Numerical Modeling of Jellyfish Galaxy at Intel Xeon Phi supercomputers

Igor Kulikov, Igor Chernykh, Victor Protasov

ICM&MG SB RAS

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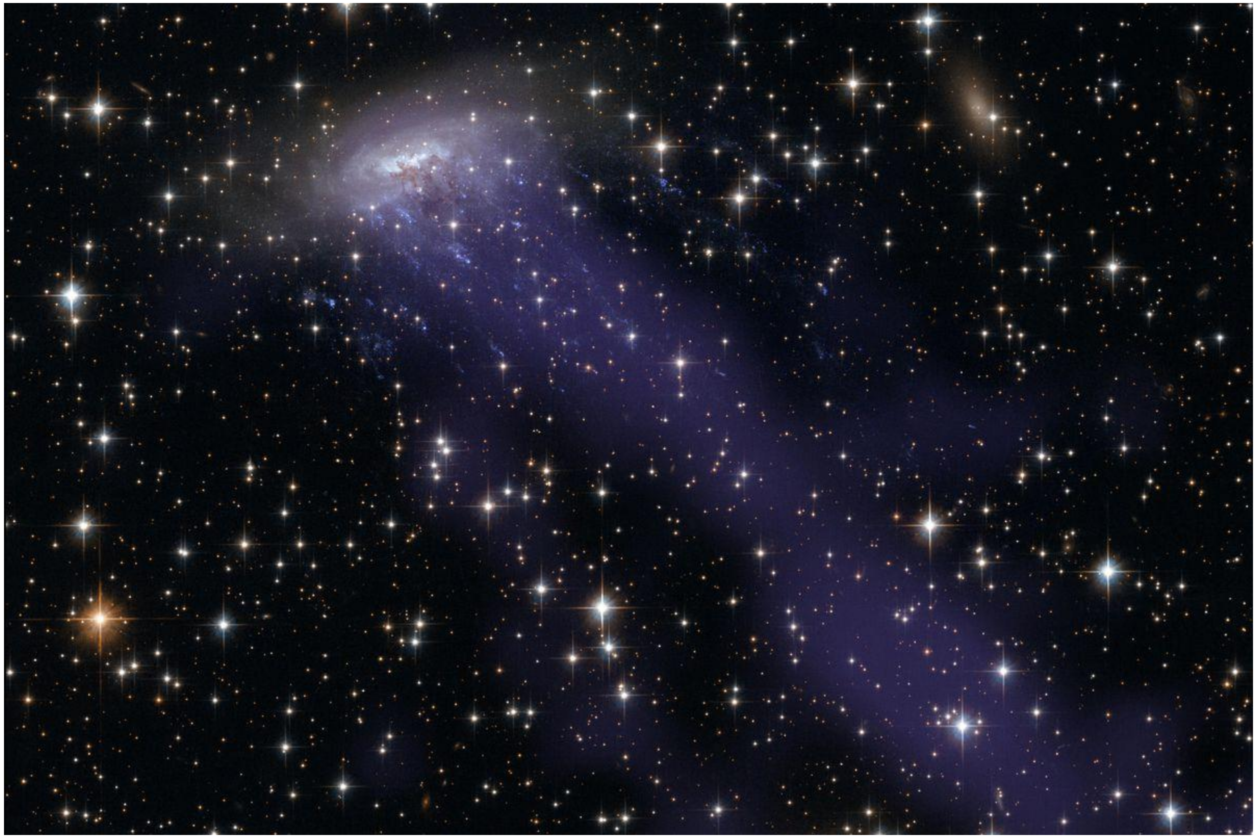
The general problem:
AGN is the driver of ram-pressure?

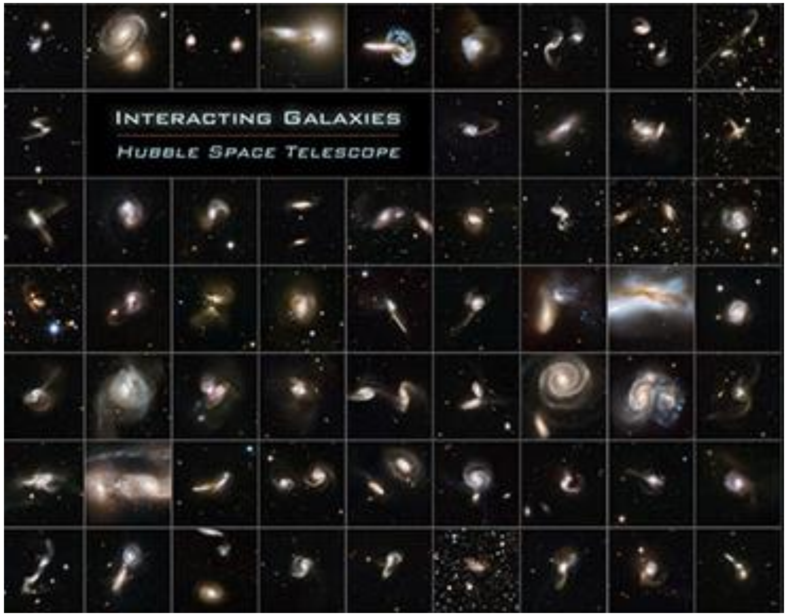


Poggianti B., Jaffé Y., Moretti A. et al. Ram-pressure feeding of supermassive black holes // Nature. – 2017. – V. 548. – P. 304-309

The motivation – (i) physics

«The movement of galaxies in dense clusters turns the collisions of galaxies into an important evolutionary factor»

Professor
Alexander Tutukov



The motivation and challenges for me are:

1. The model of galaxy
2. The numerical solver
3. The parallel implementation

Tutukov, Lazareva, Kulikov, Astron Rep., 2011

The motivation – (ii) supercomputers

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway , NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371
2	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P , NUDT National Super Computer Center in Guangzhou China	3,120,000	33,862.7	54,902.4	17,808
3	**Piz Daint** - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100 , Cray Inc. Swiss National Supercomputing Centre (CSCS) Switzerland	361,760	19,590.0	25,326.3	2,272
4	**Gyoukou** - ZettaScaler-2.2 HPC system, Xeon D-1571 16C 1.3GHz, Infiniband EDR, PEZY-SC2 700Mhz , ExaScaler Japan Agency for Marine-Earth Science and Technology Japan	19,860,000	19,135.8	28,192.0	1,350
5	**Titan** - Cray XK7, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x , Cray Inc. DOE/SC/Oak Ridge National Laboratory United States	560,640	17,590.0	27,112.5	8,209
6	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom , IBM DOE/NNSA/LLNL United States	1,572,864	17,173.2	20,132.7	7,890
7	**Trinity** - Cray XC40, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect , Cray Inc. DOE/NNSA/LANL/SNL United States	979,968	14,137.3	43,902.6	3,844
8	**Cori** - Cray XC40, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect , Cray Inc. DOE/SC/LBNL/NERSC United States	622,336	14,014.7	27,880.7	3,939
9	**Oakforest-PACS** - PRIMERGY CX1640 M1, Intel Xeon Phi 7250 68C 1.4GHz, Intel Omni-Path , Fujitsu Joint Center for Advanced High Performance Computing Japan	556,104	13,554.6	24,913.5	2,719
10	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect , Fujitsu RIKEN Advanced Institute for Computational Science (AICS) Japan	705,024	10,510.0	11,280.4	12,660

The hybrid supercomputers

The motivation – (iii) design concept

- The physical model
- The mathematical formalization
- The numerical solver
- The structures of data
- The architecture of supercomputer
- The tools of parallel programming

The motivation – (iii) co-design concept

- The physical model
- The mathematical formalization
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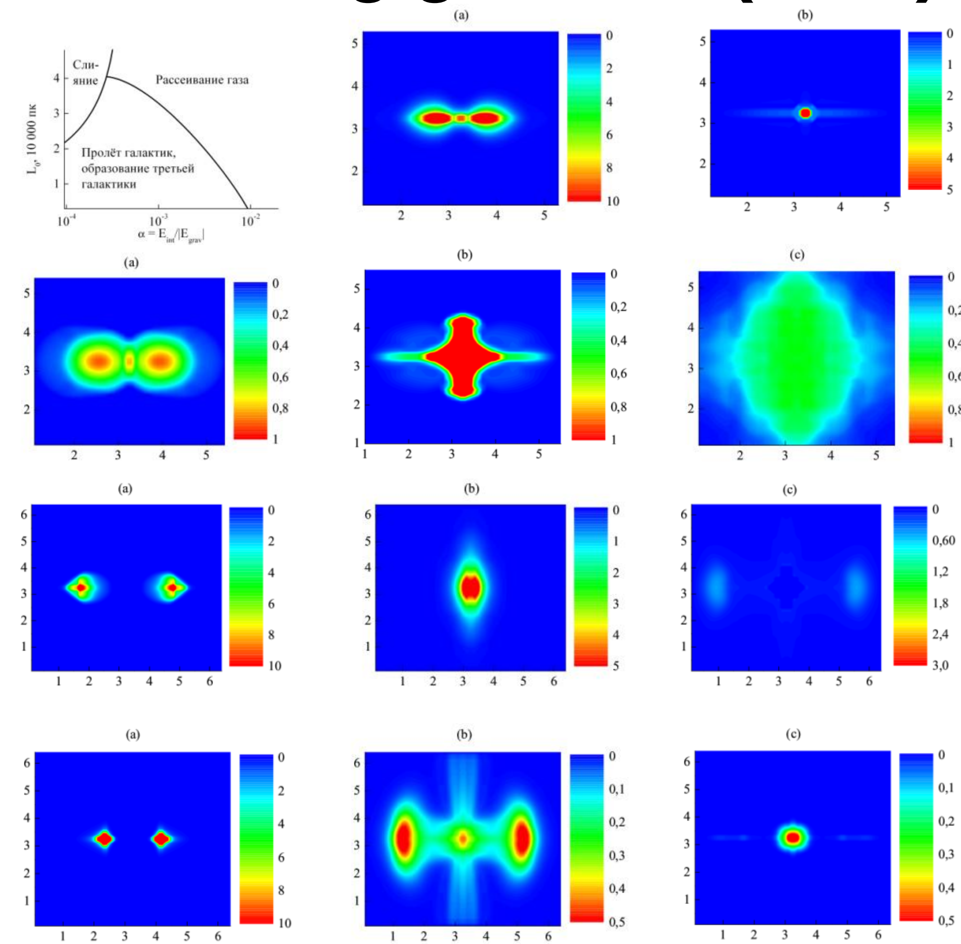
- The tools of parallel programming

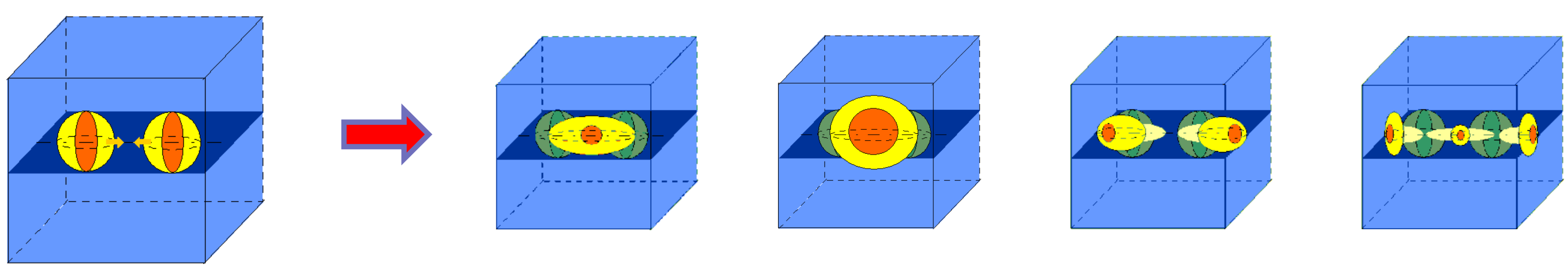
The hydrodynamics of interacting galaxies (2011)

In hydrodynamic model with <u>analytical stellar component</u> was shown four scenarios of central collision of two galaxies:

1. **The coalescence**
2. **The dissipation of the gas components of the galaxies**
3. **The free expansion**
4. **The expansion with the formation of a new galaxy with no stellar component**

1. Vshivkov, Lazareva, Snytnikov, Kulikov, Tutukov, ApJS, 2011
2. Tutukov, Lazareva, Kulikov, Astron Rep., 2011





The model of collisionless component

The disadvantages of N-body model

- a spurious generation of entropy
- a problem of choice of the kernel function in cell
- a necessary minimal number of particles in cell
- increased communication overhead
- poor load balancing
- a thermodynamically unconsistent of star formation

The hydrodynamic alternative

- The pressureless hydrodynamic
- The collisionless hydrodynamic*

*** Mitchell, Vorobyov, Hensler, MNRAS, 2013**

The model of collisionless component

$$\frac{\partial f}{\partial t} + v_i \frac{\partial f}{\partial x_i} + a_i \frac{\partial f}{\partial v_i} = 0$$

$$d^3 v = dv_x dv_y dv_z$$

$$\rho = \int m f d^3 v$$

$$u = \rho^{-1} \int m f v d^3 v$$

$$\sigma_{ij}^2 = \rho^{-1} \int m f \left(v_i - u_i\right)\left(v_j - u_j\right) d^3 v = \sigma_{ji}^2$$

- It is important to movement of the cluster and not single particle
- No thermal transfer effects (*the property of almost all the astrophysical problems*)
- The velocity dispersion is much less than the velocity squared

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho u\right) = 0$$

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot \left(\rho u u\right) = -\nabla\left(\rho \sigma^2\right) - \rho \nabla \Phi$$

$$\frac{\partial \rho E_{ij}}{\partial t} + \nabla \cdot \left(\rho E_{ij} u\right) = -\nabla \cdot \left(2 \rho \sigma_{ij}^2 u\right) - 2\left(\rho u, \nabla \Phi\right)$$

$$\rho E_{ij} = \rho \sigma_{ij}^2 + \rho u_i u_j$$

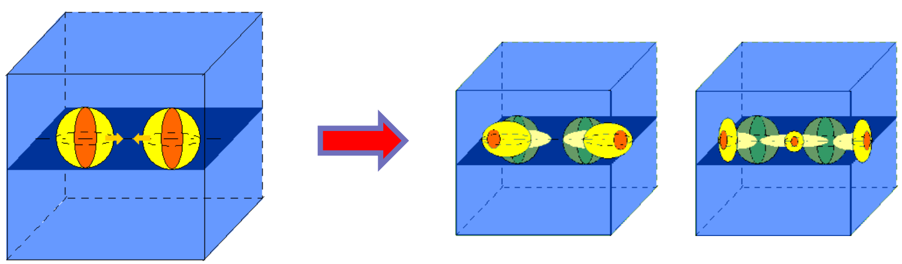
The model of collisionless component

The advantages of collisionless hydrodynamic

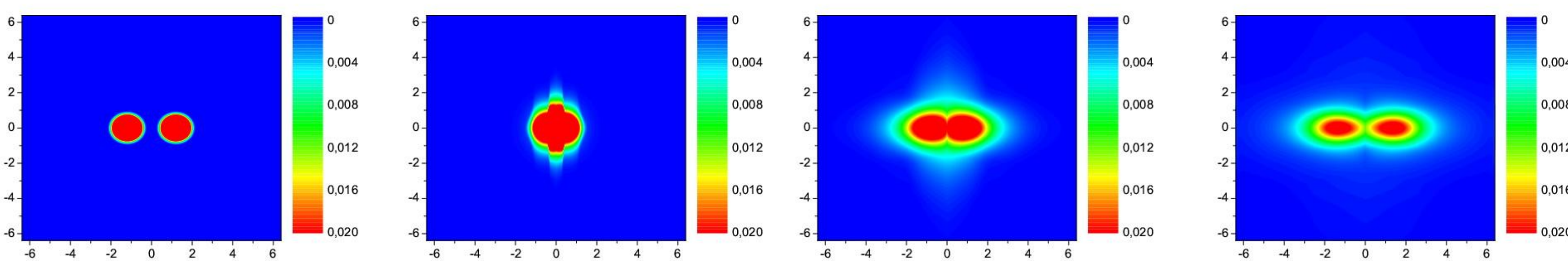
- a thermodynamically consistent of star formation
- one numerical method for gaseous and stellar components

The disadvantages of collisionless hydrodynamic

- The applicability of approach in each a specific problem



Kulikov, ApJS, 2014



The numerical methods

SPH approach

- Robustness of the algorithm
- Galilean-invariant solution
- Simplicity of implementation
- Flexible geometries of problems
- High accurate gravity solvers

- Artificial viscosity is parameterized
- Variations of the smoothing length
- The problem of shock wave and discontinuous solutions
- Instabilities suppressed
- The method is not scalable

AMR approach

- Approved numerical methods
- No artificial viscosity
- Higher order shock waves
- Resolution of discontinuities
- No suppression of instabilities
- Correct turbulence solution

- The complexity of implementation
- The effects of mesh
- Problem of the minimal mesh resolution
- Not Galilean-invariant solution
- The method is not scalable

The numerical methods

- **The moving mesh approach (***AREPO, Springel, 2010***)**
- **The classic ALE-approach (***BETHE-Hydro, Murphy & Burrows, 2008***)**
- **The hybrid method on regular mesh (***Kulikov, 2004, from bachelor thesis***)**

The main features of original methods

- **The over definition hydrodynamic equations**
- **The operator-splitting approach**
- **The combination Godunov – Roe – PPML methods**
- **Using a regular mesh**

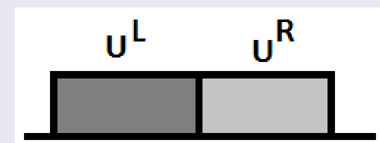
The numerical methods

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho\vec{v}\\ \rho E\\ \rho\varepsilon\end{pmatrix} + \nabla\bullet\begin{pmatrix}\rho\cdot\vec{v}\\ \rho\vec{v}\cdot\vec{v}\\ \rho E\cdot\vec{v}\\ \rho\varepsilon\cdot\vec{v}\end{pmatrix} = \begin{pmatrix}0\\ -\nabla p\\ -\nabla\bullet(p\vec{v})\\ -p\nabla\bullet(\vec{v})\end{pmatrix} \xrightarrow{(1)} \frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho\vec{v}\\ \rho E\\ \rho\varepsilon\end{pmatrix} = \begin{pmatrix}0\\ -\nabla p\\ -\nabla\bullet(p\vec{v})\\ -p\nabla\bullet(\vec{v})\end{pmatrix}$$

(2)

$$\frac{\partial f}{\partial t} + \nabla\bullet(f\cdot\vec{v}) = 0$$

The Riemann problem



$$\frac{\partial u}{\partial t} + B\frac{\partial u}{\partial x} = 0 \qquad B = R\Lambda L \qquad LR = I$$

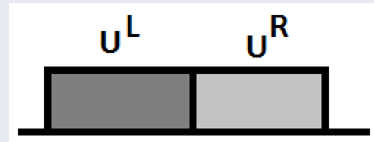
$$L\frac{\partial u}{\partial t} + LR\Lambda L\frac{\partial u}{\partial x} = 0 \qquad w = Lu$$

$$\frac{\partial w}{\partial t} + \Lambda\frac{\partial w}{\partial x} = 0 \qquad w(x,t) = w(x-\Lambda t) \qquad u = Rw$$

(*) Kulikov, et al., LNCS, 2009; APJS, 2011, 2014; AAABS, 2013; CPC 2015; JCP 2016

The numerical methods – PPML approach

The Riemann problem

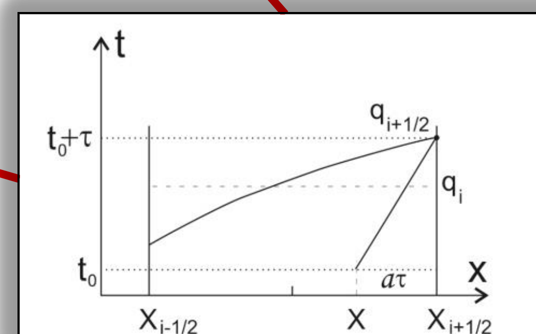


$$\frac{\partial u}{\partial t} + B\frac{\partial u}{\partial x} = 0 \qquad B = R\Lambda L \qquad LR = I$$

$$L\frac{\partial u}{\partial t} + LR\Lambda L\frac{\partial u}{\partial x} = 0 \qquad w = Lu$$

$$\frac{\partial w}{\partial t} + \Lambda\frac{\partial w}{\partial x} = 0 \qquad w(x,t) = w(x - \Lambda t) \qquad u = Rw$$

The piecewise-parabolic functions



(*) Ustyugov et al., Comp. Math. & Math. Phys., 2007, 2008, Comp. Phys., 2009

The numerical methods. The Roe solver

The Roe solver

$$[\rho] = \sqrt{\rho_L \rho_R}$$

$$H = \frac{p}{\rho} + \varepsilon$$

$$[H] = \frac{\sqrt{\rho_L}\, H_L + \sqrt{\rho_R}\, H_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}$$

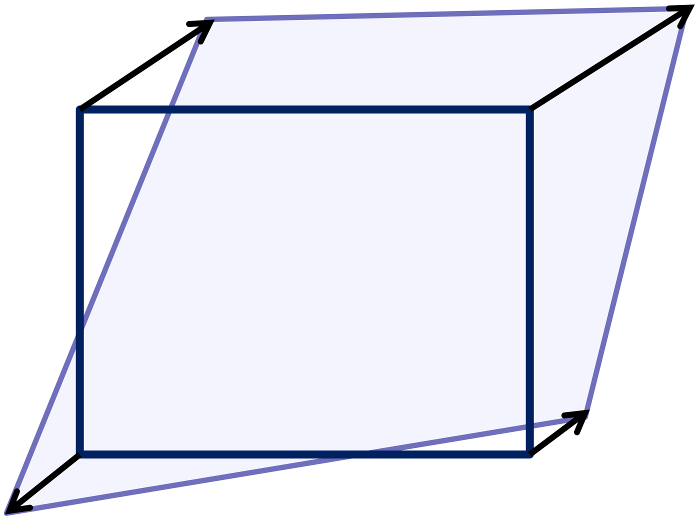
The modification of Roe solver

$$[\rho] = \frac{\rho_L^{3/2} + \rho_R^{3/2}}{\sqrt{\rho_L} + \sqrt{\rho_R}}$$

$$[p] = \frac{\sqrt{\rho_L}\, p_L + \sqrt{\rho_R}\, p_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}$$

The reason – accurate approximation of boundary gas-vacuum

The numerical methods. The advection transport



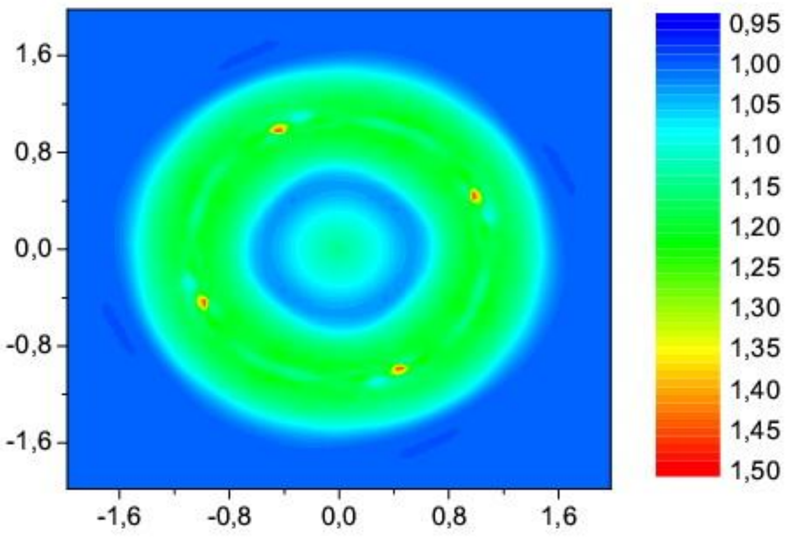
$$\frac{\partial z}{\partial t} + \nabla \cdot \left(z\vec{v} \right) = 0$$

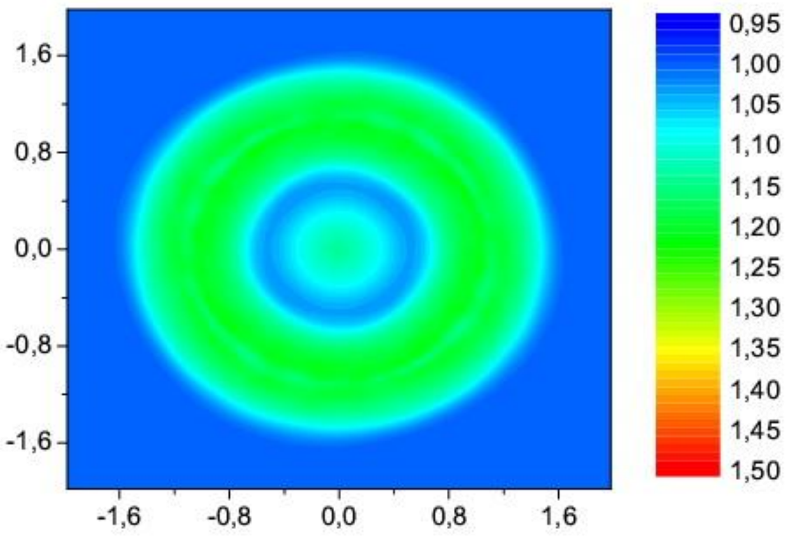
$$\left[v \right] = \frac{\sqrt{z_L}\, v_L + \sqrt{z_R}\, v_R}{\sqrt{z_L} + \sqrt{z_R}}$$

1/16	2/16	1/16
2/16	4/16	2/16
1/16	2/16	1/16

$$F_{i+1/2,kl}^{n+1/2} = \left[v \right]_{i+1/2,k,l} \times \begin{cases} z_{ikl}, & \left[v \right]_{i+1/2,k,l} \geq 0 \\ z_{i+1,kl}, & \left[v \right]_{i+1/2,k,l} < 0 \end{cases}$$

The numerical methods. The advection transport





0	0	0
0	1	0
0	0	0

1/16	2/16	1/16
2/16	4/16	2/16
1/16	2/16	1/16

The over definition hydrodynamic equation

$$\rho E = \rho\varepsilon + \frac{\rho v^2}{2}$$

$$\|V\| = \sqrt{2\left(E - \varepsilon\right)}$$

$$\rho\varepsilon = \left(\rho E - \frac{\rho v^2}{2}\right)$$

1. **The renormalization of the velocity vector length, it's direction remaining the same (*on boundary gas-vacuum*)*.**
2. **The entropy (or internal energy) correction (*on regular density*)****

Such a modification of the method keeps the detailed energy balance and entropy nondecrease guarantee

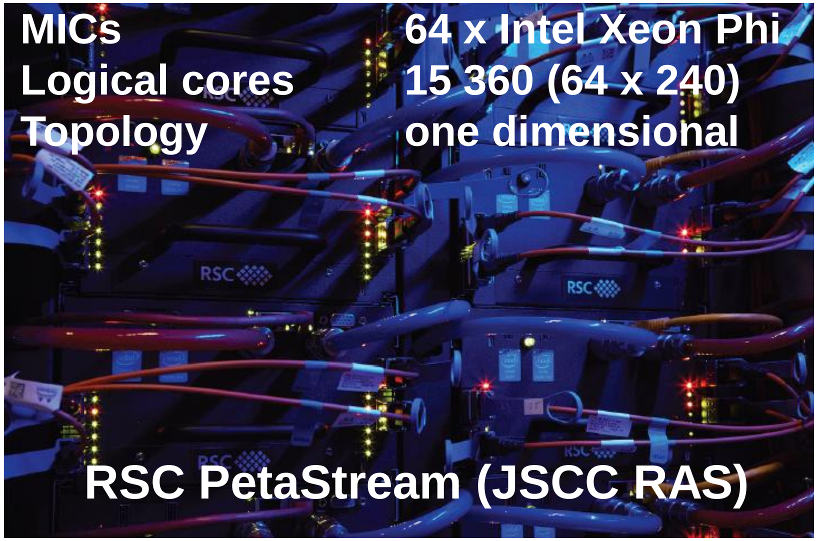
*) Vshivkov V., Lazareva G., Snytnikov A., Kulikov I., Tutukov A. Computational methods for ill-posed problems of gravitational gasodynamics // J. Inv. Ill-Posed Problems, 19. 2011, 151-166

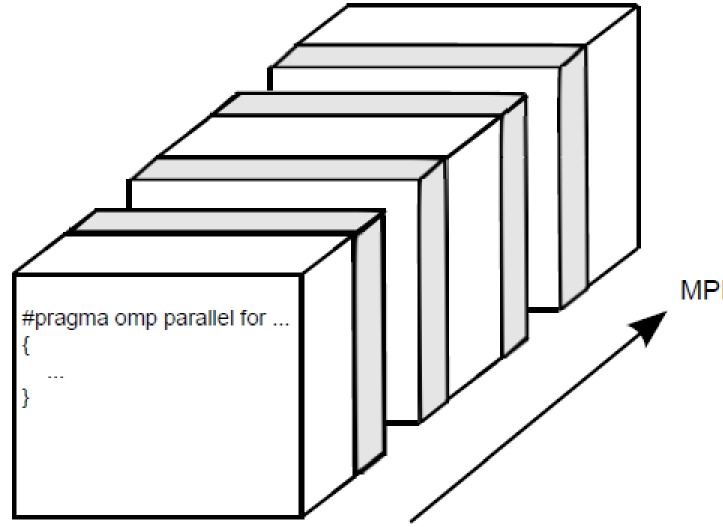
**) Godunov S., Kulikov I. Computation of Discontinuous Solutions of Fluid Dynamics Equations with Entropy Nondecrease Guarantee // J. Comp. Math & Math. Phys., 54, 2014, 1012-1024

The verification of numerical method

- **One dimensional test for shock tube (***discontinuous analytical solution***)**
- **Test of Aksenov (***continuous analytical solution***)**
- **The Kelvin-Helmholtz instability**
- **The Releigh-Taylor instability**
- **The Sedov blast wave**
- **The control of angular moment impulse test**
- **The expansion of gas into a vacuum**
- **The Evrard collapse**
- **The collapse of molecular cloud**
- **The fall of G2 onto Sgr A***
- **…**

The parallel implementation





1. The speed-up factors of <u>134</u> on 260 logical cores
2. The efficiency of <u>92%</u> on 64 MICs (or on 15 360 cores)
3. The <u>29 GFLOPS</u> of scalar performance (or 40% from peak)

The simulation of behavior of parallel implementation on <u>983 040 cores</u> by means AGNES* system the <u>80% efficiency</u> was shown

*Podkorytov et al., LNCS 2010

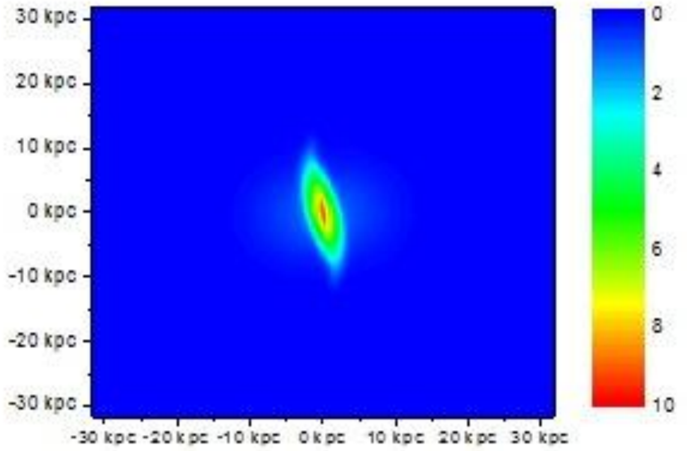
The numerical method. The summary

- The high-order (low-dissipation) numerical solution
- Not using of artificial viscosity or limiters
- The Galilean-invariant of numerical solution
- Entropy non-decrease guarantee
- Regular procedure for extension on other numerical models (*by example Boltzmann and MHD equations*)
- Simplicity of parallel implementation on hybrid and classic supercomputers
- Potential infinity scalability

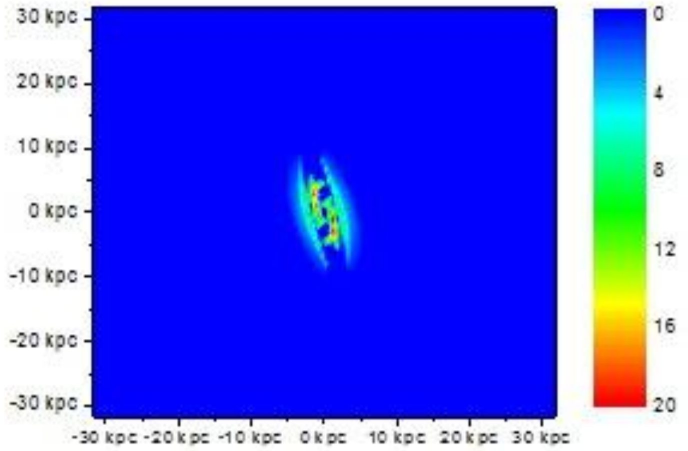
The interacting galaxies

The model:	**two-phase model (hydrodynamic + Boltzmann)**
The profiles:	**self-gravitating rotational equilibrium***
The mass of galaxy:	**10^{13} $M_\odot$**
The subgrid physics:	**star formation**
	supernovae feedback
	H_2 formation
	cooling / heating

Molecular hydrogen

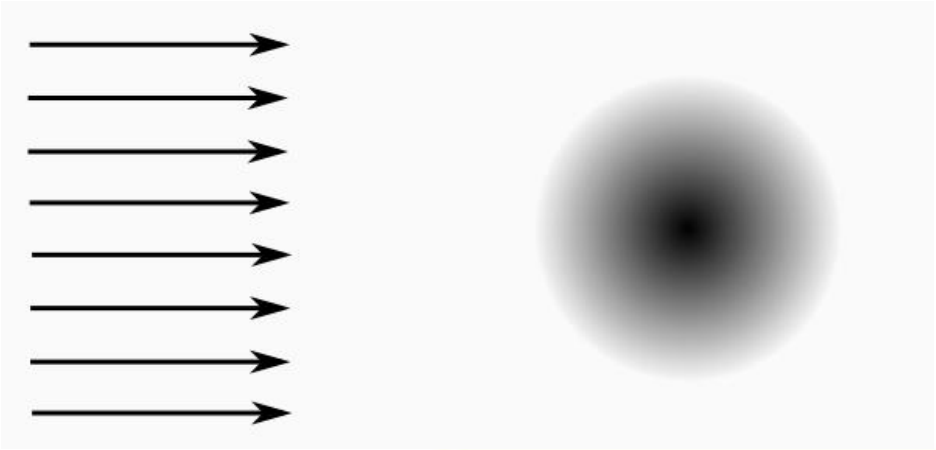


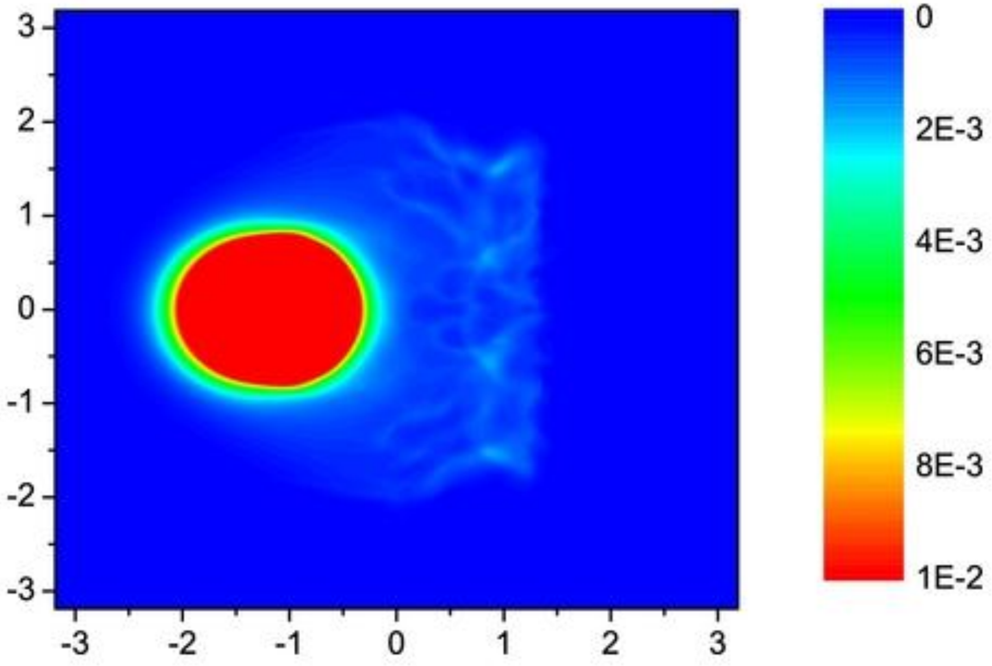
Star formation



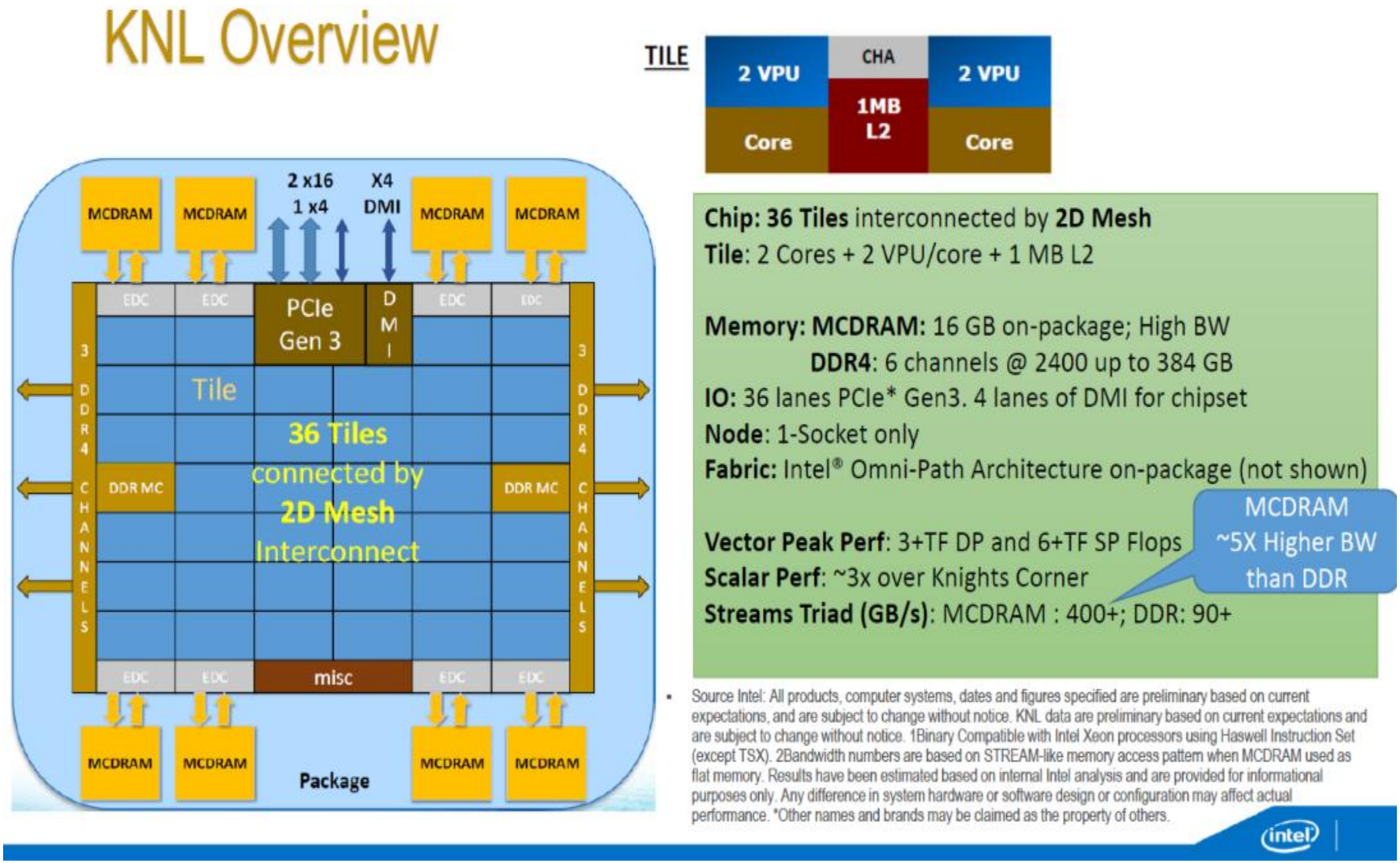
*** Vorobyov, Recchi, Hensler, A&A, 2012**

The Jellyfish galaxy

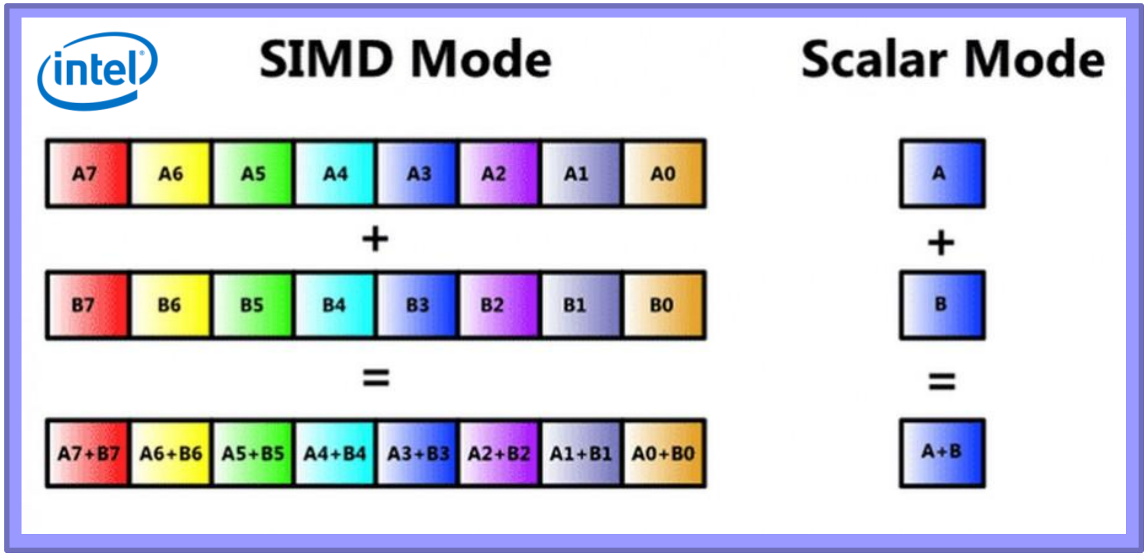




Where is TFLOPS+ on Intel Xeon Phi???



SIMD technology (SSE, AVX 512, …) + HLL solver



$$\frac{\vec{u}_k^{\,n+1}-\vec{u}_k^{\,n}}{\tau}+\frac{F_{k+1/2}-F_{k-1/2}}{h_i}=q_k$$

Vectors

$$F_{k+1/2}^{HLL}=\frac{\lambda_{k+1}F_k^n-\lambda_k F_{k+1}^n+\lambda_k\lambda_{k+1}\left(U_{k+1}^n-U_k^n\right)}{\lambda_{k+1}-\lambda_k}$$

The intrinsic of AVX 512

_mm512_set1_pd	- set value for a vector
_mm512_load_pd	- load a vector from main memory
_mm512_mul_pd	- vector multiply
_mm512_add_pd	- vector summation
_mm512_sub_pd	- vector substitution
_mm512_store_pd	- store a vector to main memory

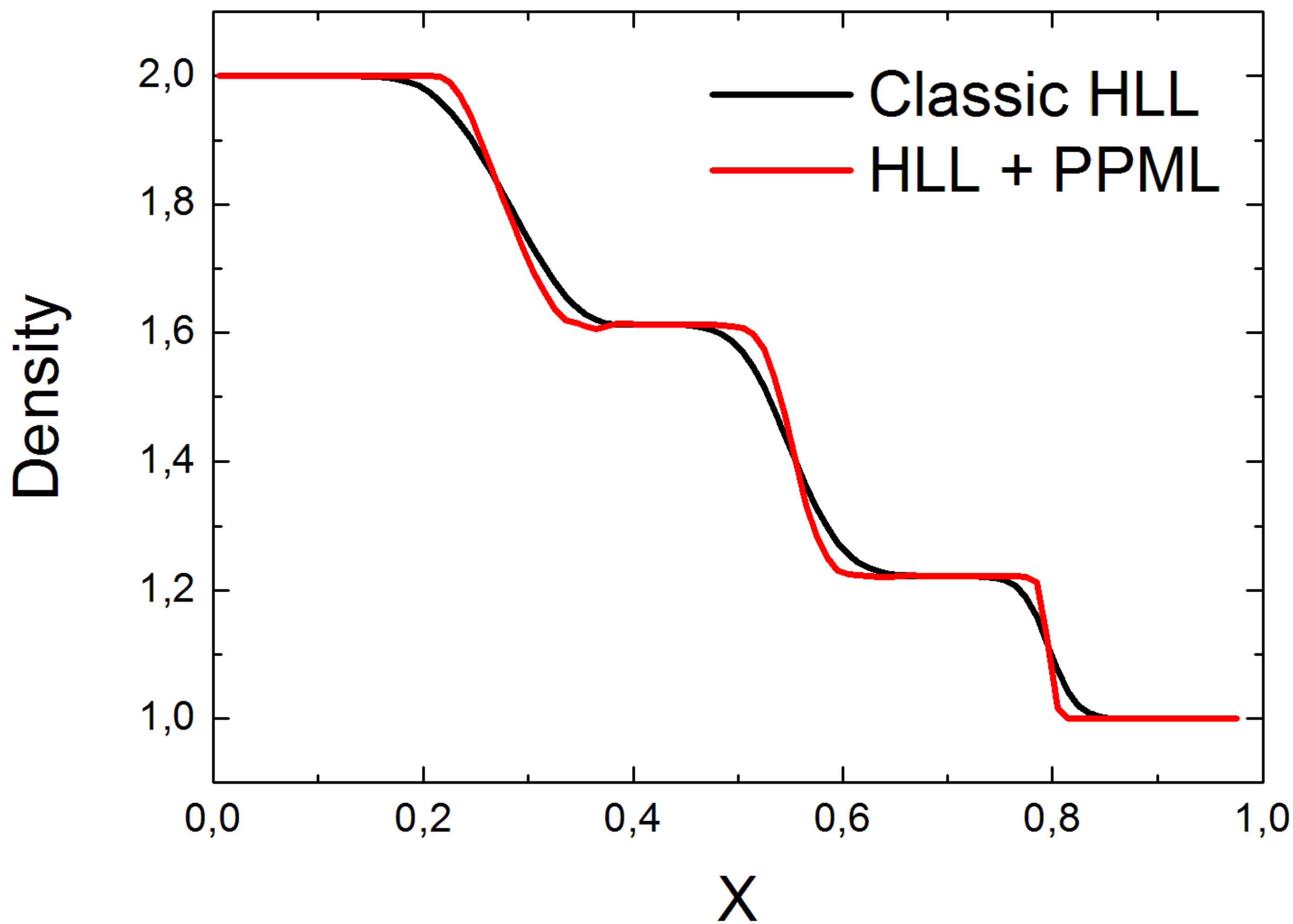
mpiicc -xMIC-AVX512 -qopenmp -O3 -o astrophi.mic astrophi.cpp -lm

Main advantages is 302 GFLOPS on Intel Xeon Phi

Main disadvantages – formation of the 8-double elements vector for computing

Pitfalls: associative of cache memory, align of memory, schedule distribution, data dependency

HLL? Where is high order and low dissipation?



The publications

1. Kulikov I. GPUPEGAS: A New GPU-accelerated Hydrodynamic Code for Numerical Simulations of Interacting Galaxies // The Astrophysical Journal Supplements Series. – 2014. – V. 214, 12. – P. 1-12

2. Kulikov I.M., Chernykh I.G., Snytnikov A.V., Glinskiy B.M., Tutukov A.V. AstroPhi: A code for complex simulation of dynamics of astrophysical objects using hybrid supercomputers // Computer Physics Communications. – 2015. – V. 186. – P. 71-80

3. Godunov S.K., Kulikov I.M. Computation of discontinuous solutions of fluid dynamics equations with entropy nondecrease guarantee // Computational Mathematics and Mathematical Physics. – 2014. – V. 54, № 6. – P. 1012-1024

4. Kulikov I., Vorobyov E. Using the PPML approach for constructing a low-dissipation, operator-splitting scheme for numerical simulations of hydrodynamic flows // Journal of Computational Physics. – 2016. – V. 317. – P. 318-346.

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Thank you for your attention!