Numerical simulation of astrophysical problems on Intel Xeon Phi based supercomputers

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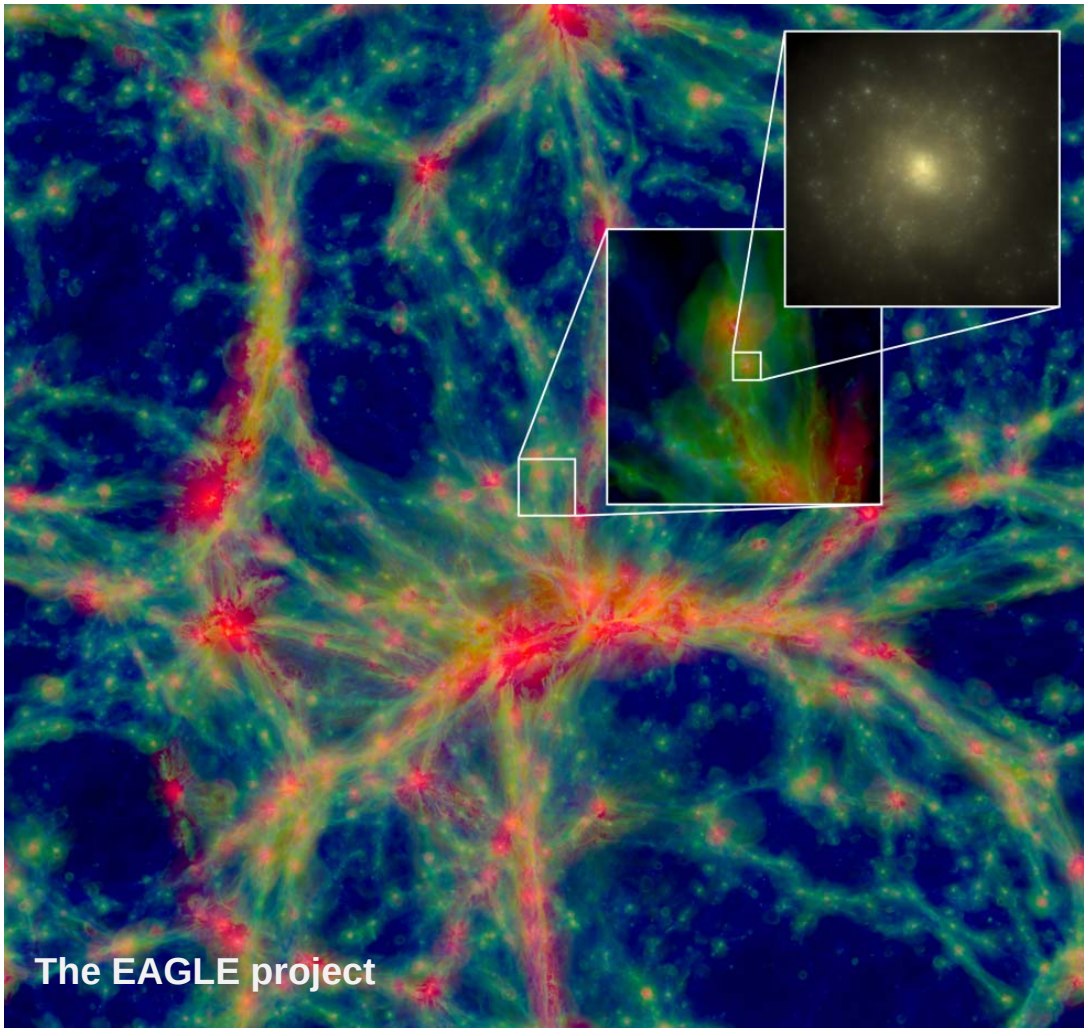
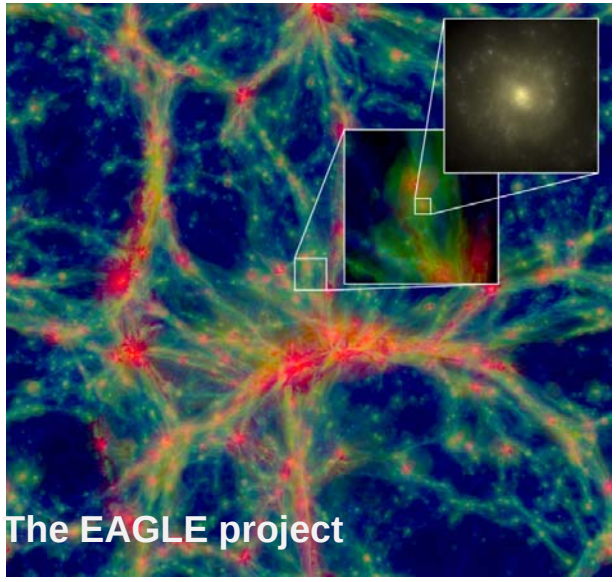
Cosmological simulation

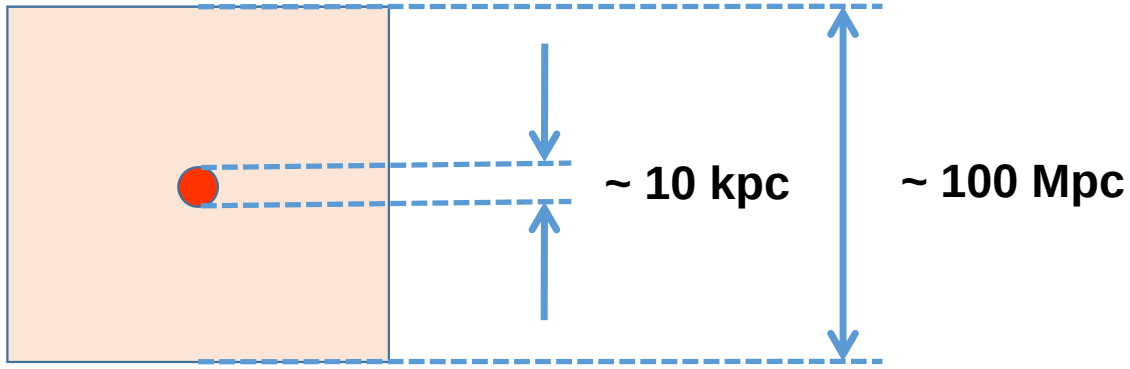


Cosmological simulation



Physics:

- Cooling/Heating
- Stars formation
- Supernova explosion
- Chemical reactions



Cosmological simulation

Hydrodynamics

$$\frac{\partial \rho}{\partial t} + \frac{1}{a}\nabla\cdot\left(\rho\vec{u}\right) = 0$$

$$\frac{\partial \rho_i}{\partial t} + \frac{1}{a}\nabla\cdot\left(\rho_i\vec{u}\right) = s_i$$

$$\frac{\partial \rho\vec{u}}{\partial t} + \frac{1}{a}\nabla\cdot\left(\rho\vec{u}\vec{u}\right) = -\frac{1}{a}\nabla p - \frac{a'}{a}\rho\vec{u} - \frac{\rho}{a^2}\nabla\Phi$$

$$\frac{\partial \rho\varepsilon}{\partial t} + \frac{1}{a}\nabla\cdot\left(\rho\varepsilon\vec{u}\right) = -\frac{1}{a}(\gamma-1)\rho\varepsilon\nabla\cdot\left(\vec{u}\right) - 2\frac{a'}{a}\rho\varepsilon + \Gamma - \Lambda$$

$$\frac{\partial \rho E}{\partial t} + \frac{1}{a}\nabla\cdot\left(\rho E\vec{u}\right) = -\frac{1}{a}\nabla\cdot\left(p\vec{u}\right) - 2\frac{a'}{a}\rho E - \frac{1}{a^2}\left(\rho\vec{u},\nabla\Phi\right) + \Gamma - \Lambda$$

Hubble's law

$$\frac{da}{dt} = H\sqrt{\Omega_M\left(a^{-1}-1\right) + \Omega_\Lambda\left(a^2-1\right)+1}$$

Cosmological simulation

Collisionless component (stars and dark matter)

$$\frac{\partial n}{\partial t}+\frac{1}{a}\nabla\cdot\left(n\vec{v}\right)=0$$

$$\frac{\partial n\vec{v}}{\partial t}+\frac{1}{a}\nabla\cdot\left(n\vec{v}\vec{v}\right)=-\frac{1}{a}\nabla\cdot(\Pi)-\frac{a'}{a}n\vec{v}-\frac{n}{a^2}\nabla\Phi$$

$$\frac{\partial \Pi_{xx}}{\partial t}+\frac{1}{a}\nabla\cdot\left(\Pi_{xx}\vec{v}\right)=-\frac{2}{a}\Pi_{xx}\frac{\partial v_x}{\partial x}-2\frac{a'}{a}\Pi_{xx}$$

$$\frac{\partial \Pi_{yy}}{\partial t}+\frac{1}{a}\nabla\cdot\left(\Pi_{yy}\vec{v}\right)=-\frac{2}{a}\Pi_{yy}\frac{\partial v_y}{\partial y}-2\frac{a'}{a}\Pi_{yy}$$

$$\frac{\partial \Pi_{zz}}{\partial t}+\frac{1}{a}\nabla\cdot\left(\Pi_{zz}\vec{v}\right)=-\frac{2}{a}\Pi_{zz}\frac{\partial v_z}{\partial z}-2\frac{a'}{a}\Pi_{zz}$$

$$\frac{\partial nW}{\partial t}+\frac{1}{a}\nabla\cdot\left(nW\vec{v}\right)=-\frac{1}{a}\nabla\cdot\left(\Pi\vec{v}\right)-2\frac{a'}{a}nW-\frac{1}{a^2}\left(n\vec{v},\nabla\Phi\right)$$

$$\Delta\Phi=4\pi G\left(\left(\rho+n\right)-\left(\rho+n\right)_0\right)$$

Numerical Method

$$\frac{\partial \mathbb{Q}}{\partial t} + \nabla \bullet \left(\mathbb{Q} \cdot \vec{v} \right) = \Im \left(\mathbb{Q}, \nabla \mathbb{Q} \right)$$

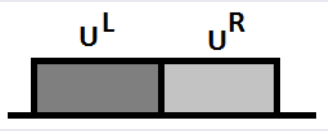
(1)

$$\frac{\partial \mathbb{Q}}{\partial t} = \Im \left(\mathbb{Q}, \nabla \mathbb{Q} \right)$$

(2)

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

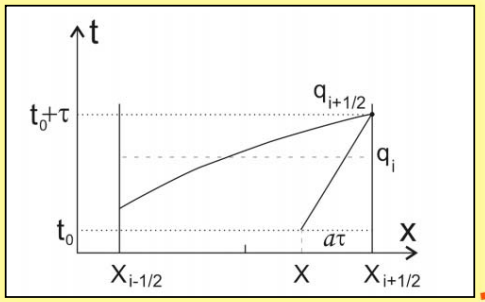
Riemann problem



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

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

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



piecewise-parabolic functions

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

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

Overdefined equation system

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

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

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

1. **Renormalization of velocity vector *at the boundary area between gas and vacuum**.**
2. **Correction of entropy****

This modification helps to control 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

Numerical method

- High-order method
- The absence of artificial viscosity
- Galilean-invariant solution
- Entropy nondecrease guarantee
- Possible extension of the model by other hyperbolic equations (fro example MHD equations)
- Simple parallelization
- «Potentially infinite scalability»

Chemical reactions

$$H + e \rightarrow H^+ + 2e \qquad H^+ + e \rightarrow H + \gamma$$

$$H + e \rightarrow H^- + \gamma \qquad H^- + H \rightarrow H_2 + e$$

$$H + H^+ \rightarrow H_2^+ + \gamma \qquad H_2^+ + H \rightarrow H_2 + H^+$$

$$H_2 + H^+ \rightarrow H_2^+ + H \qquad H_2 + e \rightarrow 2H + e$$

$$H^- + e \rightarrow H + 2e \qquad H^- + H \rightarrow 2H + e$$

$$H^- + H^+ \rightarrow 2H + \gamma \qquad H^- + H^+ \rightarrow H_2^+ + e$$

$$H_2^+ + e \rightarrow 2H + \gamma \qquad H_2^+ + H^- \rightarrow H + H_2$$

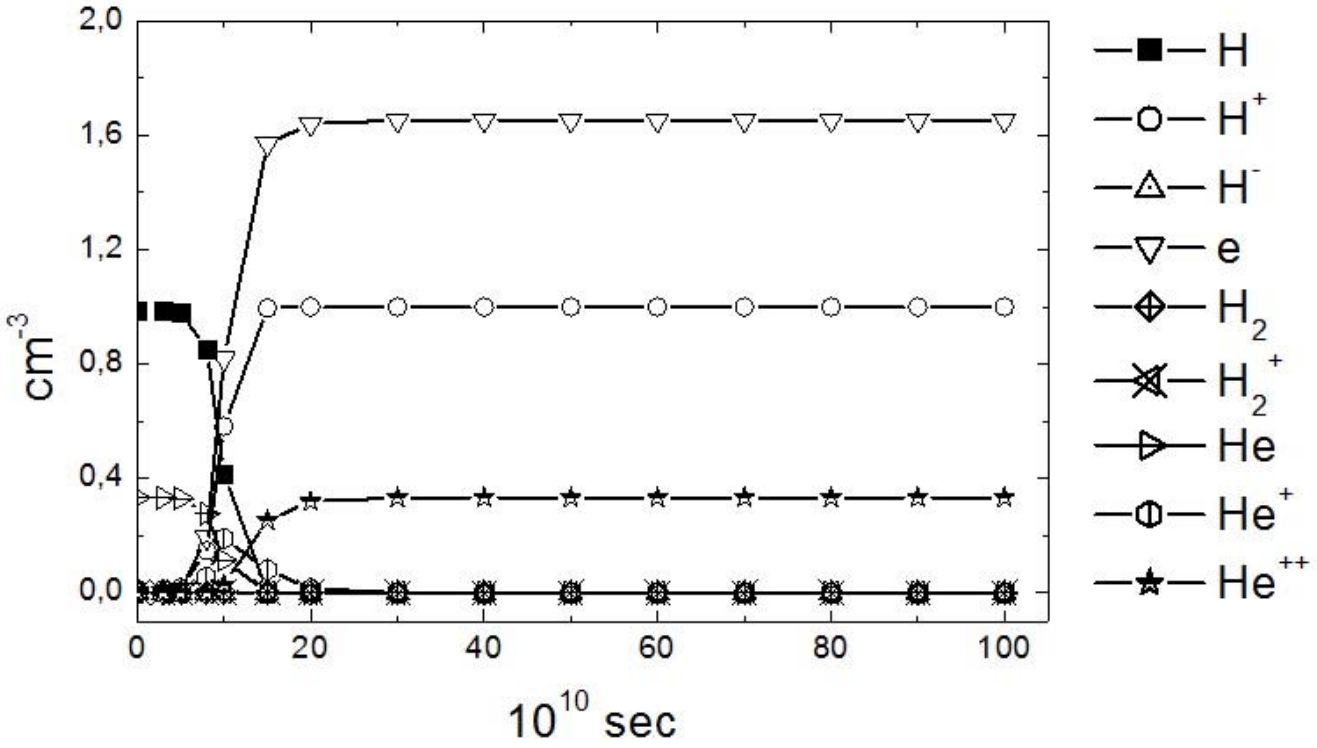
$$3H \rightarrow H_2 + H \qquad H_2 + H \rightarrow 3H$$

$$He + e \rightarrow He^+ + 2e \qquad He^+ + e \rightarrow He + \gamma$$

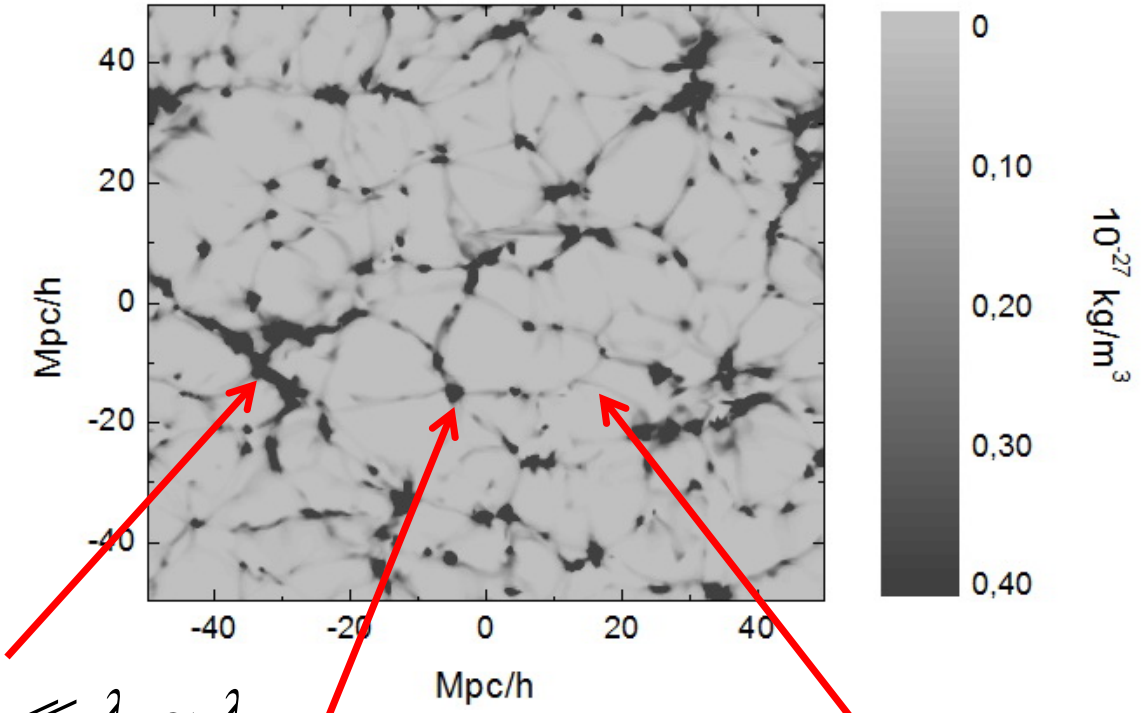
$$He^+ + e \rightarrow He^{++} + 2e \qquad He^{++} + e \rightarrow He^+ + \gamma$$

(Grassi et al., MNRAS, 2013)

Chemical reactions



Cosmological simulation



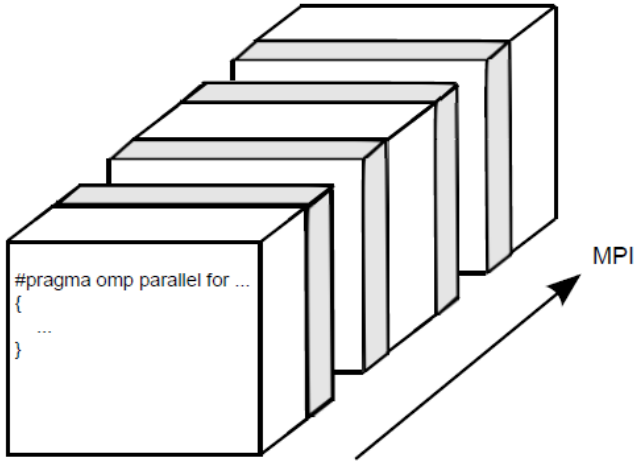
walls (pancake) $\lambda_1 \ll \lambda_2 \sim \lambda_3$

filaments $\lambda_1 \sim \lambda_2 \ll \lambda_3$

cluster $\lambda_1 \sim \lambda_2 \sim \lambda_3$

Parallel realization

134x speedup on 240 Intel Xeon Phi cores



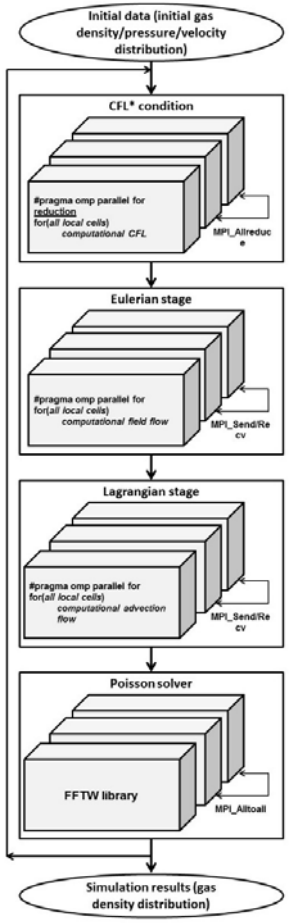
RSC PetaStream (JSCC RAS)

MICs	**64 x Intel Xeon Phi**
Logical cores	**15 360 (64 x 240)**

RSC PetaStream (Polytechnic)

MICs	**256 x Intel Xeon Phi**
Logical cores	**61 440 (256 x 240)**

Parallel realization



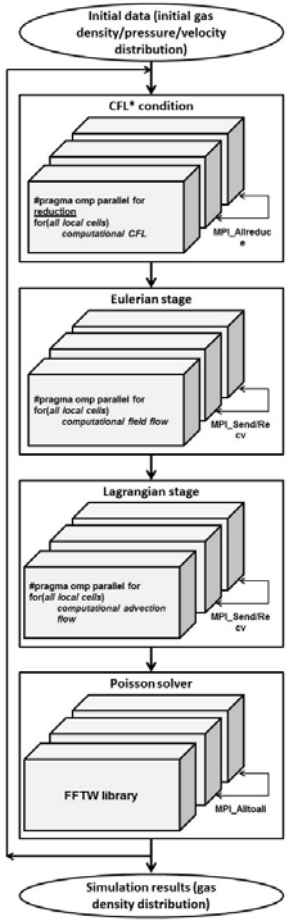
Configuration	MPI/OpenMP Communications
Intel Core-i7 3820 (4 cores, 128^3 grid size)	2.37 %
Intel Xeon E7-4870 (4 cores, 256^3 grid size)	1.65 %
Intel Xeon E5-2650v2 (16 cores, 512^3 grid size)	2.03 %
Intel Xeon Phi 7120D (60 MICs, 256^3 grid size)	8.52 %
Intel Xeon Phi 7120D (60 MICs, 512^3 grid size)	7.13 %

Number of accelerators	Efficiency (MVS-10P)	Efficiency (Polytechnic)
1	1,0000	1,0000
2	1,0345	1,0058
4	1,0335	0,9864
8	0,9771	0,9857
16	0,9417	0,9591
32	0,9345	0,9101
64	0,9235	0,8659
96	—	0,8326
128	—	0,8101
192	—	0,7711
224	—	0,7565

TABLE 2
Efficiency on a different accelerators number for MVS-10P and Polytechnic supercomputers.

73% efficiency (weak scalability) on 256x Intel Xeon Phi accelerators, 15360 cores (61440 threads) used

Vectorization



Initial code	Vectorized code

Data operations:
void EulerStage (...) {…
#pragma omp parallel for default(none) shared(…)private(…) num_threads(MIC_THREADS)
…
R_diff = …;
for(curr_ind=0 ; curr_ind <NX;curr_ind++) {
RVx[curr_ind] += -
taumic*R_diff[curr_ind]/2/hmic;
}
…}
	Data operations:
	void EulerStage (...) {…
	#pragma omp parallel for default(none) shared(…)private(…) num_threads(MIC_THREADS) …
	R_diff = … ;
	__m512d taumic = _mm256_set1_pd(tau / 2.0 / hmic)
	for(curr_ind=0 ; curr_ind <NX;curr_ind+=8) {
	RVxv =_mm512_load_pd(RVx+curr_ind);
	Rdifv =_mm512_load_pd(R_diff+curr_ind);
	RVxv=_mm512_fnmadd_pd(taumic,Rdifv,RVxv);
	mm512_store_pd(RVx+curr_ind,RVxv);
	}
	… }

Kulikov, Chernykh, Glinskiy, Nenashev, Shmelev, Andreev, Egunov, Kharkov. Numerical simulations of astrophysical problems on a massively parallel supercomputer (2016, in print)

Vectorization

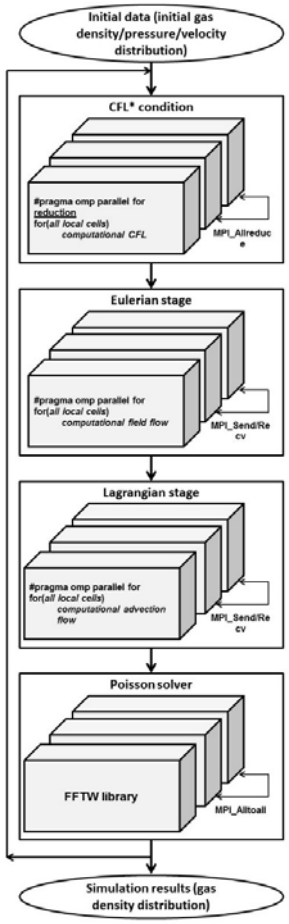


Fig 2. Optimization of memory operations, commands for working with unaligned memory

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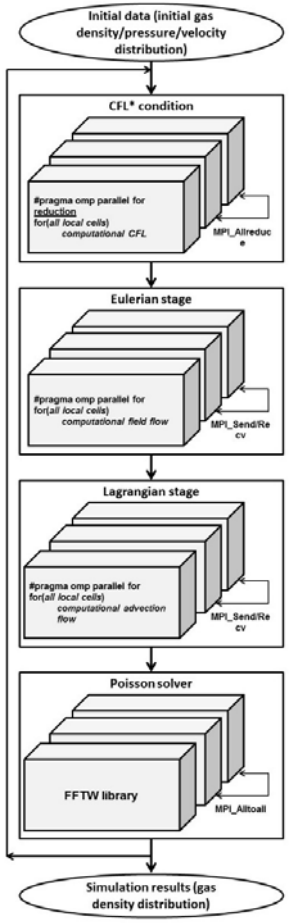
Vectorization




```
rvppp = _mm512_mask_blend_pd(_mm512_cmp_pd_mask(vppp, zero, _CMP_LT_OS), rvppp, next);
rvpmp = _mm512_mask_blend_pd(_mm512_cmp_pd_mask(vpmp, zero, _CMP_LT_OS), rvpmp, next);
rvmpp = _mm512_mask_blend_pd(_mm512_cmp_pd_mask(vmpp, zero, _CMP_LT_OS), rvmpp, next);
rvmmp = _mm512_mask_blend_pd(_mm512_cmp_pd_mask(vmmp, zero, _CMP_LT_OS), rvmmp, next);
rvppm = _mm512_mask_blend_pd(_mm512_cmp_pd_mask(vppm, zero, _CMP_GT_OS), rvppm, prev);
rvpmm = _mm512_mask_blend_pd(_mm512_cmp_pd_mask(vpmm, zero, _CMP_GT_OS), rvpmm, prev);
rvmpm = _mm512_mask_blend_pd(_mm512_cmp_pd_mask(vmpm, zero, _CMP_GT_OS), rvmpm, prev);
rvmmm = _mm512_mask_blend_pd(_mm512_cmp_pd_mask(vmmm, zero, _CMP_GT_OS), rvmmm, prev);
FZP = _mm512_mul_pd(_mm512_add_pd(_mm512_add_pd(_mm512_mul_pd(vppp, rvppp), _mm512_mul_pd(vpmp,
rvpmp)), _mm512_add_pd(_mm512_mul_pd(vmpp, rvmpp), _mm512_mul_pd(vmmp, rvmmp))), four);//(vppp*rvppp +
vppm*rvppm + vpmp*rvpmp + vpmm*rvpmm) / 4.0;
FZM = _mm512_mul_pd(_mm512_add_pd(_mm512_add_pd(_mm512_mul_pd(vppm, rvppm),
_mm512_mul_pd(vpmm, rvpmm)), _mm512_add_pd(_mm512_mul_pd(vmpm, rvmpm), _mm512_mul_pd(vmmm,
rvmmm))), four);//(vmpp*rvmpp + vmpm*rvmpm + vmmp*rvmmp + vmmm*rvmmm) / 4.0;
__m512d aVect = _mm512_loadu_pd(a + i*NZ*NY + k*NZ + l);
__m512d dmvVect = _mm512_set1_pd(dmv);
__m512d result = _mm512_sub_pd(aVect,
_mm512_mul_pd(_mm512_add_pd(_mm512_add_pd(_mm512_sub_pd(FXP, FXM), _mm512_sub_pd(FYP, FYM)),
_mm512_sub_pd(FZP, FZM)), dmvVect));
```

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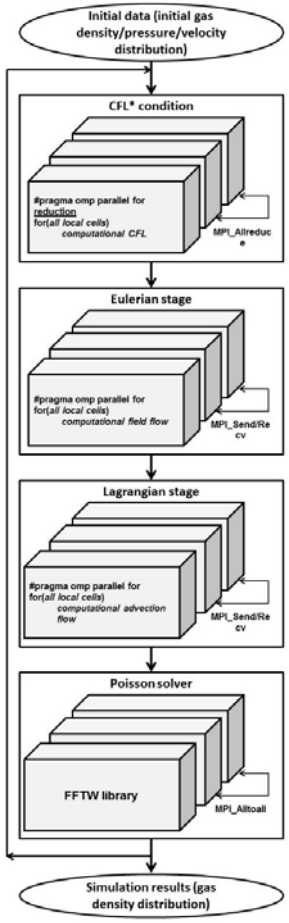
Vectorization



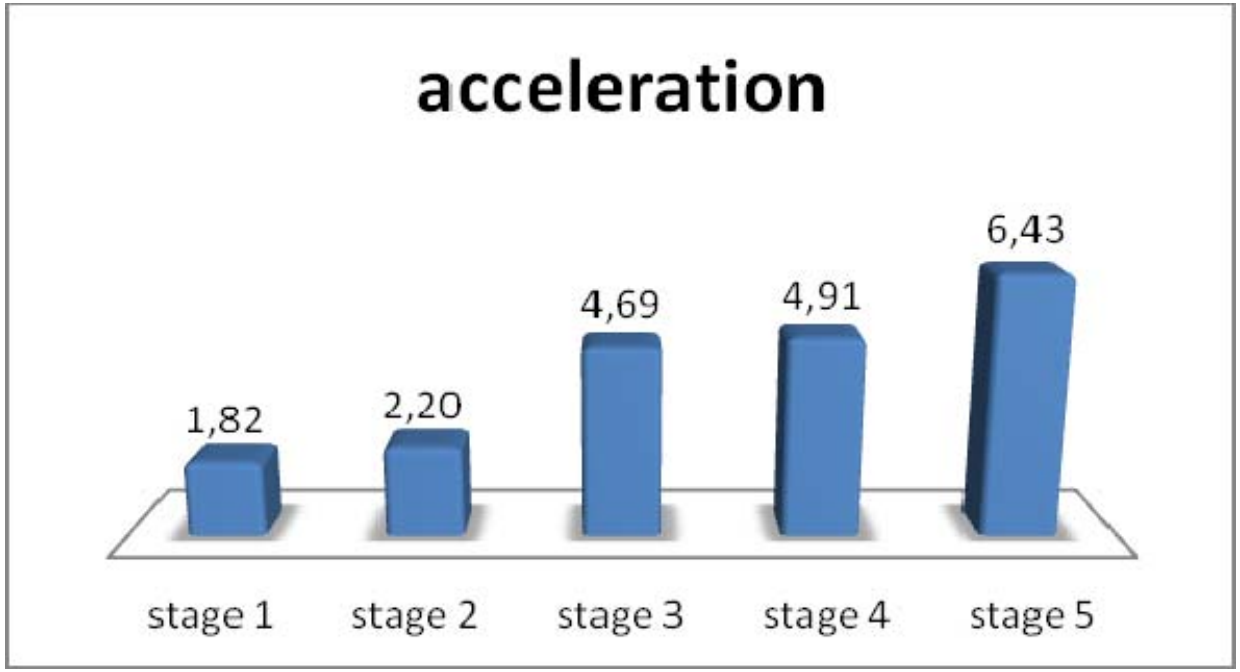


Fig. 3. Acceleration of the AstroPhi code via vectorization. Stage 1 – algorithm optimization. Stage 2 – optimization of arithmetic operations. Stage 3 – optimization of memory operations. Stage 4 – reducing a number of memory load operations. Stage 5 – transition to FMA commands.

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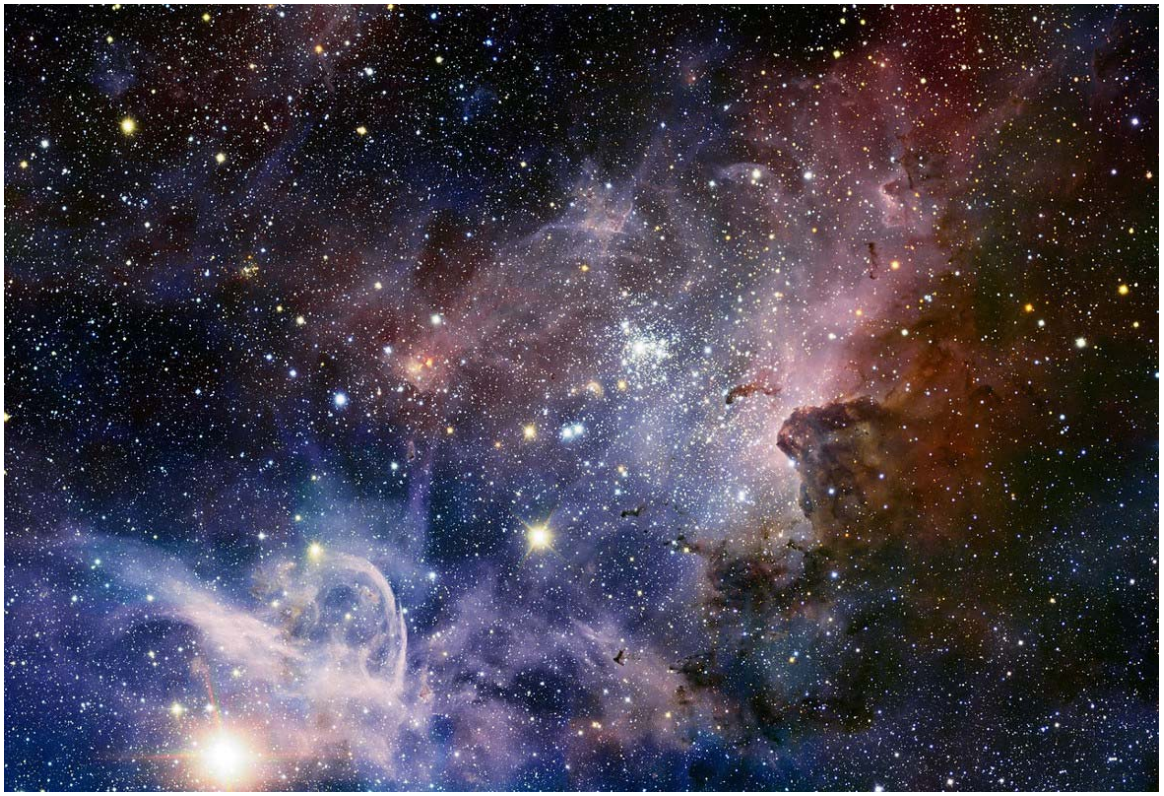
Future work

- Global MHD simulation of the solar wind interaction with comets, natural satellites and planets (the movement of galaxies through the intergalactic gas)
- A supernova explosion with chemical kinetics(178 "chemical" and nuclear reactions) in the gas-dynamic and relativistic hydrodynamics model
- Implementation of the astrophysical code to state-of-art level (Top10 astrophysical code in 2020)



Thank you for your attention