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Experimental Study of Macrogrid Domain Decomposition Methods with Approximate Block Bisection

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Работа поддержана грантом РНФ № 24-21-00402

N* NOVOSIBIRSK STATE UNIVERSITY *The real science

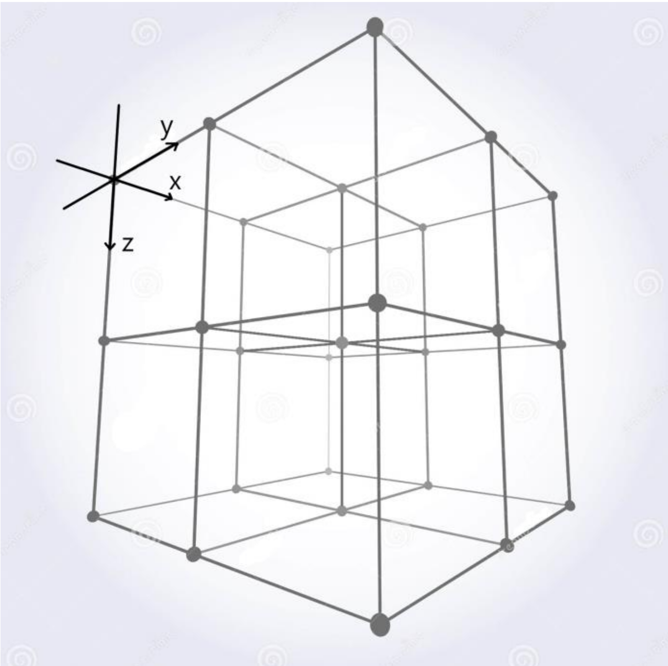
ICM&MG

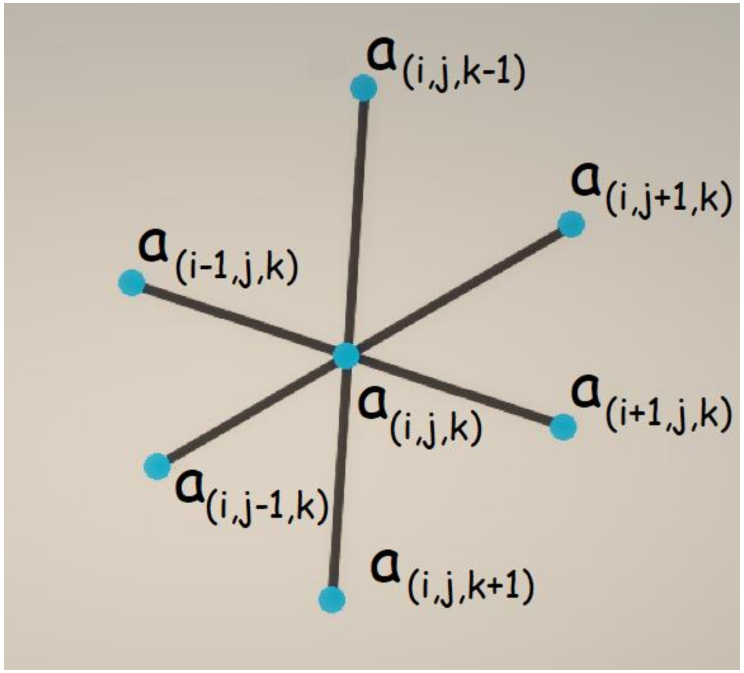
Постановка задачи:

$$\begin{cases} \Delta u = f \ , \ \Omega \in R^3 \\ u = 1 \text{ на } \partial\Omega \end{cases}$$

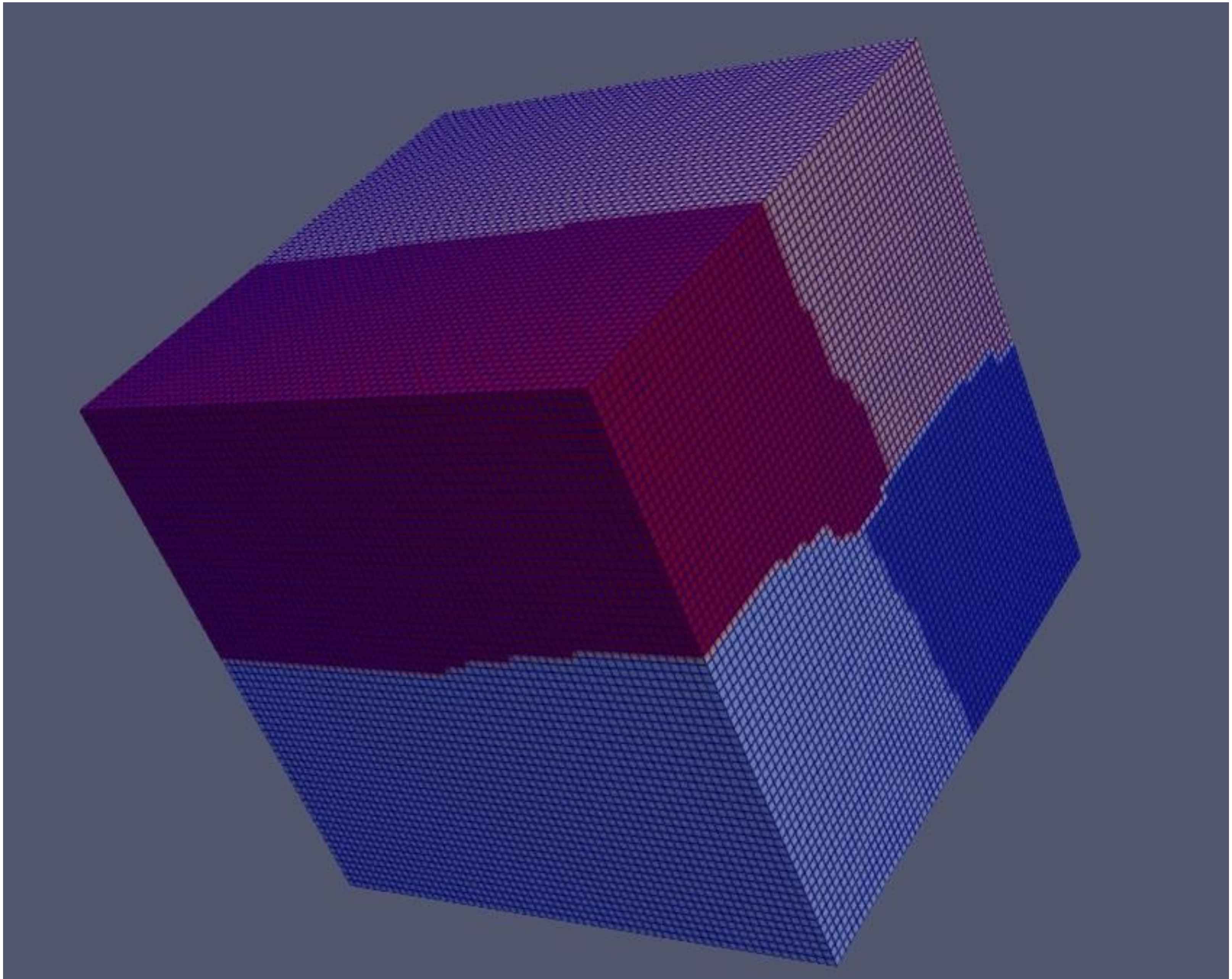
$$\Omega = [x_0, x_{Nx+1}] \times [y_0, y_{Ny+1}] \times [z_0, z_{Ny+1}]$$

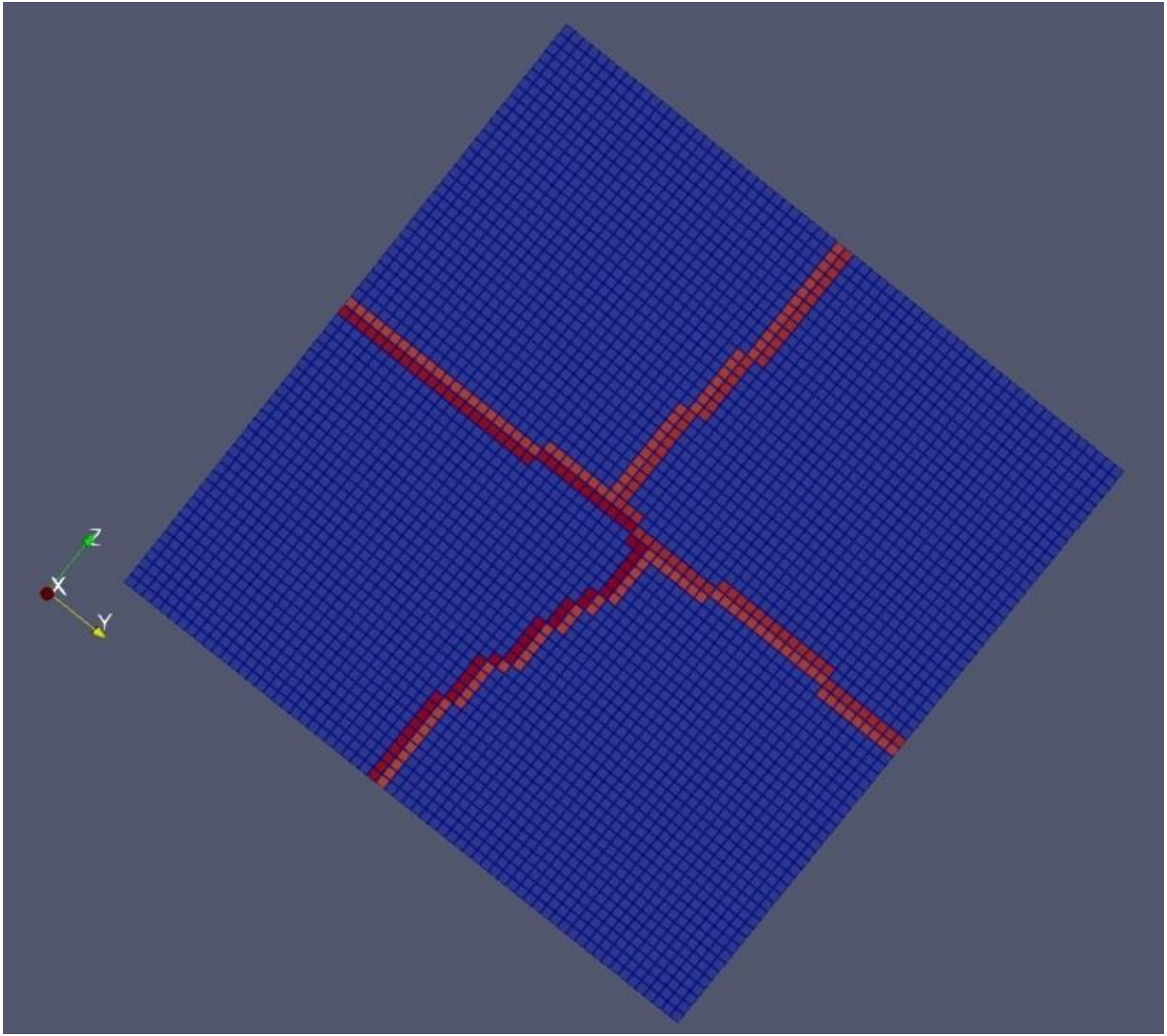
$$\Omega^h : (x_i, y_j, z_k) \ i = 1, ..., N_x; \ j = 1, ..., N_y; \ k = 1, ..., N_z;$$





Построение макросетки




Z
X
Y

$$Au = f$$

$$f = A \begin{bmatrix} 1 \\ 1 \\ .. \\ 1 \end{bmatrix}, Au = \begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{bmatrix} \begin{bmatrix} u_a \\ u_b \end{bmatrix} = \begin{bmatrix} f_a \\ f_b \end{bmatrix}$$

$$A = \begin{bmatrix} A_{1,1} & 0 \\ A_{2,1} & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & S \end{bmatrix} \begin{bmatrix} I & A_{1,1}^{-1} A_{1,2} \\ 0 & I \end{bmatrix}$$

$$S = A_{2,2} - A_{2,1} A_{1,1}^{-1} A_{1,2}$$

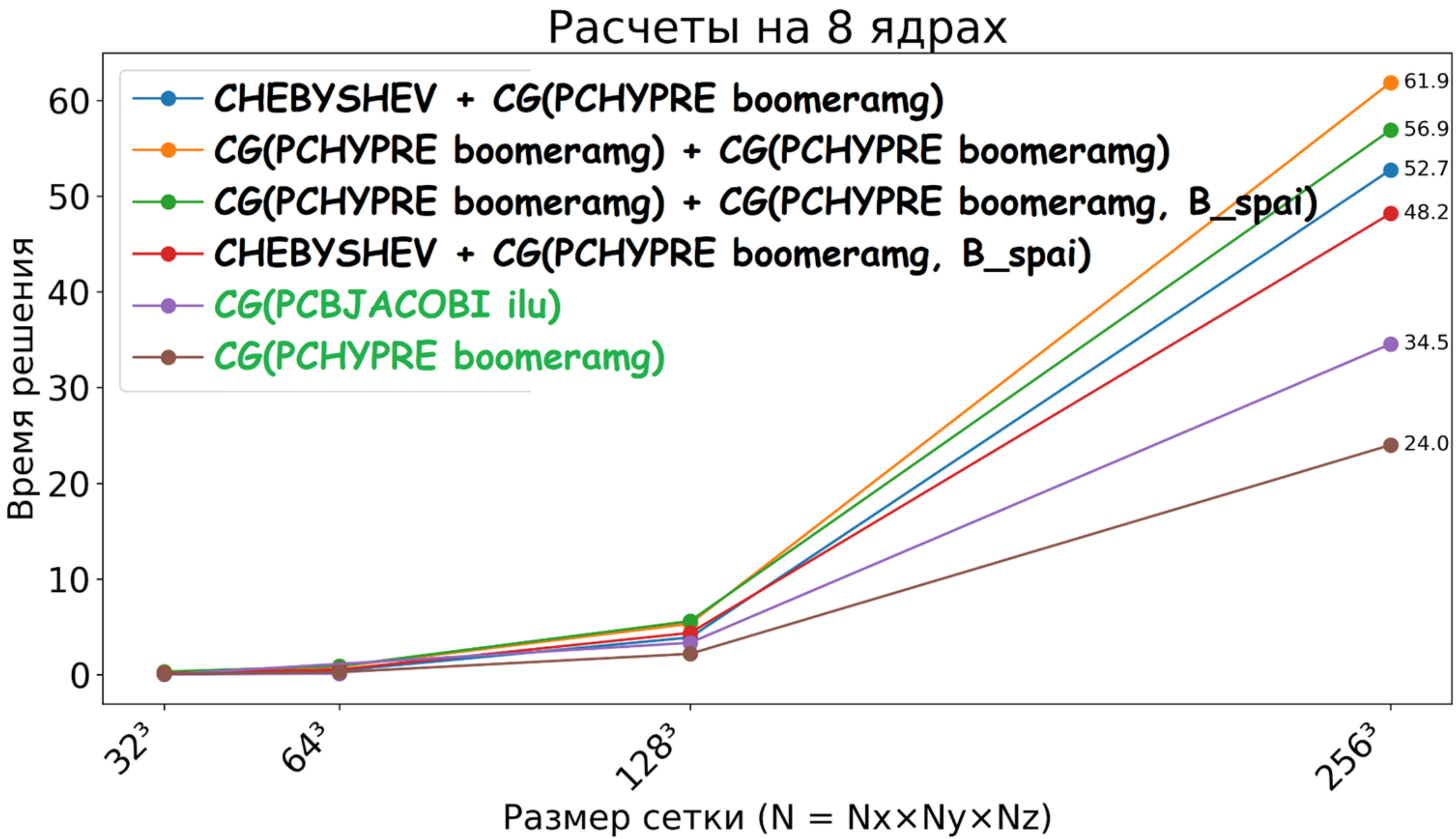
1. $$\bar{f} = \begin{bmatrix} \bar{f}_a \\ \bar{f}_b \end{bmatrix}, \quad \begin{aligned} \bar{f}_a &= A_{1,1}^{-1} f_a \\ \bar{f}_b &= f_b - A_{2,1} \bar{f}_a \end{aligned}$$

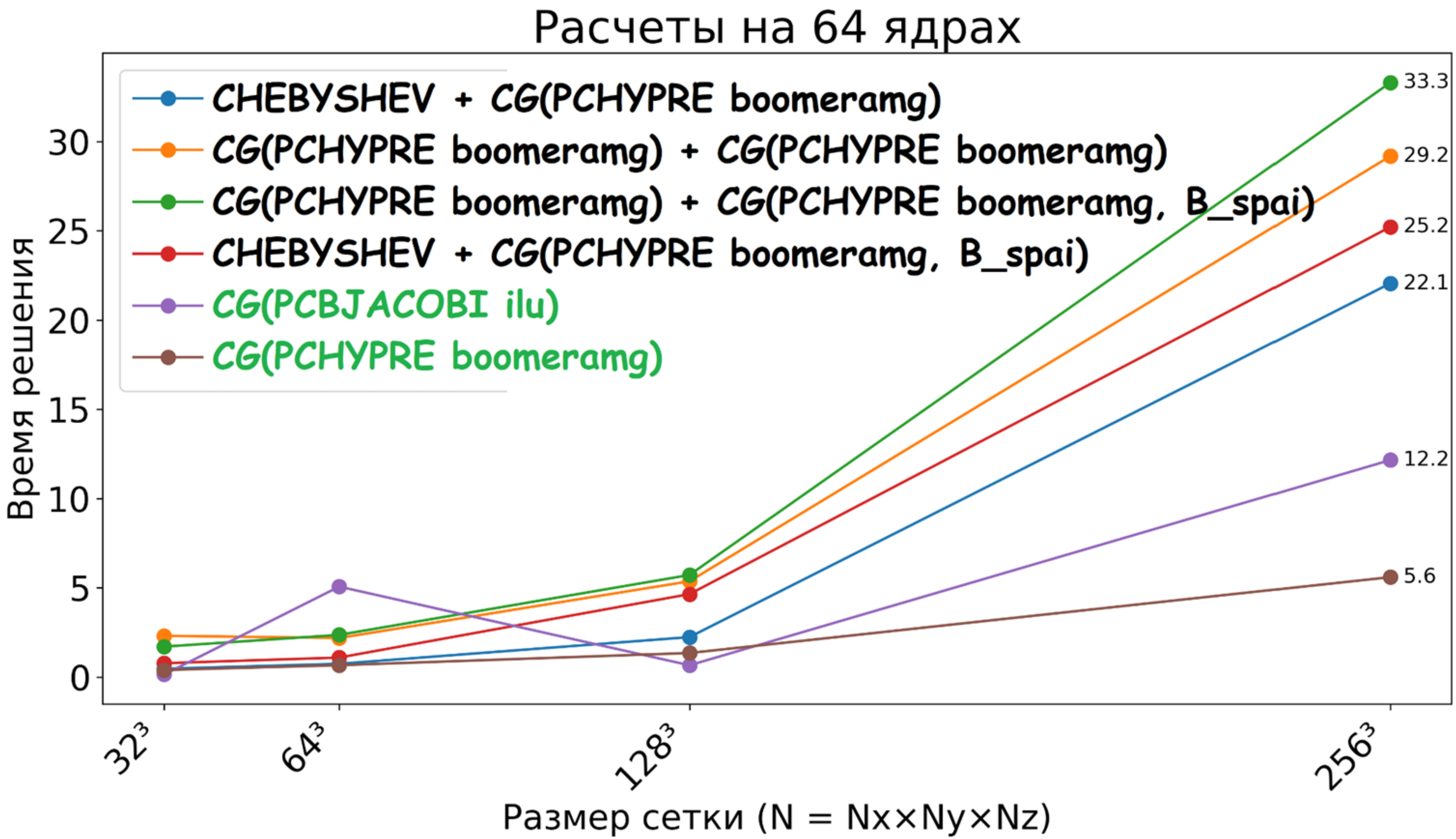
$$\lambda_{max} = ||A_{1,1}||_\infty, \; \lambda_{min} = 1$$

2. $$S\bar{u}_b = \bar{f}_b \; , \; S \approx B_S = A_{2,2} - \theta C$$

$$\theta \in [0,1] \; , \; Ce = A_{2,1} A_{1,1}^{-1} A_{1,2} e$$

3. $$\bar{u}_a = \bar{f}_a \; , \; u = \begin{bmatrix} I & A_{1,1}^{-1} A_{1,2} \\ 0 & I \end{bmatrix} \bar{u}$$


Расчеты на 8 ядрах
CHEBYSHEV + CG(PCHYPRE boomeramg)
CG(PCHYPRE boomeramg) + CG(PCHYPRE boomeramg)
CG(PCHYPRE boomeramg) + CG(PCHYPRE boomeramg, B_spai)
CHEBYSHEV + CG(PCHYPRE boomeramg, B_spai)
CG(PCBJACOBI ilu)
CG(PCHYPRE boomeramg)
61.9
56.9
52.7
48.2
34.5
24.0
Время решения
0
10
20
30
40
50
60
32³
64³
128³
256³
Размер сетки (N = Nx×Ny×Nz)



Расчеты на 64 ядрах
CHEBYSHEV + CG(PCHYPRE boomeramg)
CG(PCHYPRE boomeramg) + CG(PCHYPRE boomeramg)
CG(PCHYPRE boomeramg) + CG(PCHYPRE boomeramg, B_spai)
CHEBYSHEV + CG(PCHYPRE boomeramg, B_spai)
CG(PCBJACOBI ilu)
CG(PCHYPRE boomeramg)
33.3
29.2
25.2
22.1
12.2
5.6
Время решения
0
5
10
15
20
25
30
32^3
64^3
128^3
256^3
Размер сетки (N = Nx×Ny×Nz)

PCSetType(pc_S, PCBJACOBI);

	32^3	64^3	128^3	256^3
8 ядер	n = 45 Δ = 5.88e-07 t = 0.015868 r = 9.36e-08	n = 80 Δ = 8.85e-07 t = 0.133642 r = 1.12e-07	n = 147 Δ = 1.52e-06 t = 3.330689 r = 1.07e-07	n = 269 Δ = 3.24e-06 t = 34.544850 r = 1.08e-07
64 ядер	n = 52 Δ = 7.10e-07 t = 0.151154 r = 1.05e-07	n = 87 Δ = 1.01e-06 t = 5.072682 r = 1.26e-07	n = 152 Δ = 2.13e-06 t = 0.668400 r = 1.23e-07	n = 275 Δ = 5.31e-06 t = 12.161725 r = 1.17e-07

PCSetType(pc_S, PCHYPRE);

	32^3	64^3	128^3	256^3
8 ядер	n = 11 Δ = 3.18e-07 t = 0.075907 r = 6.46e-08	n = 12 Δ = 6.14e-07 t = 0.259020 r = 8.52e-08	n = 14 Δ = 4.29e-07 t = 2.175602 r = 3.54e-08	n = 16 Δ = 9.93e-07 t = 23.994086 r = 5.54e-08
64 ядер	n = 12 Δ = 3.17e-07 t = 0.402106 r = 6.96e-08	n = 13 Δ = 6.28e-07 t = 0.671745 r = 1.05e-07	n = 15 Δ = 6.27e-07 t = 1.354671 r = 6.60e-08	n = 17 Δ = 8.08e-07 t = 5.604505 r = 6.22e-08

CHEBYSHEV+CG(PCHYPRE boomeramg, B_spai)

	32^3	64^3	128^3	256^3
8 ядер	n = 34 A11: 0.004466 r = 7.92e-08 n = 16 S: 0.134499 r = 7.92e-08 Δ = 5.25e-06 Full: 0.152580 r = 2.06e-07	n = 31 A11: 0.006100 r = 7.23e-08 n = 25 S: 0.493347 r = 7.23e-08 Δ = 9.70e-06 Full: 0.537611 r = 1.67e-07	n = 30 A11: 0.012745 r = 9.07e-08 n = 35 S: 4.137747 r = 9.07e-08 Δ = 1.60e-05 Full: 4.364867 r = 1.90e-07	n = 29 A11: 0.051087 r = 8.54e-08 n = 50 S: 46.526033 r = 8.54e-08 Δ = 3.25e-05 Full: 48.183920 r = 1.85e-07
64 ядер	n = 47 A11: 0.124555 r = 9.02e-08 n = 19 S: 0.617294 r = 9.02e-08 Δ = 7.39e-06 Full: 0.783534 r = 2.31e-07	n = 35 A11: 0.019618 r = 7.75e-08 n = 31 S: 1.031941 r = 7.75e-08 Δ = 1.24e-05 Full: 1.100296 r = 2.48e-07	n = 34 A11: 0.681591 r = 7.54e-08 n = 44 S: 2.954330 r = 7.54e-08 Δ = 2.34e-05 Full: 4.652473 r = 2.49e-07	n = 31 A11: 0.078453 r = 7.12e-08 n = 65 S: 23.666658 r = 7.12e-08 Δ = 3.34e-05 Full: 25.219505 r = 2.61e-07

Вывод

Возможные приемы ускорения:

- Специальная блочная структура матрицы A11 позволяет эффективно использовать мелко-блочные варианты прогонок, значительно повышающие производительность расчетов.
- Дальнейшее совершенствование метода можно осуществить с помощью обобщенного принципа согласования сеточных сумм для обратной матрицы A11.
- Для решения матрицы S применять дефляционные алгоритмы, основанные на расширении Крыловского базиса с учетом предыдущих внешних итераций.

Расчеты производились на вычислительном узле a100serv НОЦ «Газпромнефть-НГУ» - 72 ядра Intel Xeon Platinum 8354H 3.1 GHz, 3 Тб оперативной памяти, графическая карта NVIDIA Tesla A100, сеть Ethernet 10 Гб/с.

Спасибо за внимание!

KSPSetType(ksp, KSPCG);
KSPSetTolerances(ksp, 1e-7, 1e-8, 1000, 1000);
KSPGetPC(ksp, &pc_S);
PCSetType(pc_S, PCBJACOBI);
PetscOptionsSetValue(NULL, -sub_pc_type, ilu);
KSPSetOperators(ksp, A, A);
VecZeroEntries(x);
KSPSolve(ksp, rhs, x);

	32^3	64^3	128^3	256^3
8 ядер	n = 45 Δ = 5.88e-07 t = 0.015868 r = 9.36e-08	n = 80 Δ = 8.85e-07 t = 0.133642 r = 1.12e-07	n = 147 Δ = 1.52e-06 t = 3.330689 r = 1.07e-07	n = 269 Δ = 3.24e-06 t = 34.544850 r = 1.08e-07
64 ядер	n = 52 Δ = 7.10e-07 t = 0.151154 r = 1.05e-07	n = 87 Δ = 1.01e-06 t = 5.072682 r = 1.26e-07	n = 152 Δ = 2.13e-06 t = 0.668400 r = 1.23e-07	n = 275 Δ = 5.31e-06 t = 12.161725 r = 1.17e-07

KSPSetType(ksp, KSPCG);
KSPSetTolerances(ksp, 1e-7, 1e-8, 1000, 1000);
KSPGetPC(ksp, &pc_S);
PCSetType(pc_S, PCHYPRE);
PCHYPRESetType(pc_S,boomeramg);
-pc_hypre_boomeramg_agg_nl, 1;
-pc_hypre_boomeramg_strong_threshold, 0.7
-pc_hypre_boomeramg_coarsen_type, HMIS
-pc_hypre_boomeramg_interp_type, ext+i
-pc_hypre_boomeramg_truncfactor, 0.2
KSPSetOperators(ksp, A, A);
PetscOptionsSetValue(NULL, -sub_pc_type, ilu);
VecZeroEntries(x);
KSPSolve(ksp, rhs, x);

	32^3	64^3	128^3	256^3
8 ядер	n = 11 Δ = 3.18e-07 t = 0.075907 r = 6.46e-08	n = 12 Δ = 6.14e-07 t = 0.259020 r = 8.52e-08	n = 14 Δ = 4.29e-07 t = 2.175602 r = 3.54e-08	n = 16 Δ = 9.93e-07 t = 23.994086 r = 5.54e-08
64 ядер	n = 12 Δ = 3.17e-07 t = 0.402106 r = 6.96e-08	n = 13 Δ = 6.28e-07 t = 0.671745 r = 1.05e-07	n = 15 Δ = 6.27e-07 t = 1.354671 r = 6.60e-08	n = 17 Δ = 8.08e-07 t = 5.604505 r = 6.22e-08

```
KSPSetOperators(ksp_cheb, A11, A11);
KSPGetPC(ksp_cheb, &pc_cheb);
PCSetType(pc_cheb,PCNONE );
KSPSetType(ksp_cheb, KSPCHEBYSHEV);
KSPChebyshevSetEigenvalues(ksp_cheb, h_max, h_min);
KSPSetTolerances(ksp_cheb, 1e-7, 1e-8, 1e2, 1000);
VecZeroEntries(fa_bar);
KSPSolve(ksp_cheb,fa,fa_bar);

KSPSetType(ksp_S, KSPCG);
KSPSetTolerances(ksp_S, 1e-7, 1e-8, 1000, 1000);
KSPGetPC(ksp_S, &pc_S);
PCSetType(pc_S, PCHYPRE);
PCHYPRESetType(pc_S,boomeramg);
-pc_hypre_boomeramg_agg_nl, 1;
-pc_hypre_boomeramg_strong_threshold, 0.7
-pc_hypre_boomeramg_coarsen_type, HMIS
-pc_hypre_boomeramg_interp_type, ext+i
-pc_hypre_boomeramg_truncfactor, 0.2
KSPSetOperators(ksp_S, S, B_S);
VecZeroEntries(x);
KSPSolve(ksp_S,fb_bar,ub_bar);
```

```
KSPSetOperators(ksp_S, A11, A11);
KSPSetType(ksp_S, KSPCG);
KSPSetTolerances(ksp_S, 1e-7, 1e-8, 1000, 1000);
KSPGetPC(ksp_S, &pc_S);
PCSetType(pc_S, PCHYPRE);
PCHYPRESetType(pc_S,boomeramg);
-pc_hypre_boomeramg_agg_nl, 1;
-pc_hypre_boomeramg_strong_threshold, 0.7
-pc_hypre_boomeramg_coarsen_type, HMIS
-pc_hypre_boomeramg_interp_type, ext+i
-pc_hypre_boomeramg_truncfactor, 0.2
KSPSetTolerances(ksp_cheb, 1e-7, 1e-8, 1e2, 1000);
VecZeroEntries(fa_bar);
KSPSolve(ksp_S,fa,fa_bar);

KSPSetOperators(ksp_S, S, B_S);
VecZeroEntries(x);
KSPSolve(ksp_S,fb_bar,ub_bar);
```

	32^3	64^3	128^3	256^3
8 ядер	n = 34 A11: 0.004618 r = 7.92e-08 n = 18 S: 0.110706 r = 7.92e-08 Δ = 5.53e-06 Full: 0.123731 r = 1.56e-07	n = 31 A11: 0.005807 r = 7.23e-08 n = 28 S: 0.410750 r = 7.23e-08 Δ = 9.04e-06 Full: 0.429039 r = 1.57e-07	n = 30 A11: 0.012017 r = 9.07e-08 n = 38 S: 3.830442 r = 9.07e-08 Δ = 1.73e-05 Full: 3.886811 r = 2.05e-07	n = 29 A11: 0.059373 r = 8.54e-08 n = 56 S: 52.339505 r = 8.54e-08 Δ = 3.25e-05 Full: 52.736405 r = 1.90e-07
64 ядер	n = 47 A11: 0.017729 r = 9.02e-08 n = 21 S: 0.431624 r = 9.02e-08 Δ = 6.95e-06 Full: 0.473744 r = 2.07e-07	n = 35 A11: 0.017360 r = 7.75e-08 n = 33 S: 0.698123 r = 7.75e-08 Δ = 1.19e-05 Full: 0.749903 r = 2.59e-07	n = 34 A11: 0.054229 r = 7.54e-08 n = 50 S: 2.154716 r = 7.54e-08 Δ = 2.20e-05 Full: 2.246164 r = 2.50e-07	n = 31 A11: 0.066916 r = 7.12e-08 n = 74 S: 21.799548 r = 7.12e-08 Δ = 3.35e-05 Full: 22.059736 r = 2.70e-07

	32^3	64^3	128^3	256^3
8 ядер	n = 3 A11: 0.045084 r = 1.29e-08 n = 18 S: 0.231033 r = 1.29e-08 Δ = 5.18e-07 Full: 0.290216 r = 1.10e-07	n = 3 A11: 0.084981 r = 5.79e-09 n = 28 S: 0.729587 r = 5.79e-09 Δ = 1.09e-06 Full: 0.838139 r = 1.11e-07	n = 3 A11: 0.291383 r = 7.99e-09 n = 38 S: 4.957728 r = 7.99e-09 Δ = 2.60e-06 Full: 5.322741 r = 1.50e-07	n = 3 A11: 2.121518 r = 6.44e-09 n = 56 S: 59.319539 r = 6.44e-09 Δ = 6.61e-06 Full: 61.866181 r = 1.45e-07
64 ядер	n = 3 A11: 0.831521 r = 2.41e-08 n = 21 S: 1.416708 r = 2.41e-08 Δ = 1.34e-06 Full: 2.319806 r = 2.06e-07	n = 3 A11: 0.231185 r = 2.33e-08 n = 33 S: 1.904302 r = 2.33e-08 Δ = 1.42e-06 Full: 2.196113 r = 1.82e-07	n = 3 A11: 0.338638 r = 1.37e-08 n = 50 S: 4.940102 r = 1.37e-08 Δ = 3.85e-06 Full: 5.372162 r = 1.86e-07	n = 3 A11: 1.015650 r = 9.40e-09 n = 74 S: 27.914539 r = 9.40e-09 Δ = 9.02e-06 Full: 29.184595 r = 1.75e-07

```
KSPSetOperators(ksp_S, A11, A11);
KSPSetType(ksp_S, KSPCG);
KSPSetTolerances(ksp_S, 1e-7, 1e-8, 1000, 1000);
KSPGetPC(ksp_S, &pc_S);
PCSetType(pc_S, PCHYPRE);
PCHYPRESetType(pc_S,boomeramg);
-pc_hypre_boomeramg_agg_nl, 1;
-pc_hypre_boomeramg_strong_threshold, 0.7
-pc_hypre_boomeramg_coarsen_type, HMIS
-pc_hypre_boomeramg_interp_type, ext+i
-pc_hypre_boomeramg_truncfactor, 0.2
KSPSetTolerances(ksp_cheb, 1e-7, 1e-8, 1e2, 1000);
VecZeroEntries(fa_bar);
KSPSolve(ksp_S,fa,fa_bar);

build_SPAI(A11,&A11_inv);
B_spai = A22 - A21*A11_inv*A12
KSPSetOperators(ksp_S, S, B_spai);
VecZeroEntries(ub_bar);
KSPSolve(ksp_S,fb_bar,ub_bar);
```

	32^3	64^3	128^3	256^3
8 ядер	n = 3 A11: 0.044498 r = 1.29e-08 n = 16 S: 0.241166 r = 1.29e-08 Δ = 1.31e-06 Full: 0.305467 r = 1.77e-07	n = 3 A11: 0.083594 r = 5.79e-09 n = 25 S: 0.765913 r = 5.79e-09 Δ = 1.49e-06 Full: 0.898320 r = 1.21e-07	n = 3 A11: 0.287360 r = 7.99e-09 n = 35 S: 5.056906 r = 7.99e-09 Δ = 3.13e-06 Full: 5.594019 r = 1.31e-07	n = 3 A11: 2.086673 r = 6.44e-09 n = 50 S: 53.052982 r = 6.44e-09 Δ = 4.52e-06 Full: 56.899013 r = 1.36e-07
64 ядер	n = 3 A11: 0.240569 r = 2.41e-08 n = 19 S: 1.384750 r = 2.41e-08 Δ = 1.53e-06 Full: 1.712454 r = 2.20e-07	n = 3 A11: 0.240217 r = 2.33e-08 n = 31 S: 2.046254 r = 2.33e-08 Δ = 1.19e-06 Full: 2.369924 r = 1.53e-07	n = 3 A11: 0.965634 r = 1.37e-08 n = 44 S: 4.586069 r = 1.37e-08 Δ = 2.76e-06 Full: 5.725825 r = 1.73e-07	n = 3 A11: 1.073831 r = 9.40e-09 n = 65 S: 31.290830 r = 9.40e-09 Δ = 1.01e-05 Full: 33.302043 r = 1.64e-07

```
KSPSetOperators(ksp_cheb, A11, A11);
KSPGetPC(ksp_cheb, &pc_cheb);
PCSetType(pc_cheb,PCNONE );
KSPSetType(ksp_cheb, KSPCHEBYSHEV);
KSPChebyshevSetEigenvalues(ksp_cheb, h_max, h_min);
KSPSetTolerances(ksp_cheb, 1e-7, 1e-8, 1e2, 1000);
VecZeroEntries(fa_bar);
KSPSolve(ksp_cheb,fa,fa_bar);

KSPSetType(ksp_S, KSPCG);
KSPSetTolerances(ksp_S, 1e-7, 1e-8, 1000, 1000);
KSPGetPC(ksp_S, &pc_S);
PCSetType(pc_S, PCHYPRE);
PCHYPRESetType(pc_S,boomeramg);
-pc_hypre_boomeramg_agg_nl, 1;
-pc_hypre_boomeramg_strong_threshold, 0.7
-pc_hypre_boomeramg_coarsen_type, HMIS
-pc_hypre_boomeramg_interp_type, ext+i
-pc_hypre_boomeramg_truncfactor, 0.2
build_SPAI(A11,&A11_inv);
B_spai = A22 - A21*A11_inv*A12
KSPSetOperators(ksp_S, S, B_spai);
VecZeroEntries(ub_bar);
KSPSolve(ksp_S,fb_bar,ub_bar);
```

	32^3	64^3	128^3	256^3
8 ядер	n = 34 A11: 0.004466 r = 7.92e-08 n = 16 S: 0.134499 r = 7.92e-08 Δ = 5.25e-06 Full: 0.152580 r = 2.06e-07	n = 31 A11: 0.006100 r = 7.23e-08 n = 25 S: 0.493347 r = 7.23e-08 Δ = 9.70e-06 Full: 0.537611 r = 1.67e-07	n = 30 A11: 0.012745 r = 9.07e-08 n = 35 S: 4.137747 r = 9.07e-08 Δ = 1.60e-05 Full: 4.364867 r = 1.90e-07	n = 29 A11: 0.051087 r = 8.54e-08 n = 50 S: 46.526033 r = 8.54e-08 Δ = 3.25e-05 Full: 48.183920 r = 1.85e-07
64 ядер	n = 47 A11: 0.124555 r = 9.02e-08 n = 19 S: 0.617294 r = 9.02e-08 Δ = 7.39e-06 Full: 0.783534 r = 2.31e-07	n = 35 A11: 0.019618 r = 7.75e-08 n = 31 S: 1.031941 r = 7.75e-08 Δ = 1.24e-05 Full: 1.100296 r = 2.48e-07	n = 34 A11: 0.681591 r = 7.54e-08 n = 44 S: 2.954330 r = 7.54e-08 Δ = 2.34e-05 Full: 4.652473 r = 2.49e-07	n = 31 A11: 0.078453 r = 7.12e-08 n = 65 S: 23.666658 r = 7.12e-08 Δ = 3.34e-05 Full: 25.219505 r = 2.61e-07