Комплекс программ INMOST:
МКО дискретизации, реакции, и
методы решения линейных систем

Sparse System Solution Methods (S^3M)

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CFD Weekend
18 декабря, 2021

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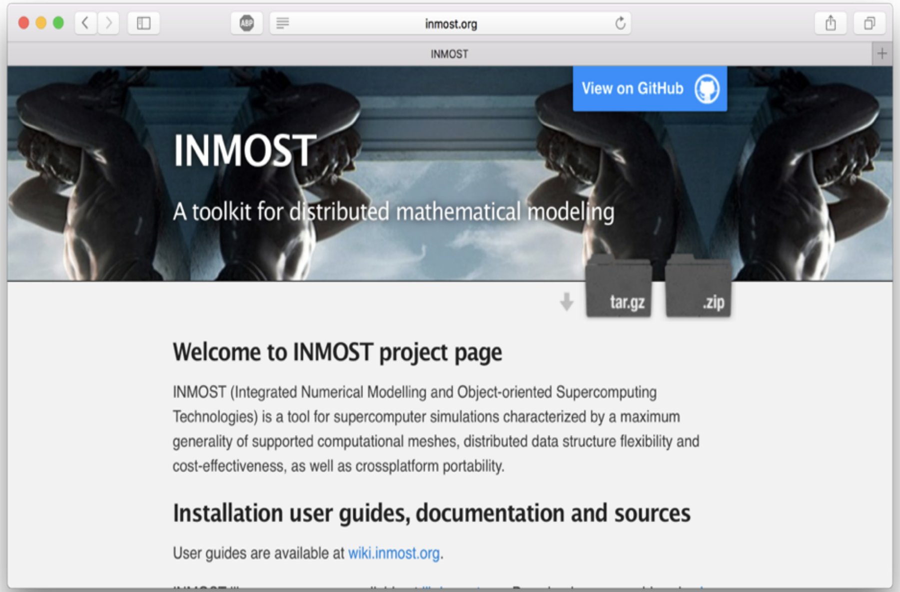
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Installation user guides, documentation and sources
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для разработки параллельных численных моделей на сетках общего вида
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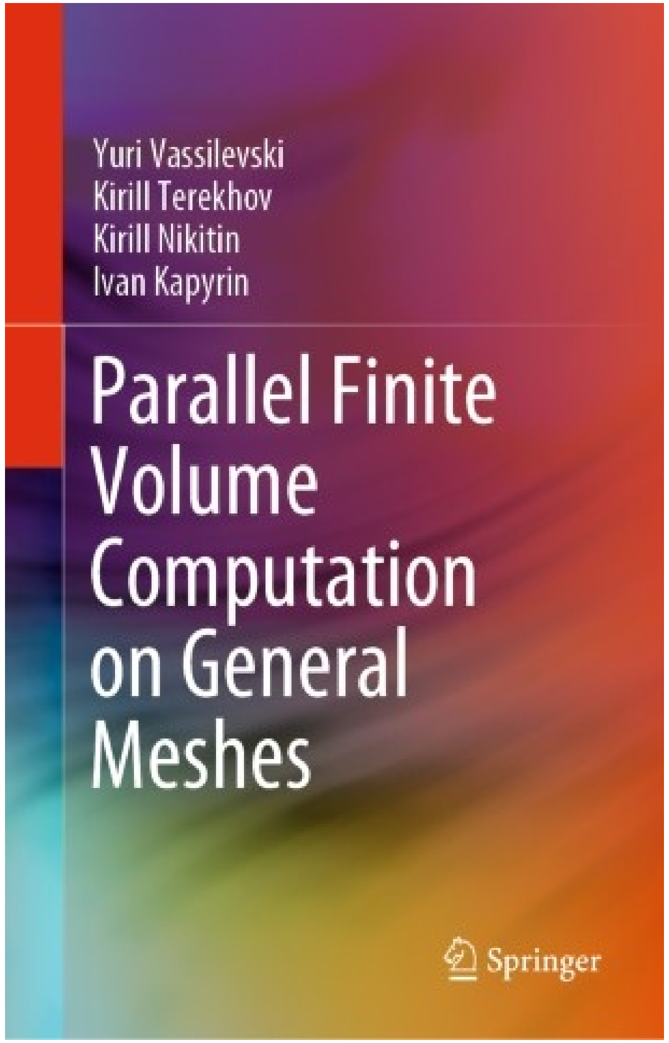
Yuri Vassilevski
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Parallel Finite Volume Computation on General Meshes
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Флагманские линейные решатели INMOST

- Preconditioned **BiCGStab(l)** method[1].
- Preconditioner parallelization using **Additive Schwarz Method**.
- **Multi-level** preconditioner based on the second-order **Crout-ILU**[2,3].
- **Condition estimation** of the inverse factors determines the **coarse system** and tunes dropping tolerances[4,5].
- **Scaling** and **reordering** of the local system on each successive level[6,7,8].

Литература

1) Sleijpen, G.L.G., Diederik R. F.**:** ***BiCGstab (l) for linear equations involving unsymmetric matrices with complex spectrum.*** **Electronic Transactions on Numerical Analysis** 1.11 (1993): 2000. **(Krylov method)**

2) Li N., Saad Y., Chow E.: ***Crout versions of ILU for general sparse matrices.*** **SIAM Journal on Scientific Computing** 25.2 (2003): 716-728. **(Crout-ILU)**

3) Kaporin, I.E.: ***High quality preconditioning of a general symmetric positive definite matrix based on its UTU+ UTR+ RTU-decomposition*****. Numerical linear algebra with applications** 5.6 (1998): 483-509. **(Second-order ILU)**

4) Bollhöfer, M.: ***A robust ILU with pivoting based on monitoring the growth of the inverse factors*****. Linear Algebra and its Applications** 338.1-3 (2001): 201-218. **(Tuning dropping tolerances)**

5) Bollhöfer, M., Saad Y.: ***Multilevel preconditioners constructed from inverse-based ILUs*****. SIAM Journal on Scientific Computing** 27.5 (2006): 1627-1650. **(Computing coarse system)**

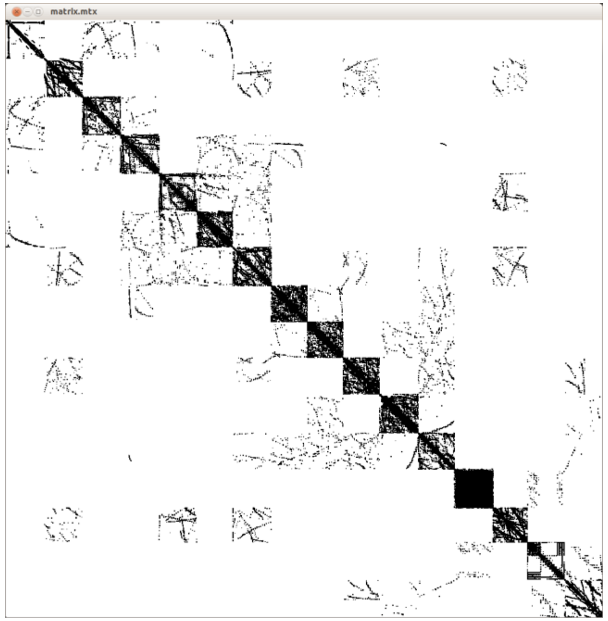
6) Cuthill, E., McKee J.: ***Reducing the bandwidth of sparse symmetric matrices.*** **Proceedings of the 1969 24th national conference.** 1969. **(Reordering for bandwidth reduction)**

7) Olschowka, M., Arnold N.: ***A new pivoting strategy for Gaussian elimination*****. Linear Algebra and its Applications** 240 (1996): 131-151. **(Maximizing diagonal product)**

8) Kaporin, I.E.: ***Scaling*****,** ***reordering*****,** ***and diagonal pivoting in ILU preconditionings*****. Russian Journal of Numerical Analysis and Mathematical Modelling** 22.4 (2007): 341-375. **(Rescaling for condition reduction)**

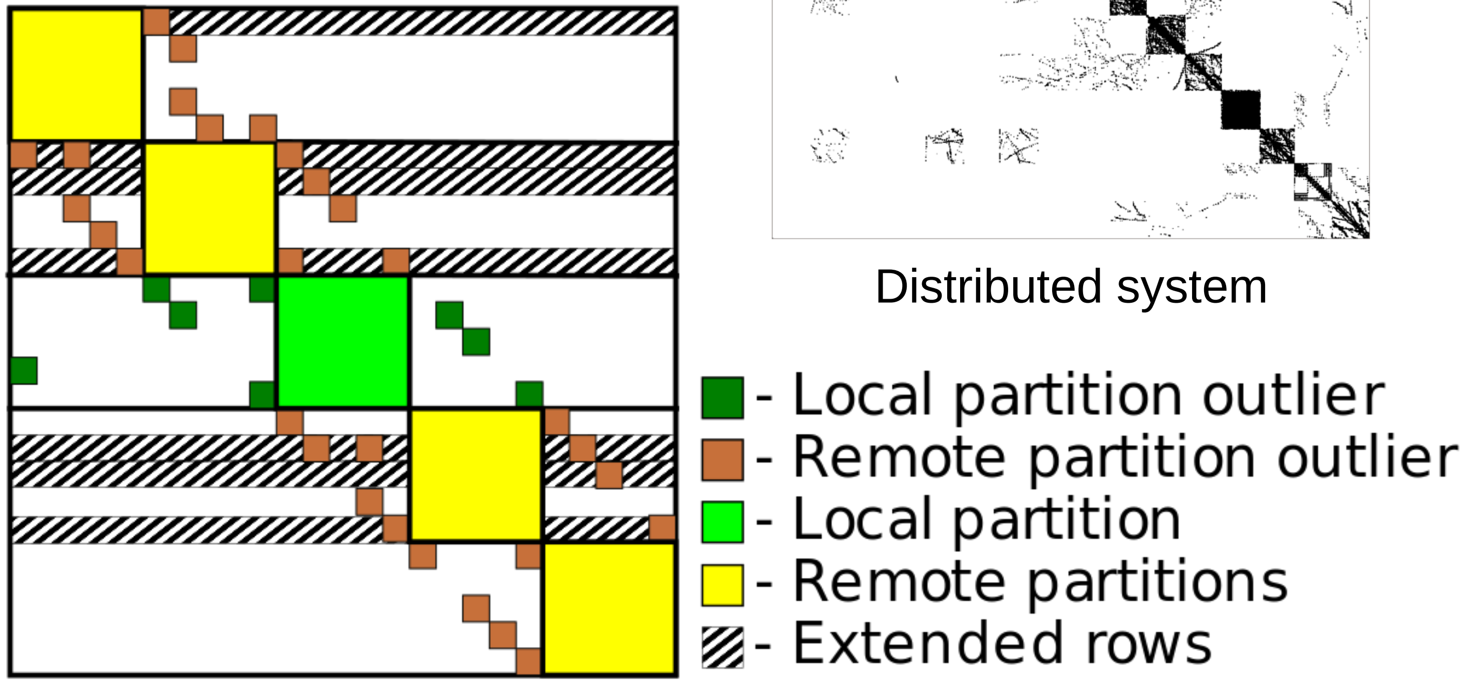
Additive Schwarz Method (AS)

- Global matrix is composed of local **blocks**.
- Extend blocks to localize the **connection**.
- **Restricted** version.



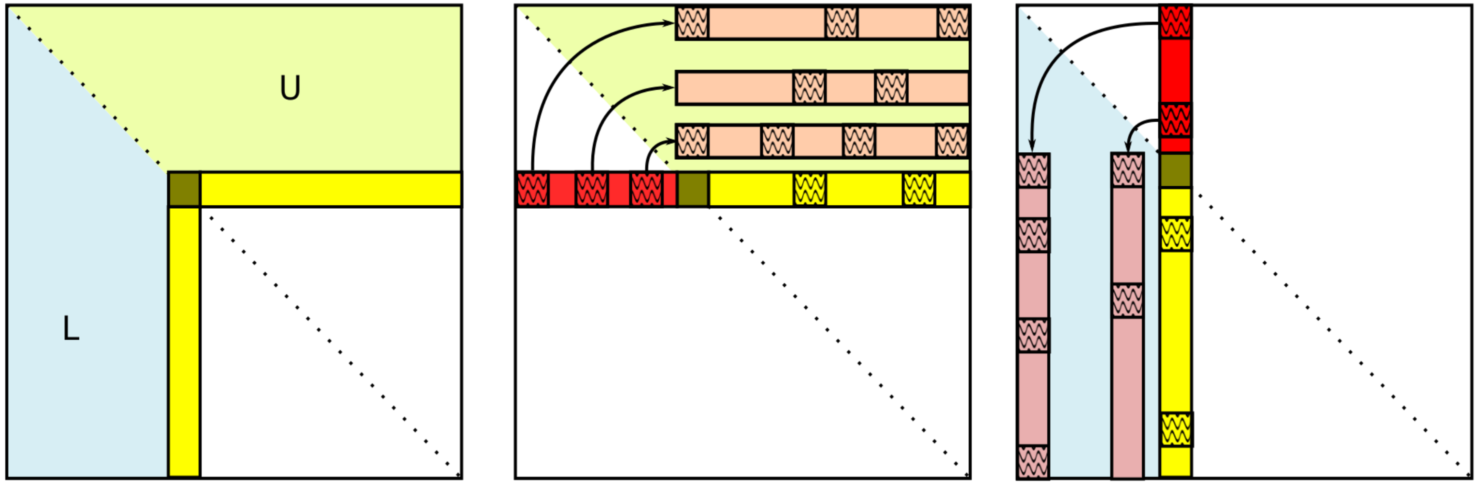
Distributed system

Matrix overlapping



Second-order Crout Incomplete LU (ILUC2)

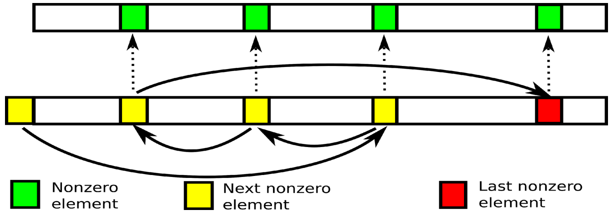
- Dual-threshold dropping:
  - τ^2 for factorization.
  - τ for iterations.
- Running condition estimation:
  - $\kappa = \max(\|L^{-1}\|, \|U^{-1}\|)$
  - $\tau/\kappa = \text{const}$ tuning.
  - Limit growth of κ.



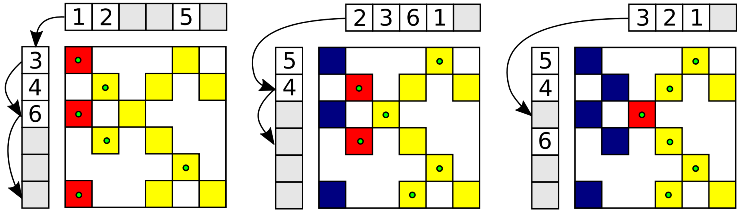
U-factor elimination

L-factor elimination

Dense row accumulator:

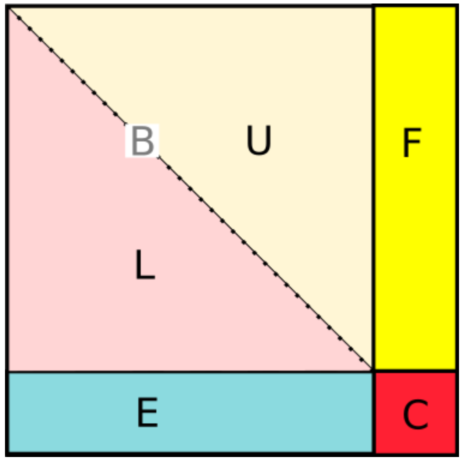


Transposed matrix traversal:

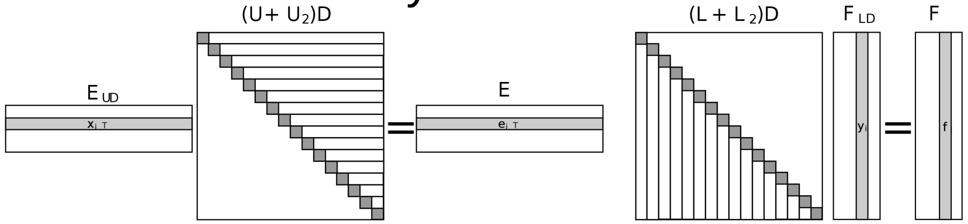


Schur Complement

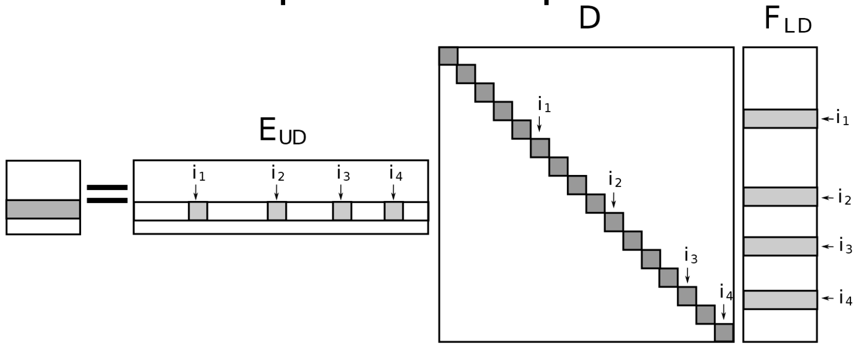
- Part that leads to growth of κ is accumulated in **C**:
  - system reordering after factorization.
- Next level system is the Schur complement:
  - $\mathbf{S} = \mathbf{C} - \mathbf{E}\,(DU)^{-1}\,D(LD)^{-1}\mathbf{F}$.
  - Requires forward and backward substitution with sparse right hand side.
  - Fill-in control is critical.



Partially factorized matrix.



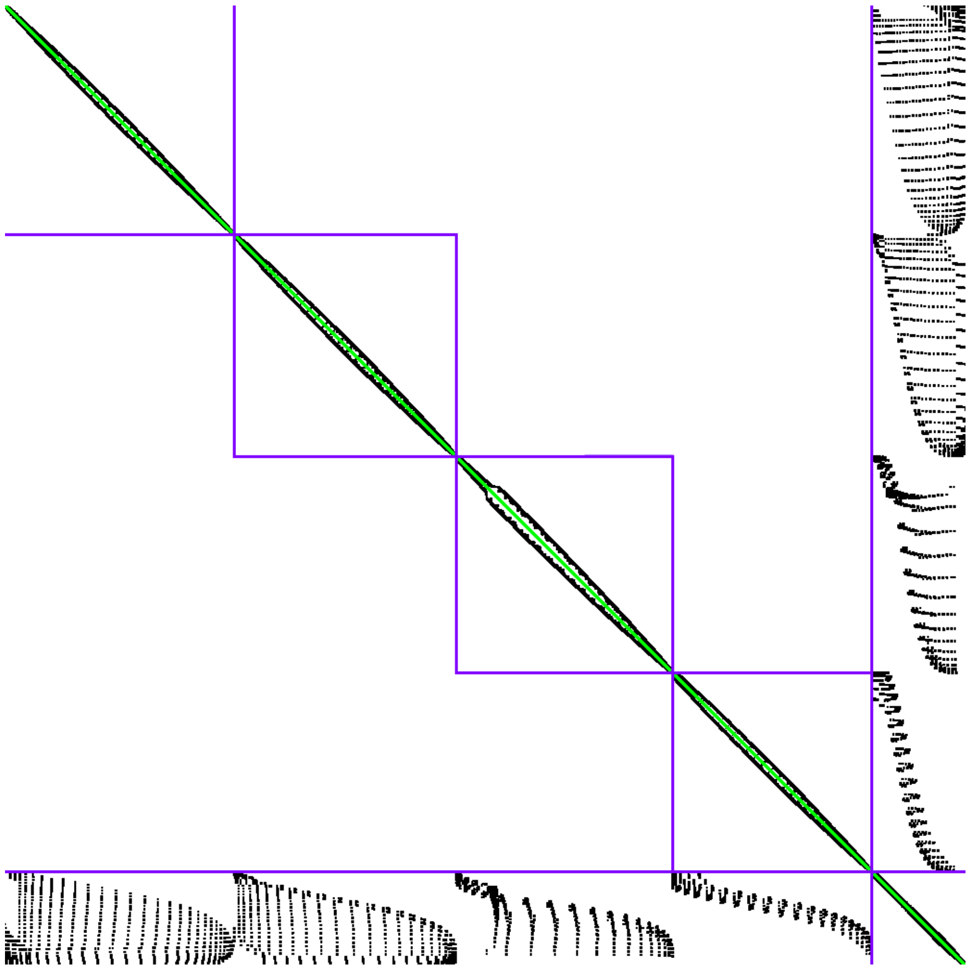
Computation of operators



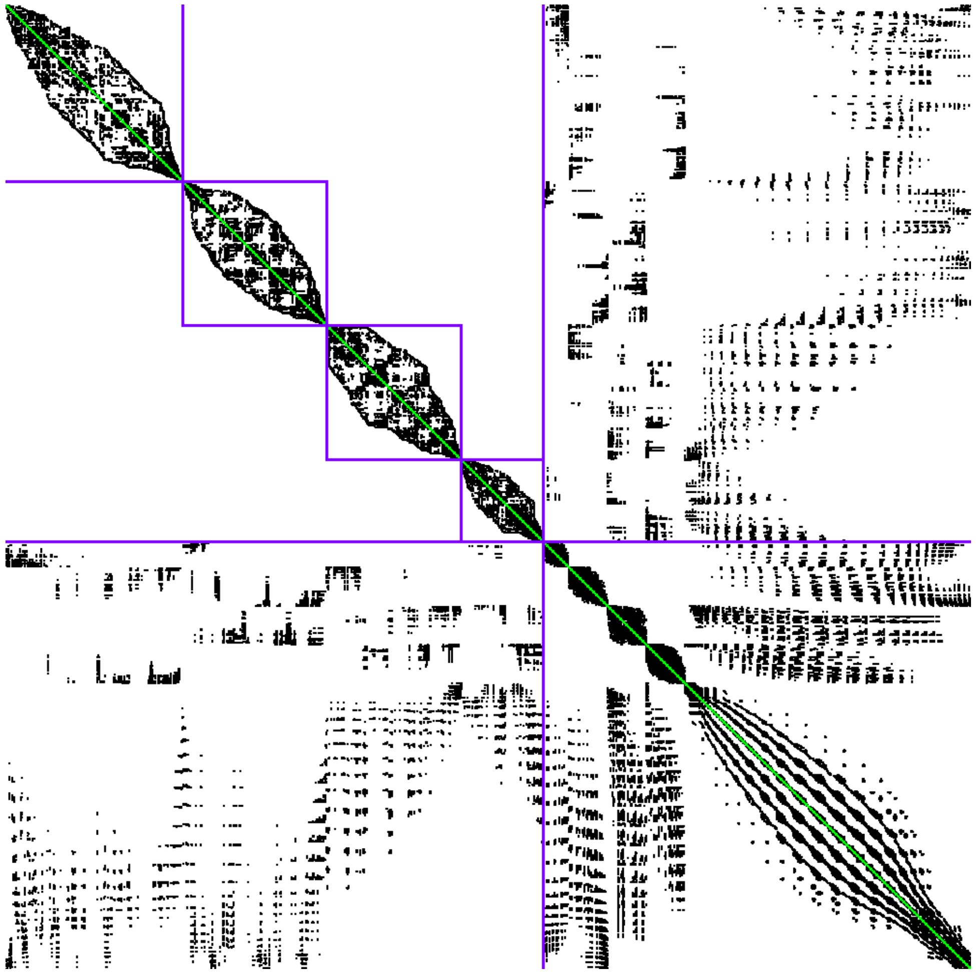
Schur complement computation

Doubly-Bordered Block-Diagonal Form

First level



Schur complement



Аналогия с Algebraic Multigrid (AMG)

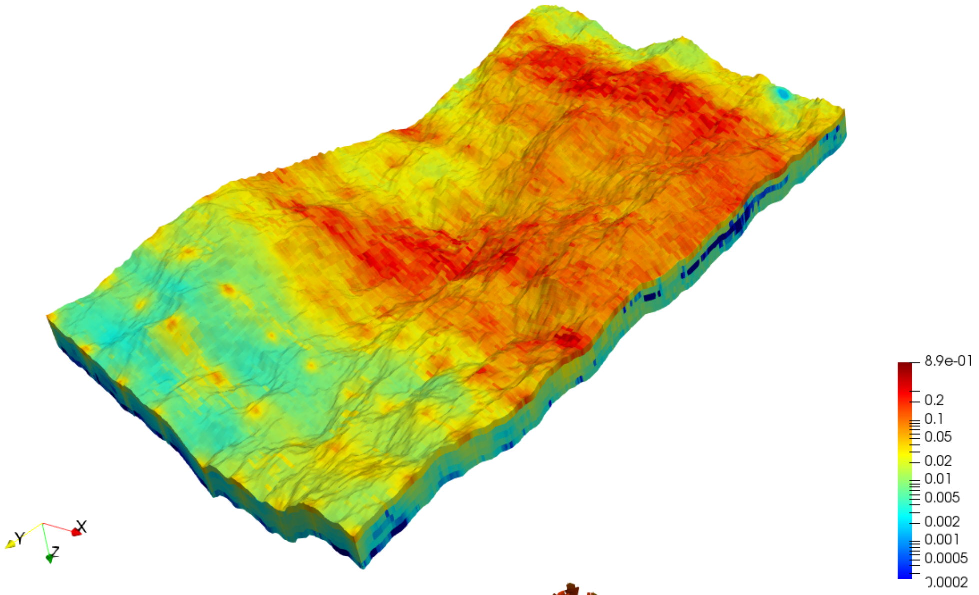
- **Coarse** system should contain the **largest error** of the **smoother**.
- Condition estimation reveals the **error** in the **smoother** and provides the ***coarse-fine splitting*** of the system.
- Ideal prolongation $P=(-EB^{-1},I)$ and restriction $R=(-FB^{-1},I)^T$.
  - (not satisfied by the present method).
- Schur complement corresponds to the **coarse** system.

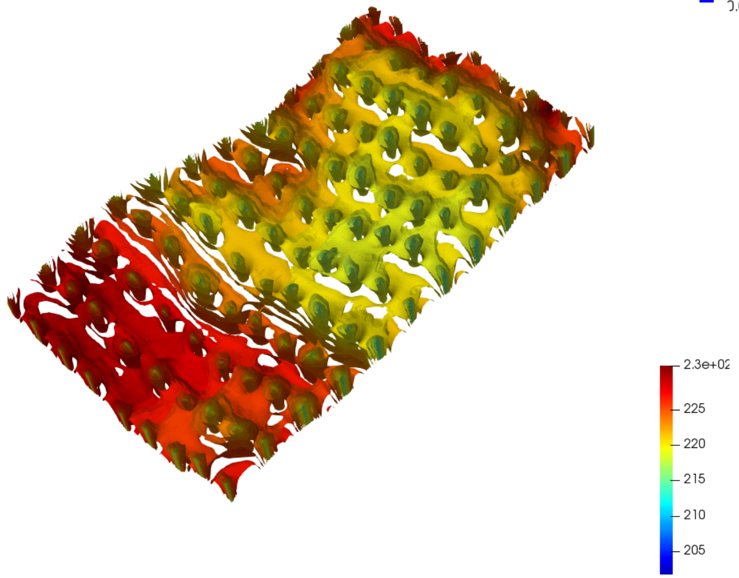
- **Universal but much more computationally complex.**
  - (definitely not linear computational complexity)

Большие задачи

- Suitable for large problem solutions:
  - Black oil problem
  - 3x unknowns per cell
  - **100M** and **200M** cells (INM RAS cluster):

Case	T_{mat}	T_{prec}	T_{iter}	T_{sol}	T_{upd}	N_n	N_l
SPE10_100M	14	18.5	55.4	78.6	0.2	402	3.5
SPE10_200M	29.6	34.7	64.1	107.5	0.38	428	3.96





- Scaled upto **1B of cells** on 9600 Cray cores by Ahmad Abushaika at HBKU, Qatar.
- Optimal preconditioner is **CPR+AMG**.

Sparse System Solution Methods (S^3M)

Concept:

- Basic operations:
  - Operations for vectors and sparse matrix-vector
  - Sparse matrix-matrix addition and multiplication, substitutions with triangular systems
  - Hidden **OpenMP** and **MPI**
    - **+ OpenMP target**
- **Portability** and ease of use:
  - MIPT practical course, SIRIUS lections

```
while( resid > ftol && resid < dtol && iters < maxiters+1 )
{
    w = A*p;
    alpha = kappa/Dot(w,p);
    x += alpha*p;
    r -= alpha*w;
    ApplyPreconditioner(r,z);
    beta = 1.0/kappa;
    kappa = Dot(r,z);
    beta *= kappa;
    resid = sqrt(fabs(kappa));
    p = z + beta*p;
    iters++;
}
```

PCG Main loop

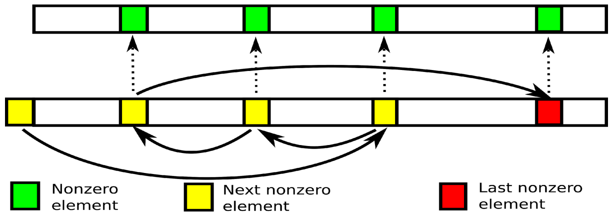
```
do
{
    beta = 1.0 / rho * alpha / omega;
    rho = Dot(r0,r);
    beta*= rho;
    p = r + beta*(p - omega*v);
    ApplyPreconditioner(p,y);
    v = A*y;
    alpha = rho / Dot(r0,v);
    s = r - alpha*v;
    ApplyPreconditioner(s,z);
    t = A*z;
    omega = Dot(t,s)/Dot(t,t);
    x += alpha*y + omega*z;
    r = s - omega*t;
    resid = Norm(r);
    iters++;
} while ( resid > ftol && resid < dtol && omega && iters < maxiters+1);
```

BiCGStab Main loop

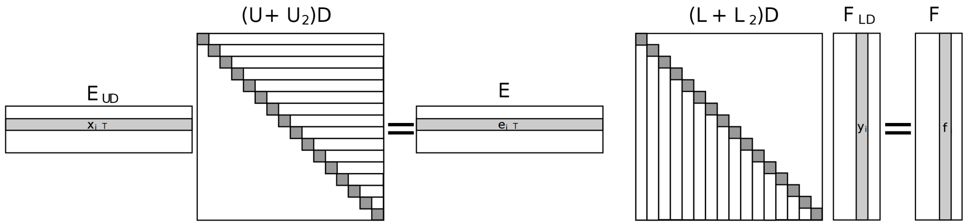
Поддержка операций

Data structures and algorithms

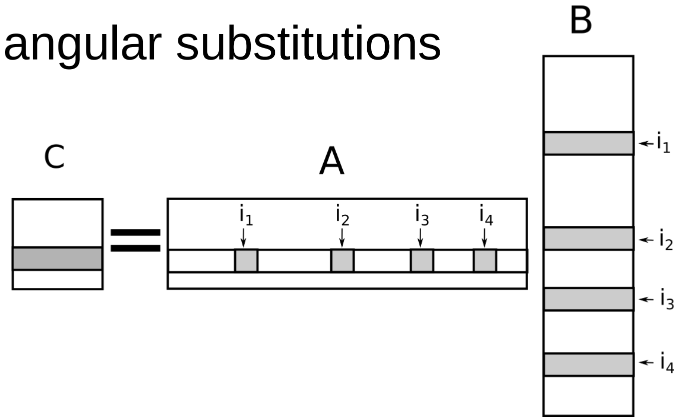
- C++ expression templates for vectors
- C++ operators for sparse matrices: add, subtract, multiply, transpose
- Dense linked lists for **O(1)** operations on sparse vectors (row accumulators)
- Triangular substitutions



Dense row accumulator



Triangular substitutions

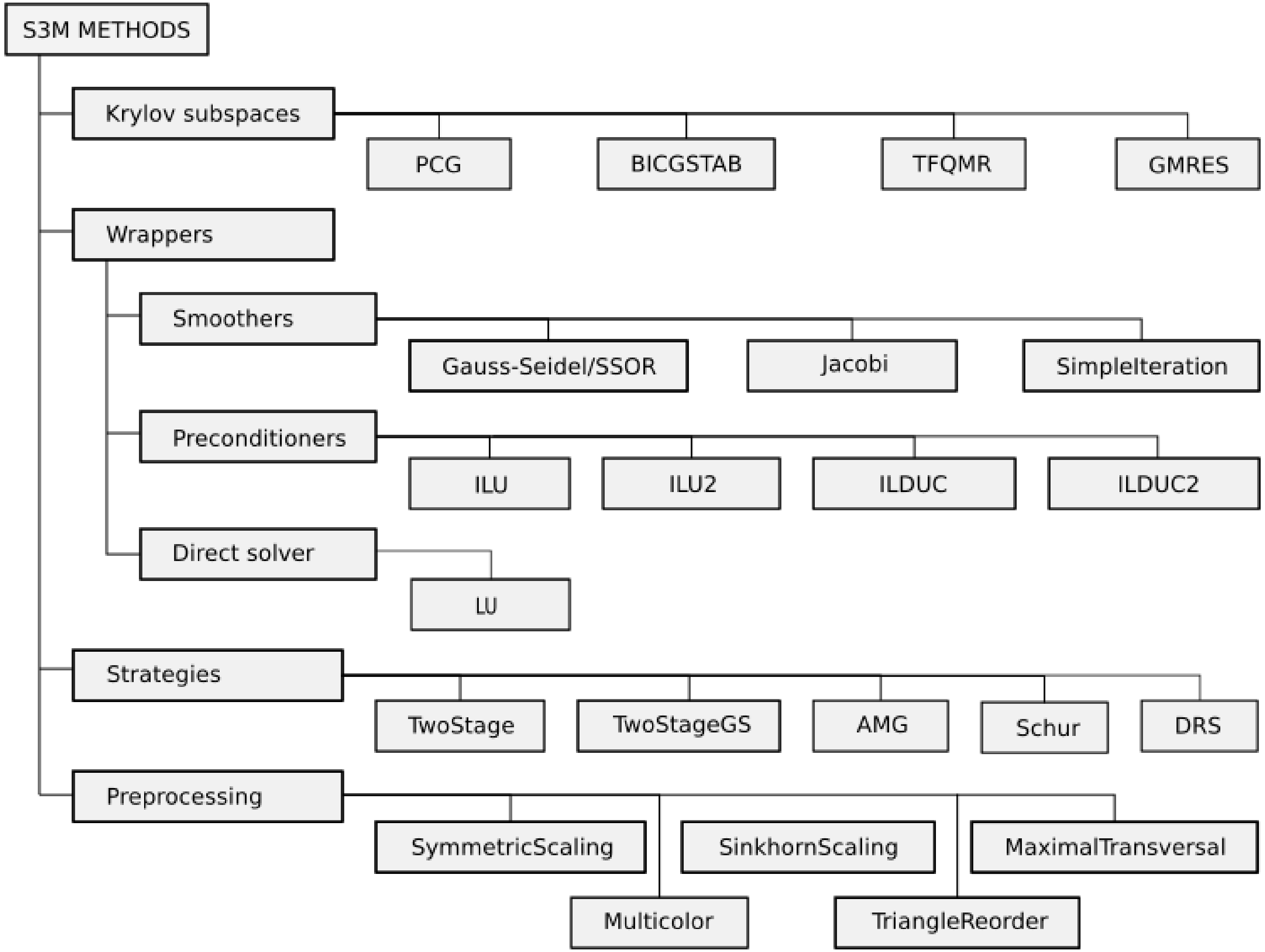


Sparse matrix multiplications (Gustavson)

Sparse System Solution Methods (S^3M)

Concept:

- Combine C++ templates for solver assembly from collections of
  - Iterative methods
  - Preconditioners and smoothers
  - Preprocessors and reorderings
  - Algebraic multigrid methods
  - **Multilevel methods** (new)
  - Multistage strategies



Sparse System Solution Methods (S^3M)

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  - **Multilevel methods** **(new)**
  - Multistage strategies

- `BICGSTAB<ILU2> Solver;`
  - **Iterative solver**: stabilized bi-conjugate gradient method
  - **Preconditioner**: second-order incomplete factorization method
- `SymmetricScaling< PCG<GaussSeidel> > Solver;`
  - **Preprocessor**: symmetric norm equilibration (Sinkhorn scaling)
  - **Iterative solver**: preconditioned conjugate gradient methd
  - **Preconditioner**: Gauss-Seidel method

Sparse System Solution Methods (S^3M)

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- `PCG< AMG<GaussSeidel,LU> > Solver;`
  - **Iterative solver**: conjugate gradient method
  - **Preconditioner**: algebraic multigrid
  - **Smoother**: Gauss-Seidel
  - **Coarsest level solver**: direct factorization
- `BICGSTAB< CPR< AMG<GaussSeidel,LU>, ILU >, TwoStageGaussSeidel > Solver;`
  - **Multistage strategy:** constrained pressure residual scaling
  - **Pressure preconditioner**: Gauss-Seidel method
  - **Saturations preconditioner**: incomplete factorization

Наборы методов

Iterative methods:

- PCG, BICGSTAB, GMRES, TFQMR

Preconditioners and **smoothers**:

- **parallel:** ConjugateGradient, SimpleIteration, Chebyshev, Jacobi, MulticolorGaussSeidel, **ParILUT** (new)
- **sequential:** GaussSeidel, ILU, ILU2, LU

Complex **preconditioners**:

- AMG, AMGRugeStuben, **MLILU**, **MLILU2** (new), amg1r6

Preprocessors:

- SinkhornScaling, SymmetricScaling, MaximumTransversal (famous MC64), RCM, METIS

Multistage strategies:

- TwoStage, TwoStageGaussSeidel, CPR, DRS, SchurMFD, SchurSeries

Parallelization strategy:

- **BlockJacobi** (new)

Многоуровневые методы

Multistage strategies:

- TwoStage – a way to combine multiple preconditioners and solve $(AM^{-1})(Mx)=b$ with

$$M^{-1} = M_1^{-1} + \sum_{i=2}^{n_{st}} M_i^{-1} \prod_{j=1}^{i-1} (I - AM_j^{-1}),$$

- TwoStageGaussSeidel – use block Gauss-Seidel with individual preconditioner M_1 and M_2:

$$\begin{bmatrix} B & E \\ F & C \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \Longrightarrow \begin{matrix} \begin{bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \end{bmatrix} = \begin{bmatrix} B & \\ F & C \end{bmatrix}^{-1} \left(\begin{bmatrix} b_1 \\ b_2 \end{bmatrix} - \begin{bmatrix} 0 & E \\ & 0 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right), \\ \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} B & E \\ & C \end{bmatrix}^{-1} \left(\begin{bmatrix} b_1 \\ b_2 \end{bmatrix} - \begin{bmatrix} 0 & \\ F & 0 \end{bmatrix} \cdot \begin{bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \end{bmatrix} \right). \end{matrix}$$

$$\tilde{x}_1 = M_1^{-1}(b_1 - Ex_2), \quad x_2 = M_2^{-1}(b_2 - F\tilde{x}_1), \quad x_1 = M_1^{-1}(b_1 - Ex_2).$$

Многоуровневые методы

Multistage strategies:

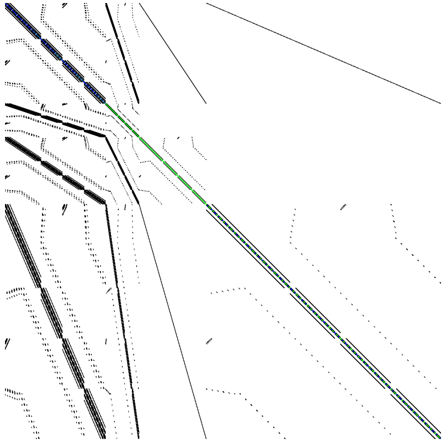
- CPR – constrained pressure residual, DRS – dynamic row scaling
  - Using black-oil problem structure, multiply from the left by a matrix to approximately decouple the pressure system:

$$\begin{bmatrix} A_{pp} & A_{ps} \\ A_{sp} & A_{ss} \end{bmatrix} \cdot \begin{bmatrix} p \\ s \end{bmatrix} = \begin{bmatrix} b_p \\ b_s \end{bmatrix} . \Longrightarrow \begin{bmatrix} B_{pp} & Z_{ps} \\ A_{sp} & A_{ss} \end{bmatrix} \cdot \begin{bmatrix} p \\ s \end{bmatrix} = \begin{bmatrix} b_p - D_{ps} D_{ss}^{-1} b_s \\ b_s \end{bmatrix} \quad \begin{matrix} B_{pp} \equiv A_{pp} - D_{ps} D_{ss}^{-1} A_{ps} \\ Z_{ps} \equiv A_{ps} - D_{ps} D_{ss}^{-1} A_{ss} \approx 0 \end{matrix}$$

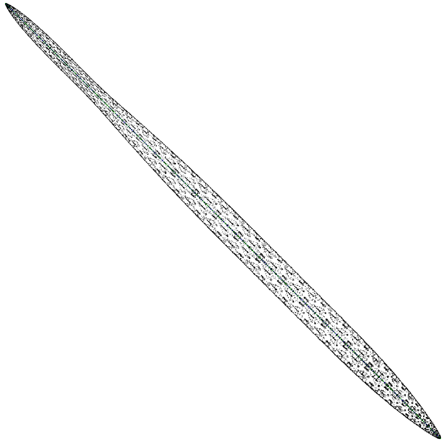
  - Use a two-stage method to solve the system.
  - M_1 - for pressure system, M_2 - for either complete system or saturations system **(block GS)**.
- SchurMFD – use mimetic finite difference method structure to compute the Schur.
- SchurSeries – use power series to invert Schur complement without assembly.

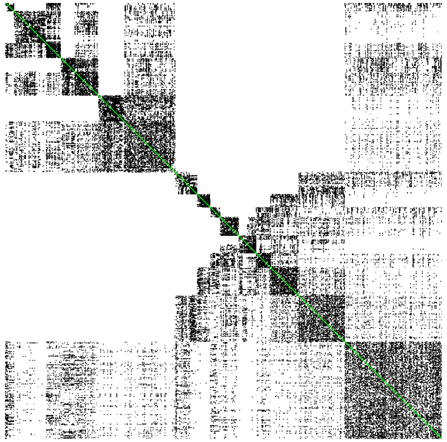
Предварительное упорядочивание

Initial System

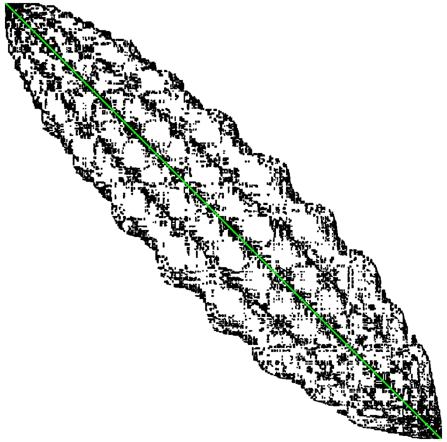


Bandwidth reduction





Fill-in reduction (METIS)



Bandwidth reduction

- Complete **blood coagulation** problem.
- 13 equations per cell.

- **Navier-Stokes** problem only.
- 4 equations per cell.
- Fill-in reduction (METIS) is 4 times slower than bandwidth reduction (RCM) algorithm.
- Quite dense matrix graph, big separator.

Контроль параметров

Flexible control of solver parameters

- Hierarchical embedding of each solver parameters
- Default parameter set, generation of files
- Common control parameters: verbosity, check, …

Input-output:

- MTX format
- Binary format for faster loading of large systems

```
Method:
    name = BICGSTAB
    dtol = 1e+50
    rtol = 1e-06
    tol = 1e-08
    maxiters = 5000
    true_residual = 0
    verbosity = 1
    Preconditioner:
        name = AMGRugeStuben
        check = 1
        cycle = V
        level = *
        operator_type = 2
        order = 0
        phi = 0.25
        refine_splitting = 0
        verbosity = 1
        write_matrix = 0
        CoarsestSolver:
            name = LU
            verbosity = 0
        /
        Smoother:
            name = Chebyshev
            maxiters = 2
            tol = 0
            verbosity = 1
        /
    /
/
```

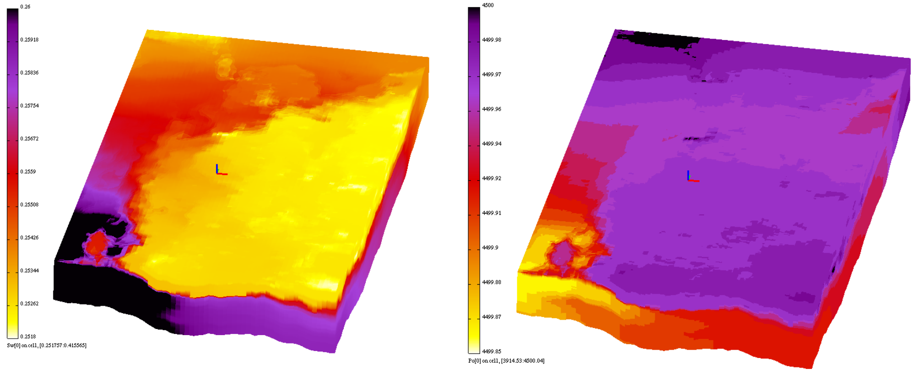
Пример применения (Black Oil)

Methods:

- MT-ILUC2 – maximum transversal with ILU
- CPR-MT-ILUC2 – CPR rescaling and then the preconditioner is applied to the full system
- CPR-TS – same as second, but multigrid is used to precondition pressure system
- CPR-TSGS – multigrid is used for pressure block and first preconditioner for saturations block

Results:

- Table does not account for setup-time memory
- Block Gauss-Seidel Requires the least memory, but looses to plain two-stage at extreme sizes



		MT-ILUC2	CPR-MT-ILUC2	CPR-TS	CPR-TSGS
spe10 (tpfa)	T	**283**	187	92	**46**
size 2 244 000	Ts	**99**	63	71	**16**
nnz 31 120 000	Tit	**184**	123.7	**20**	29
	Nit	**405**	356	**38**	76
	Lvl	—	—	10	10
	Mem	2.5 GB	2.2 GB	**2.6** GB	1.4 GB
spe10 (tpfa)	T	**4332**	2940	1067	**97** 5
size 20 196 000	Ts	**687**	522	597	**150**
nnz 281 222 400	Tit	**3645**	2417	**470**	825
	Nit	**1065**	799	**93**	225
	Lvl	—	—	12	12
	Mem	21 GB	19 GB	**22** GB	**13** GB
spe10 (tpfa)	T	**20857**	20276	**3758**	3976
size **60 588 000**	Ts	**1693**	1440	1564	**466**
nnz **845 568 000**	Tit	**19164**	18836	**2194**	2510
	Nit	2156	**2241**	**150**	321
	Lvl	—	—	12	12
	Mem	54 GB	52 GB	**63** GB	**39** GB

Заключение и дальнейшие планы

- Implemented very flexible linear solvers framework
- Used as practical illustration in MIPT course
- Future directions:
  - **MPI** and **OpenMP target** parallelization
  - Integration of **domain-decomposition** methods
  - More **multistage** strategies:
    - Poromechanics – fixed-stress strategy
    - Navier-Stokes – pressure projection, Vanka smoother
    - Maxwell - …
  - integration into INMOST for linear system solution of multiphysics problems

Supported by RSF grant №21-71-20024

Спасибо за внимание

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Links

- WWW.INMOST.ORG
- WWW.INMOST.RU
- https://github.com/kirill-terekhov/mipt-solvers