

Повышение параллельной эффективности вычислений для сложных гидрогеологических задач

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XVIII Всероссийская Конференция-школа молодых исследователей
“Современные проблемы математического моделирования”

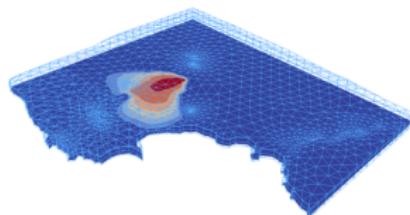
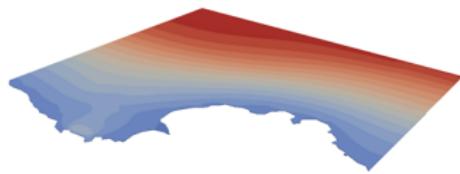
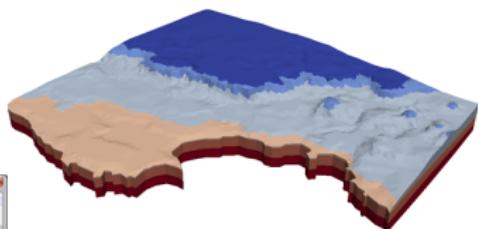
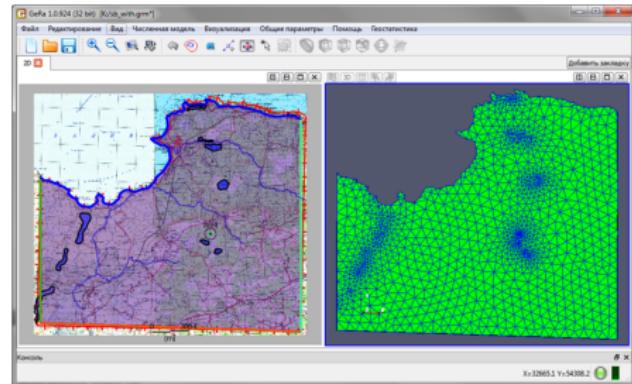


- **GeRa: модули и структура**
- Расчетная модель
- Настройка параметров линейного решателя
- Численные эксперименты

The major present-day abilities of GeRa

Modeling:

- geological
- groundwater flow
- transport in geological media



GeRa (Geomigration of Radionuclides): simulated processes

- ground-water flow in confined, unconfined and unsaturated conditions;
- transport in uniform and dual-porosity media (advection, dispersion, diffusion);
- equilibrium chemical reactions either governed by sorption isotherms or with real chemical calculations;
- radioactive decay chains;
- heat generation caused by radioactive decay;
- density and temperature driven convection.

GeRa: software used

- Qt
- INMOST +ParMetis +PETSc
- iPHREEQC
- VTK
- SVN

Most of the software is freely distributed

GeRa = 150,000+ rows of C++ code

GeRa/V1 была аттестована Ростехнадзором в 2018 году для использования Росатомом при обосновании безопасности объектов использования атомной энергии

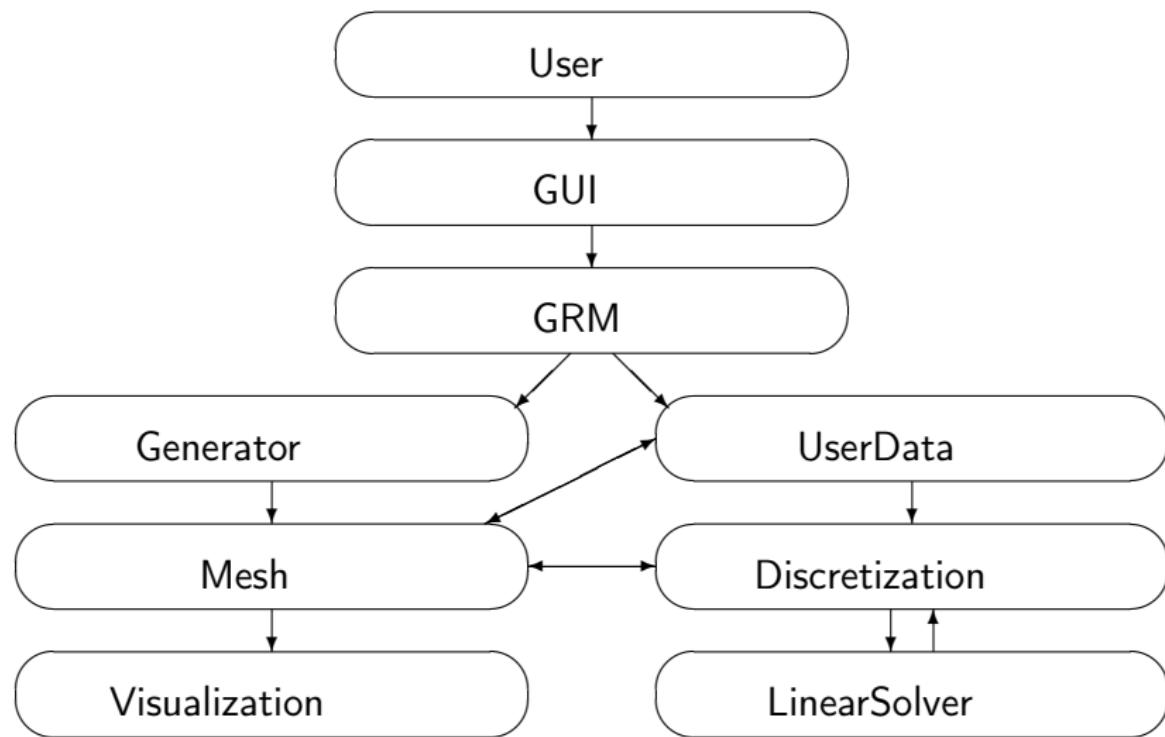
- **I**ntegrated
- **N**umerical
- **M**odelling and
- **O**bject-oriented
- **S**upercomputing
- **T**echnologies

INMOST is the software platform for developing parallel numerical models on general meshes.

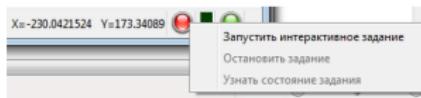
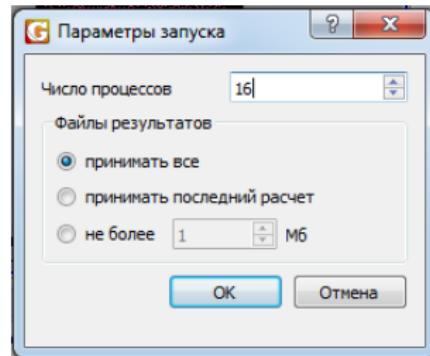
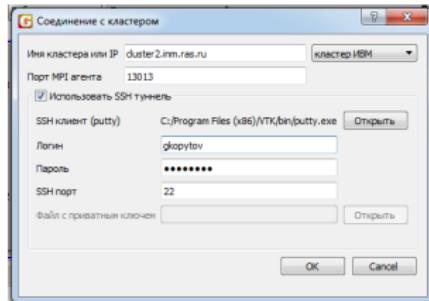
INMOST is a tool for supercomputer simulations characterized by a maximum generality of supported computational meshes, distributed data structure flexibility, cost-effectiveness, cross platform portability.

Технология INMOST используется в более чем 10 проектах в России, США, Голландии, Катаре...

User → GeRa modules/objects



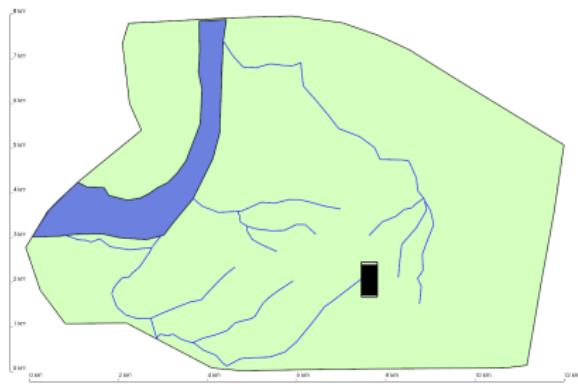
GeRa: computations on remote cluster via GUI



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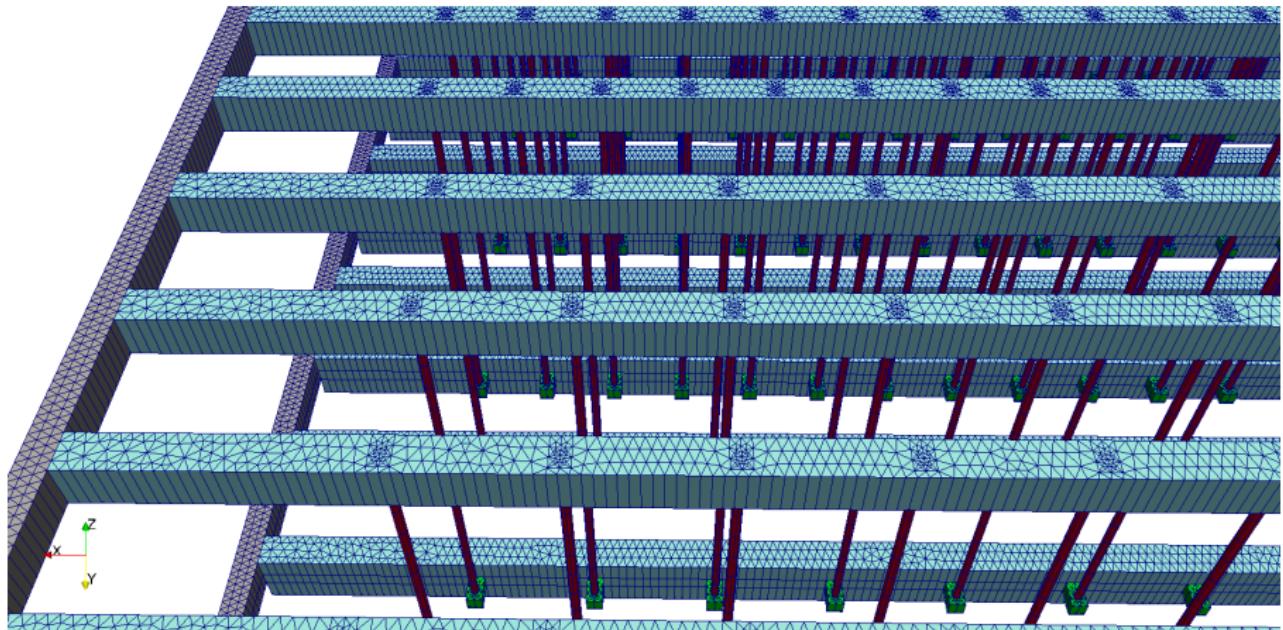
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Model: Yeniseisky site (Krasnoyarsk region)

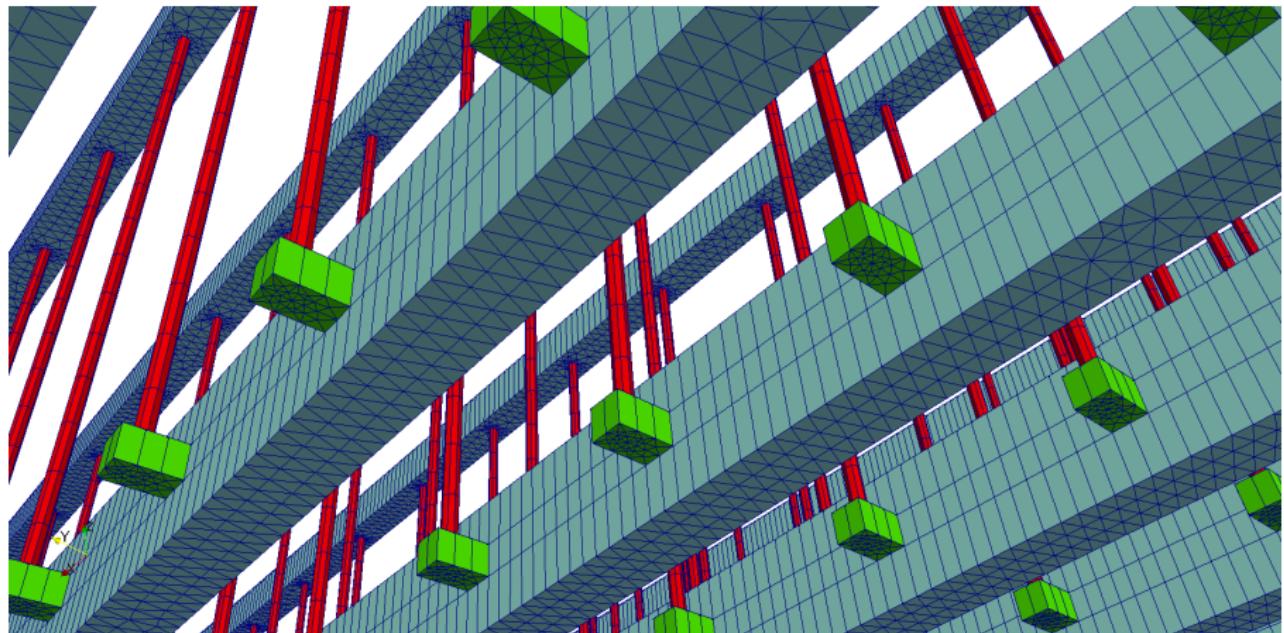


- nonstationary groundwater flow and migration of radionuclides
- reactive transport
- boundary condition of rainfall recharge
- four layers with different thickness
- different hydraulic conductivities (from 10^{-1} to 10^{-4} m/day)
- number of cells: $>10^7$

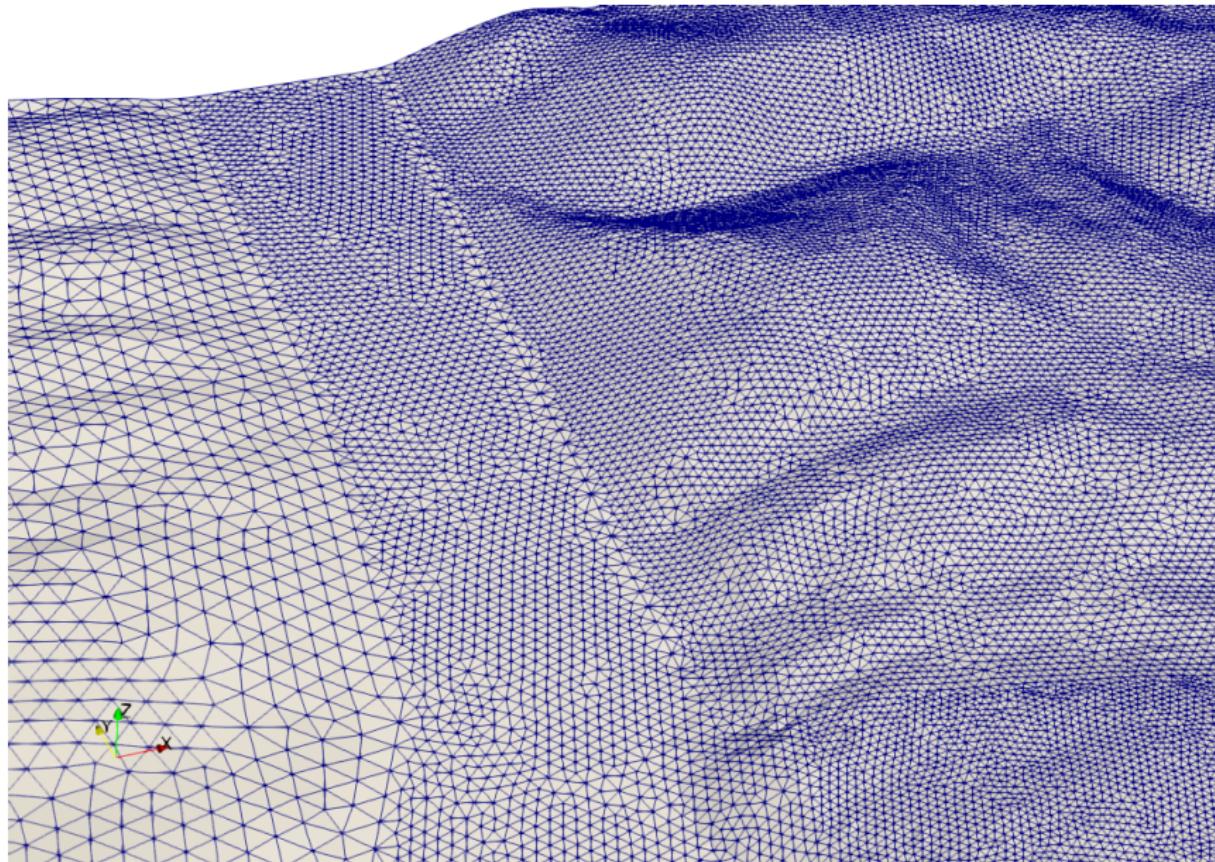
Prismatic grid of the upper horizon



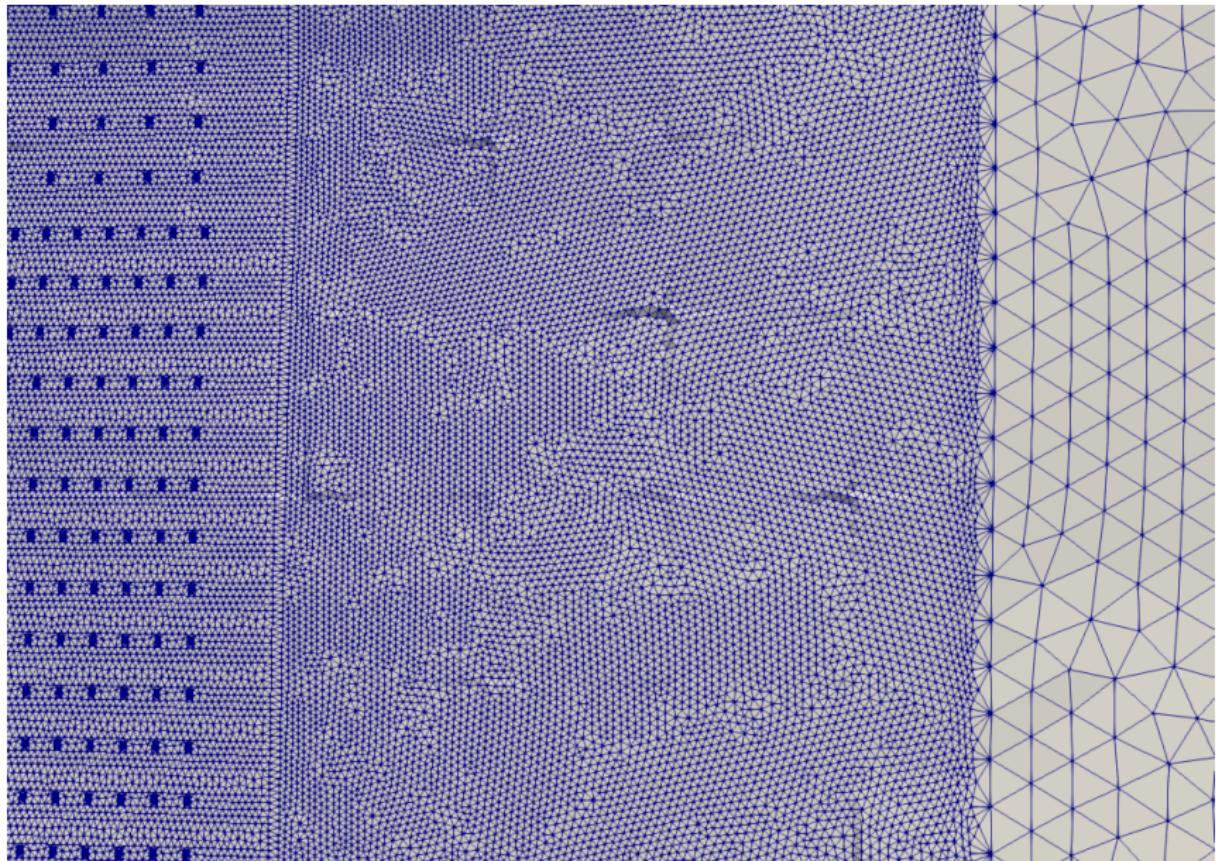
Prismatic grid of the lower horizon



Fragment of the computational mesh (near river)

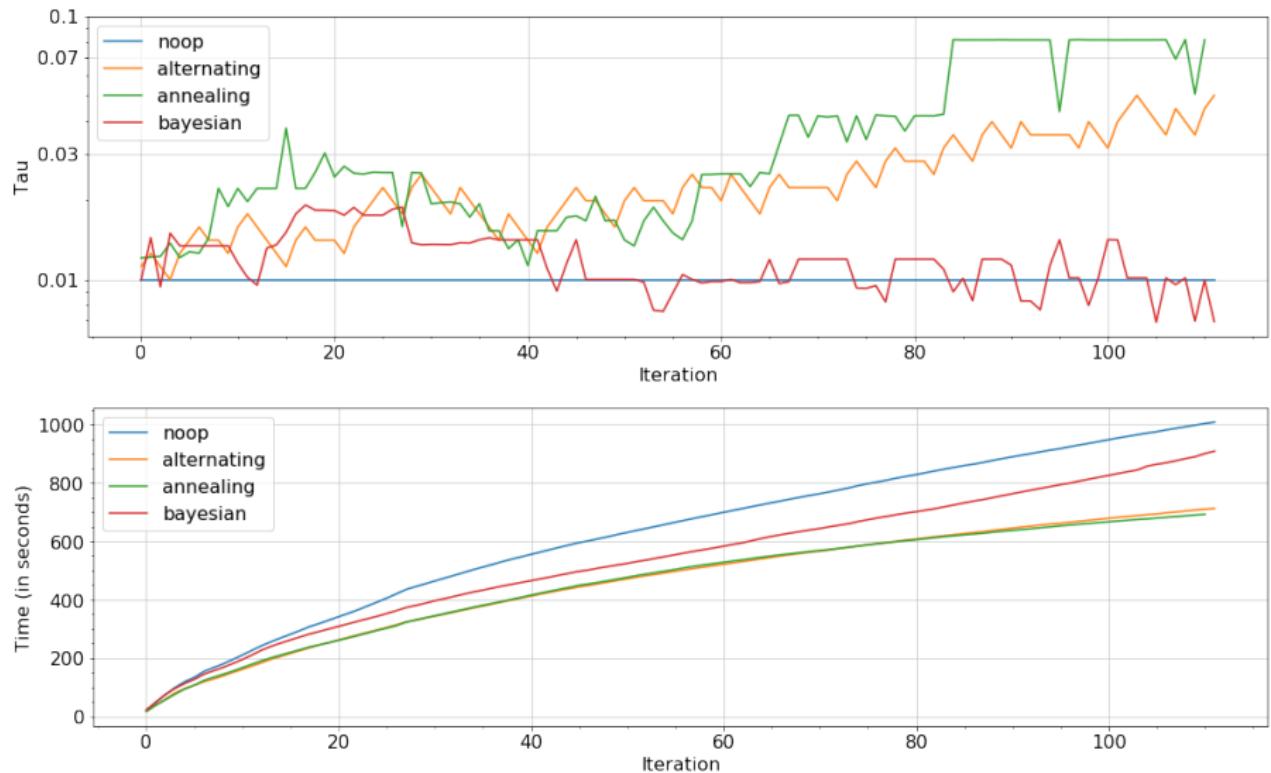


Fragment of the computational mesh (near wells)

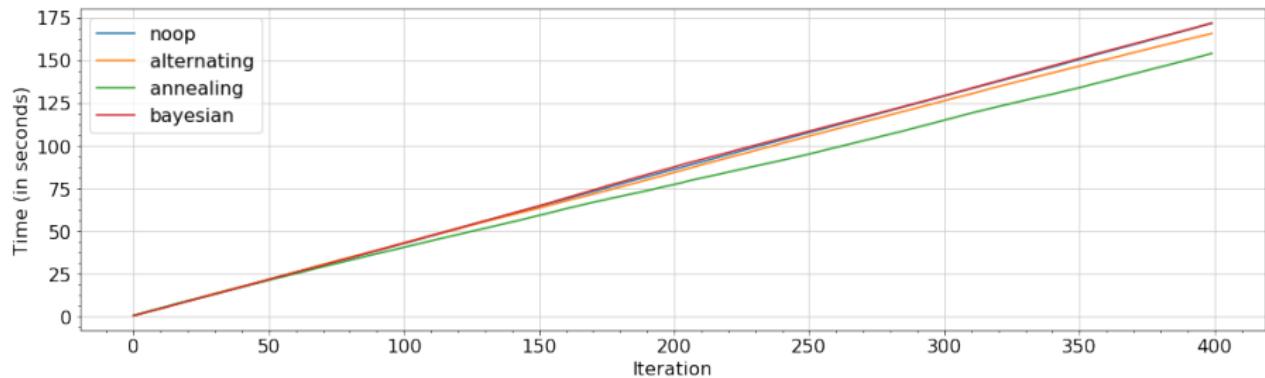
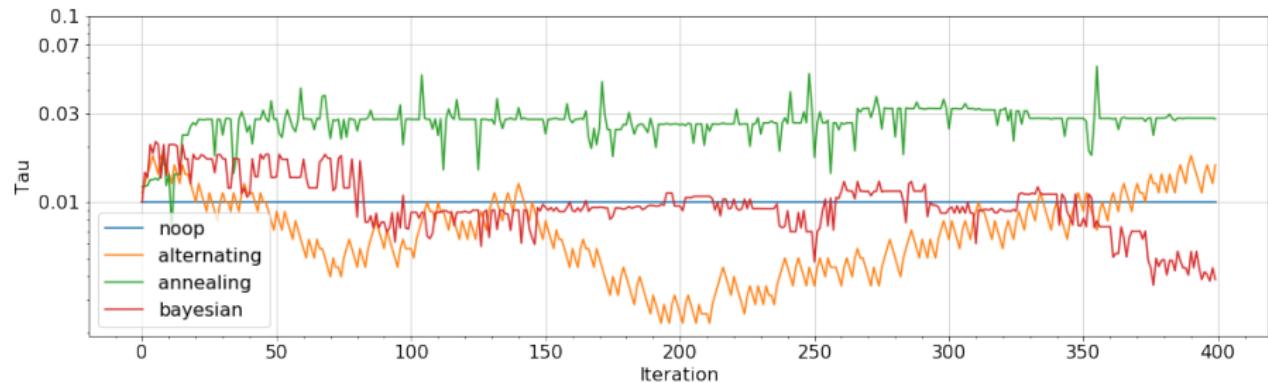


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- **Настройка параметров линейного решателя**
- Численные эксперименты

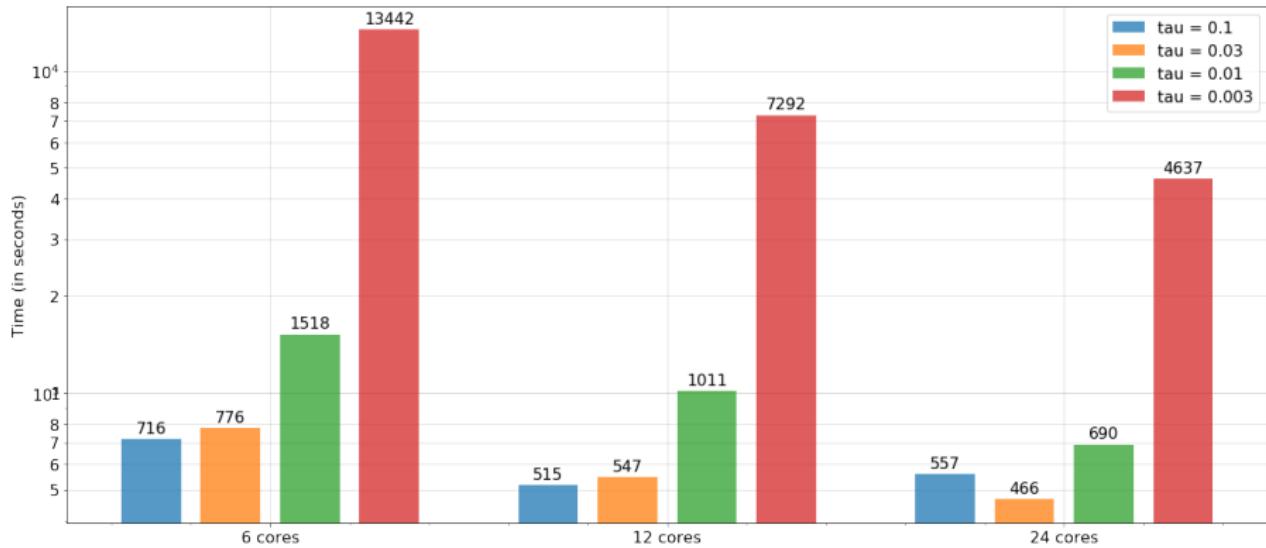
[gw]: Optimization on τ for the GW flow modeling



[tr]: Optimization on τ for the transport process



Solution time on 6, 12, 24 cores for different fixed values of τ



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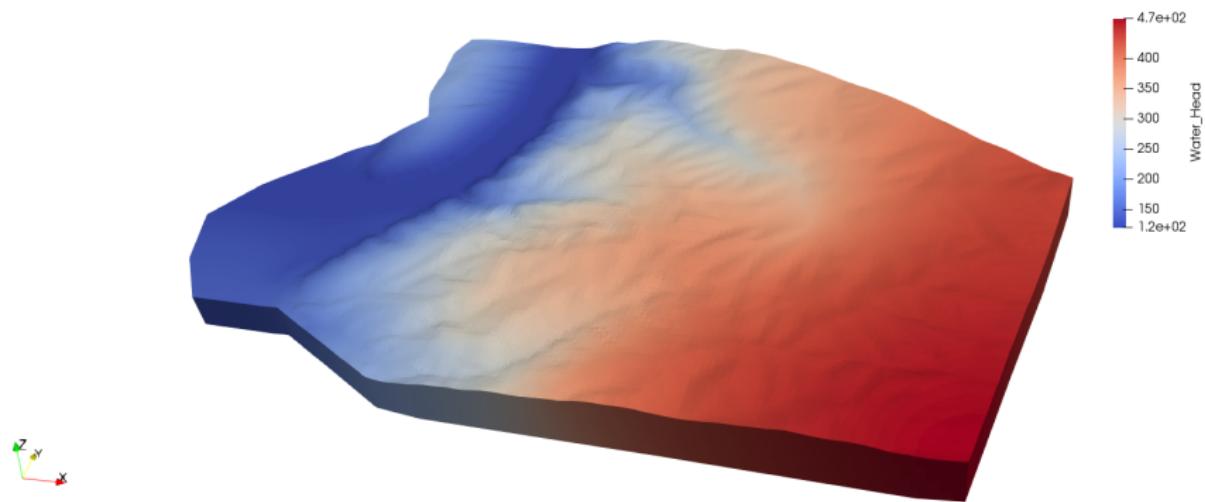
Calculation results on the INM RAS cluster

p	T_{gw}	S_{gw}	T_{tr}	S_{tr}	T_{total}	S_{total}
3	2995.2	1.00	3478.9	1.00	6474.1	1.00
6	2102.4	1.42	2213.7	1.57	4316.1	1.50
12	1570.4	1.90	1376.2	2.52	2946.6	2.19
24	807.9	3.70	737.2	4.71	1545.1	4.19
48	388.9	7.70	478.6	7.26	867.5	7.46
96	330.1	9.70	302.0	11.51	632.1	10.24
192	159.3	18.80	226.3	15.37	385.6	16.78

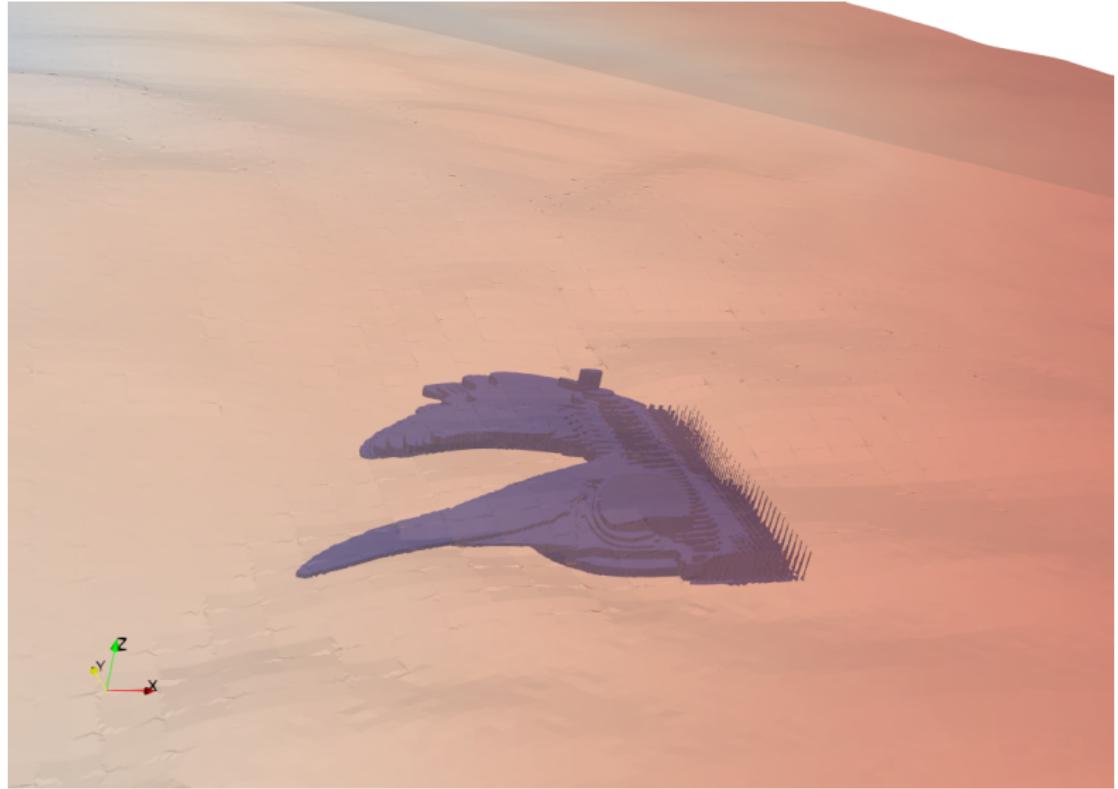
- p – number of cores used
- $T = T(p)$ – simulation time on p cores (in sec.)
- S – relative speedup wrt. to run on 3 cores, $S = T(3)/T(p)$

- INMOST → BiILU2(τ, q) linear solver
- $\tau_{\text{gw}}^* = 0.01$, $q_{\text{gw}}^* = 3$ and $\tau_{\text{tr}}^* = 0.02$, $q_{\text{tr}}^* = 2$
- BiCGstab iterations up to relative residual 10^9 times reduction

[gw]: Calculated GW head



[tr]: Predicted pollution plume with a relative concentration above $5 \cdot 10^{-6}$ at a time point of 8000 years



Summary

- GeRa gives reasonable scalability up to 192 cores
- linear solver parameters tuning can be performed automatically
- the use of a fine ($> 10^7$ cells) grid allow to obtain a detailed prediction