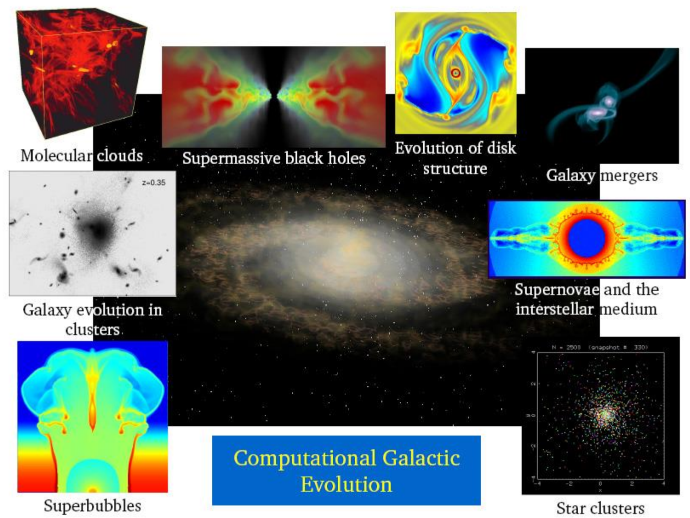
Different physics:

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

Hertzsprung-Russell diagram

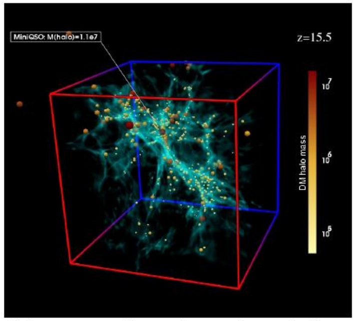




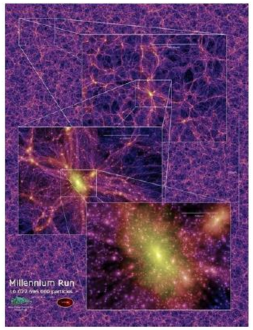


Computation on the Cosmological Scale…

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



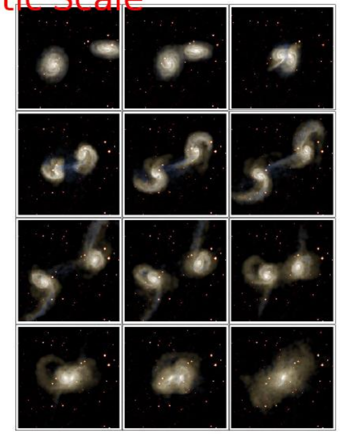
The first mini quasar effects on the surrounding IGM (Kuhlen et al.)



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)

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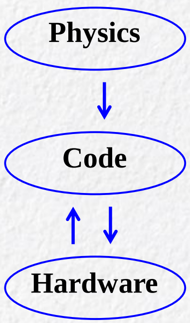
Simulations

Major aspects:



ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდელირება 2, ალ. თევზაძე (2016)

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

PLUTO

http://plutocode.ph.unito.it/ A Riemann solver for HD/MHD/RMHD with AMR. Parallel. C/C++

SNOOPY

http://ipag.osug.fr/~lesurg/snoopy.html Spectral, incompressible MHD, parallel

PENCIL

http://www.nordita.org/software/pencil-code/ MHD Cartesian. A higher order non-conservative advection method. Turbulence. Parallel. FORTRAN

FLASH

http://flash.uchicago.edu/website/home/ Cartesian HD, modules, AMR, parallel.

ZEUS

http://www.astro.princeton.edu/jstone/zeus.html (M)HD. Staggered grid, Cartesian, cylindrical, polar, gravity, self-gravity and radiation transfer.

ATHENA

http://www.astro.princeton.edu/jstone/athena.html Riemann solvers (including also Roe's algorithm). Cartesian. MHD, AMR, parallelization (MPI) etc.

GADGET

http://www.mpa-garching.mpg.de/gadget/ SPH and N-body code for astrophysics.

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

http://top500.org/lists/2011/06

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

TOP 10 Sites for June 2016

For more information about the sites and systems in the list, click on the links or view the complete list.

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	National Supercomputing Center in Wuxi China	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway NRCPC	10,649,600	93,014.6	125,435.9	15,371
2	National Super Computer Center in Guangzhou China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808
3	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209
4	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890
5	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705,024	10,510.0	11,280.4	12,660
6	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786,432	8,586.6	10,066.3	3,945
7	DOE/NNSA/LANL/SNL United States	**Trinity** - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Aries interconnect Cray Inc.	301,056	8,100.9	11,078.9	
8	Swiss National Supercomputing Centre (CSCS) Switzerland	**Piz Daint** - Cray XC30, Xeon E5-2670 8C 2.600GHz, Aries interconnect , NVIDIA K20x Cray Inc.	115,984	6,271.0	7,788.9	2,325
9	HLRS - Höchstleistungsrechenzentrum Stuttgart Germany	**Hazel Hen** - Cray XC40, Xeon E5-2680v3 12C 2.5GHz, Aries interconnect Cray Inc.	185,088	5,640.2	7,403.5	
10	King Abdullah University of Science and Technology Saudi Arabia	**Shaheen II** - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Aries interconnect Cray Inc.	196,608	5,537.0	7,235.2	2,834

NASA Pleiades Supercomputer

11,472 nodes
4.09 Pflop/s LINPACK
(#15 on June 2016 top500)

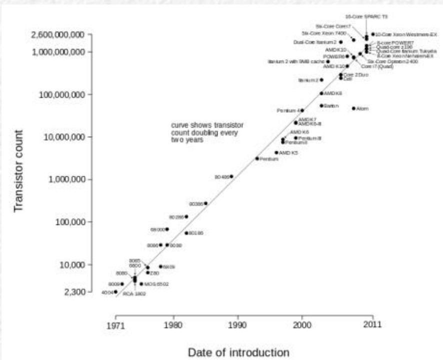
Total CPU cores: 246,048
Total memory: 938 TB

Beowulf cluster

Perspective

Moor's law

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

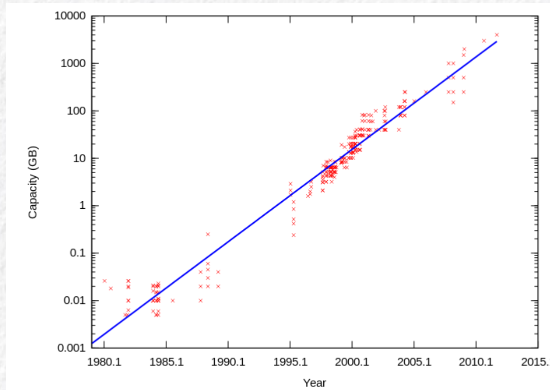


2016 – End of the Moors roadmap?

Perspective

Kryder's law

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



BASIC CONCEPTS

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 2, ალ. თევზაძე (2016)

Workflow

Configuration

- Initial conditions
- Boundary conditions

Calculus

- Compilation
- Run

Data analysis

- Post processing
- Visualization

ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდელირება 2, ალ. თევზაძე (2016)

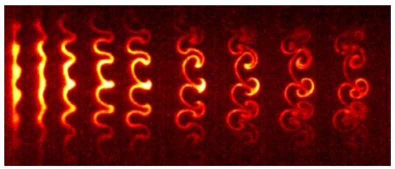
Are my results correct?

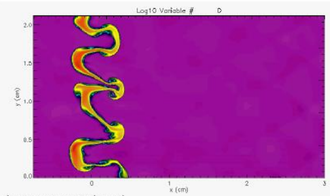
Indicators:

- Resolution Study
- Exact Analytic Solutions
- Different Numerical Methods
- Code Validation

ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდელირება 2, ალ. თევზაძე (2016)

Code Validation





(FLASH Center and LLNL)

Catastrophic cancellation

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

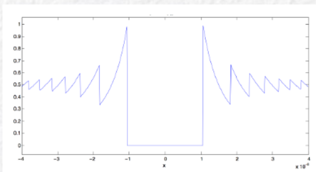
$$y = 333.75b^6 + a^2(11a^2b^2 - b^6 - 121b^4 - 2) + 5.5b^8 + \frac{a}{2b}$$

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



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.

Courant-Friedrichs-Lewy condition

CFL number: numerical stability

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

CFL < 1

2D:

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

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

Properties of Numerical Models

A robust simulation has the following properties:

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

ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდელირება 2, ალ. თევზაძე (2016)

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 $t \geq 0$.

ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდელირება 2, ალ. თევზაძე (2016)

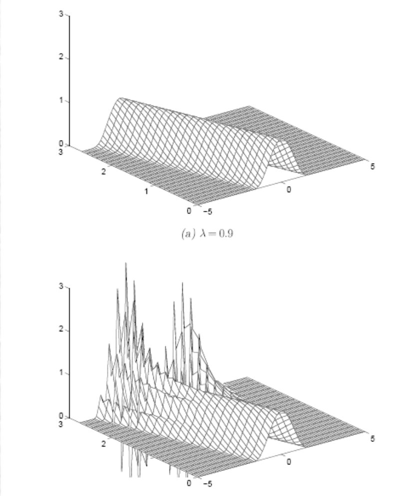
Numerical Stability

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)

ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდელირება 2, ალ. თევზაძე (2016)

Numerical Instability



(a) $\lambda = 0.9$

(b) $\lambda = 1.1$

Numerical Methodology

- Direct Numerical Simulations
(Godunov, finite difference, finite volume, split, unsplit, etc.)
"Numerical Experiment"

- Spectral Methods (Fourier, Chebishev)

- Pseudo-Spectral

- N-body (SPH)

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

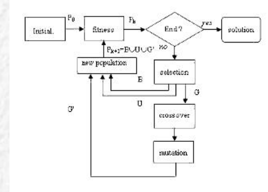
PC, Beowulf, HPC,

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

ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდელირება 2, ალ. თევზაძე (2016)

Pseudocode

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

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;
   }
}
```

ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდელირება 2, ალ. თევზაძე (2016)

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

ასტროფიზიკის და პლაზმის ფიზიკის ამოცანების მოდელირება 2, ალ. თევზაძე (2016)

PDE classification

Elliptic equation: *Poisson equation*

Parabolic 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:

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

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

http://www.tevza.org/home/course/modelling-II_2016/