# Повышение параллельной эффективности вычислений для сложных гидрогеологических задач

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

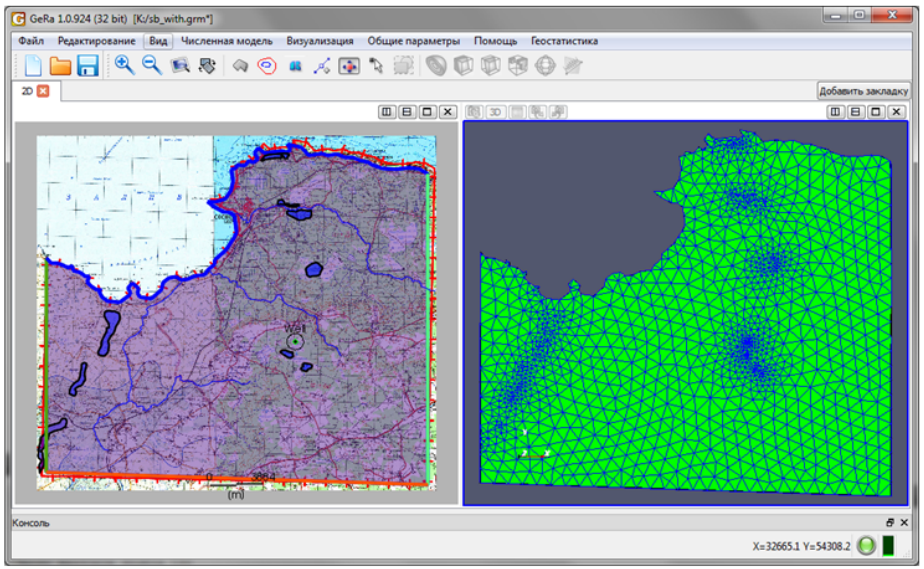
- **GeRa: модули и структура**
- Расчетная модель
- Настройка параметров линейного решателя
- Численные эксперименты

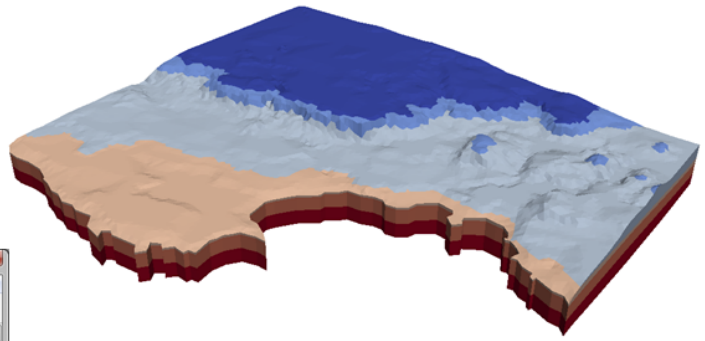
# GeRa: hydro-geological modeling code

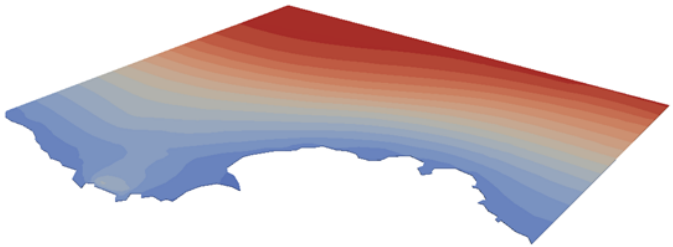
## The major present-day abilities of GeRa

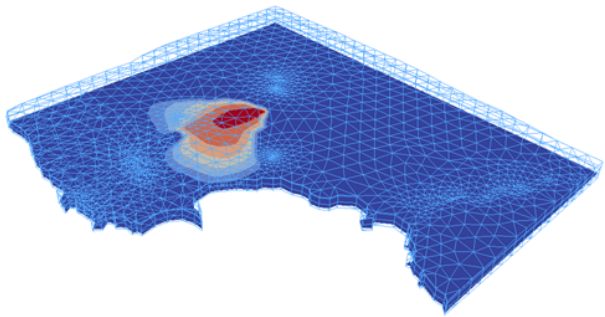
Modeling:

- 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

# INMOST: http://www.INMOST.org

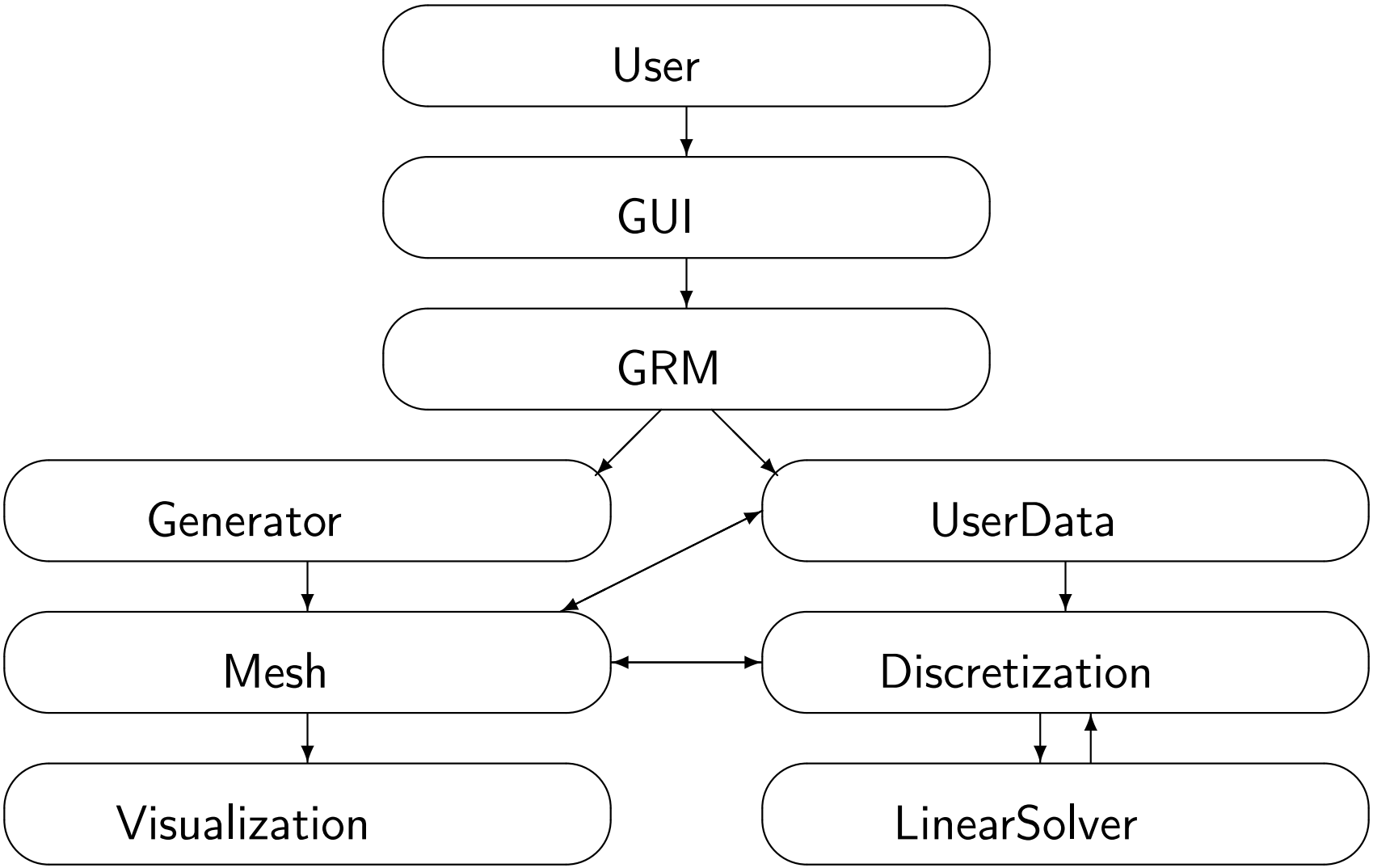
- **I**ntegrated
- **N**umerical
- **M**odelling and
- **O**bject-oriented
- **S**upercomputing
- **T**echnologies

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

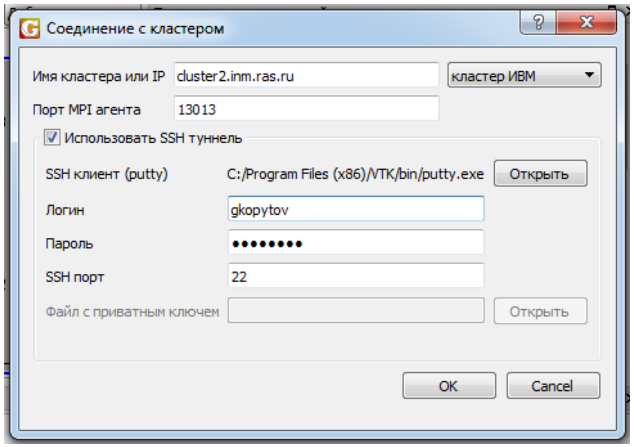
INMOST is a tool for supercomputer simulations characterized by a maximum generality of supported computational meshes, distributed data structure flexibility, cost-effectiveness, cross platform portability.

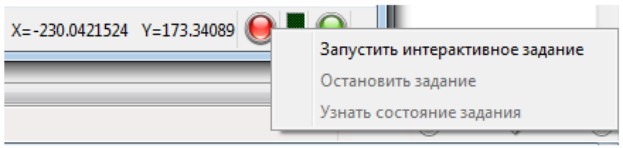
Технология INMOST используется в более чем 10 проектах в России, США, Голландии, Катаре...

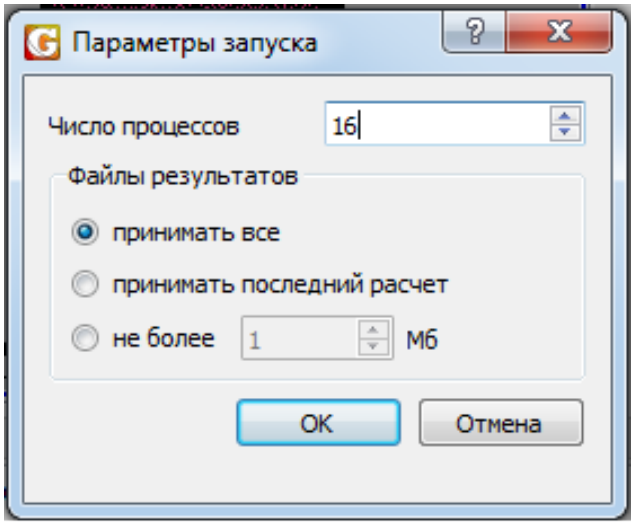
# User $\longrightarrow$ GeRa modules/objects

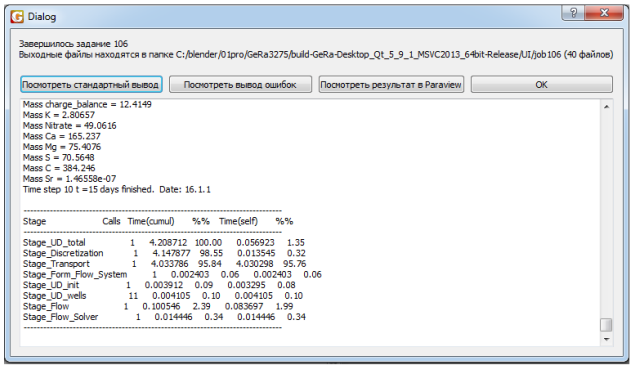


# GeRa: computations on remote cluster via GUI



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- **Расчетная модель**
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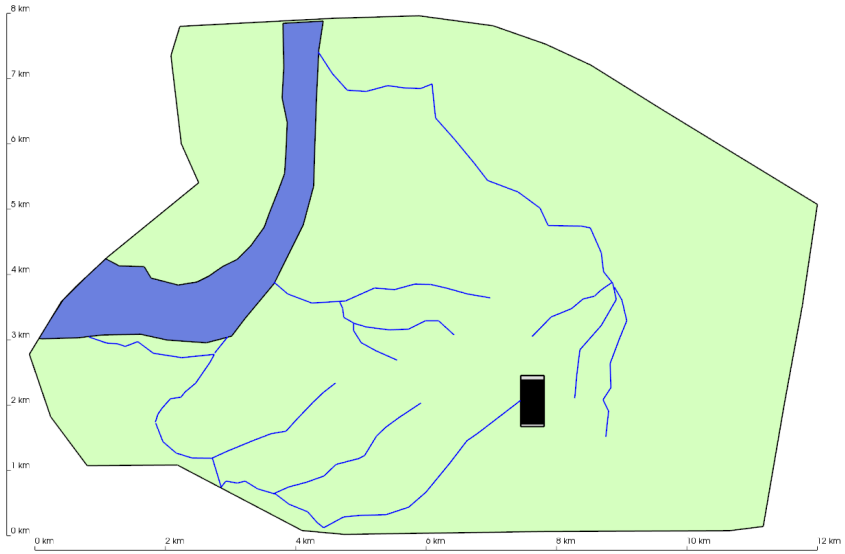
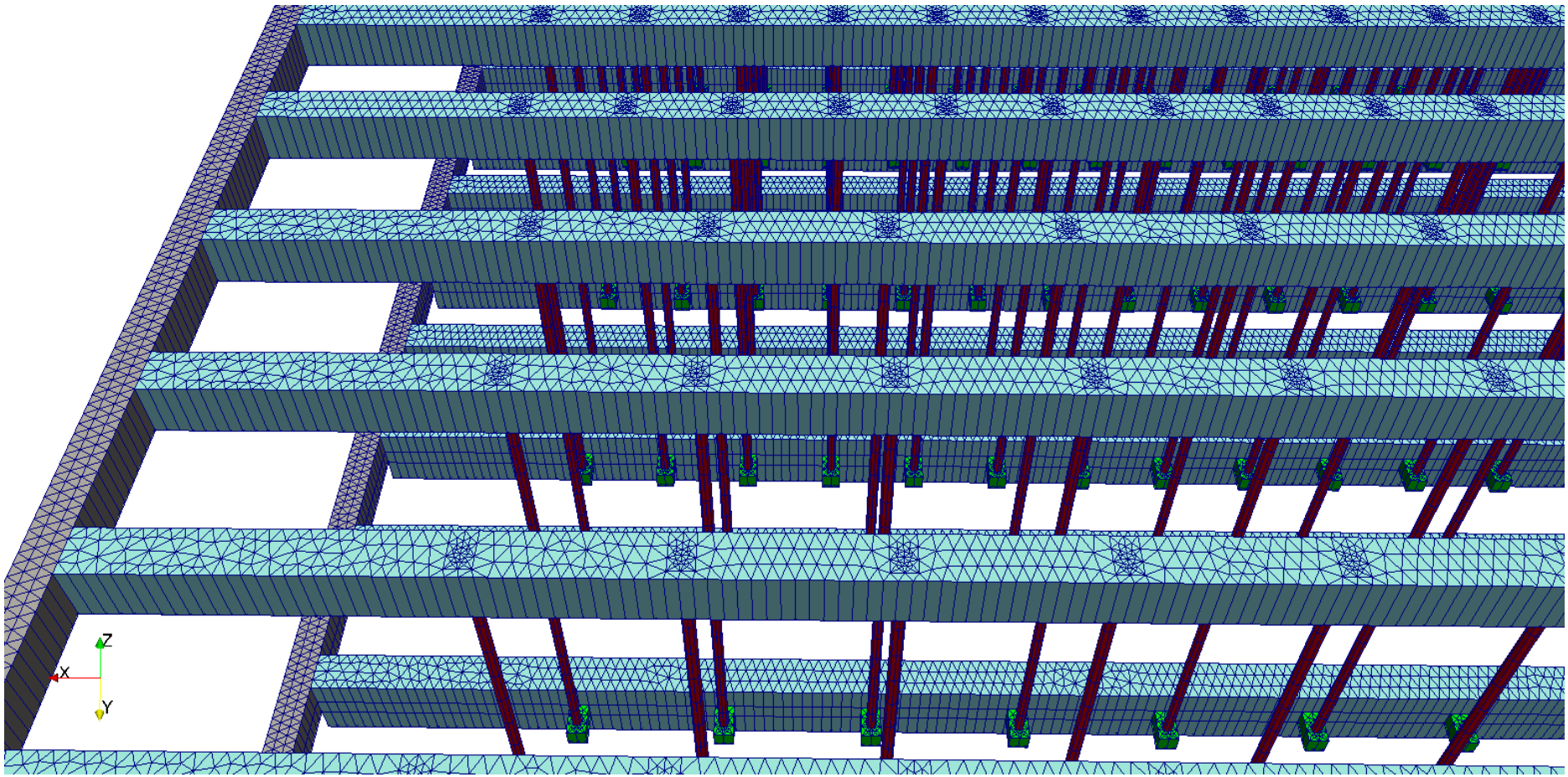
# Model: Yeniseisky site (Krasnoyarsk region)

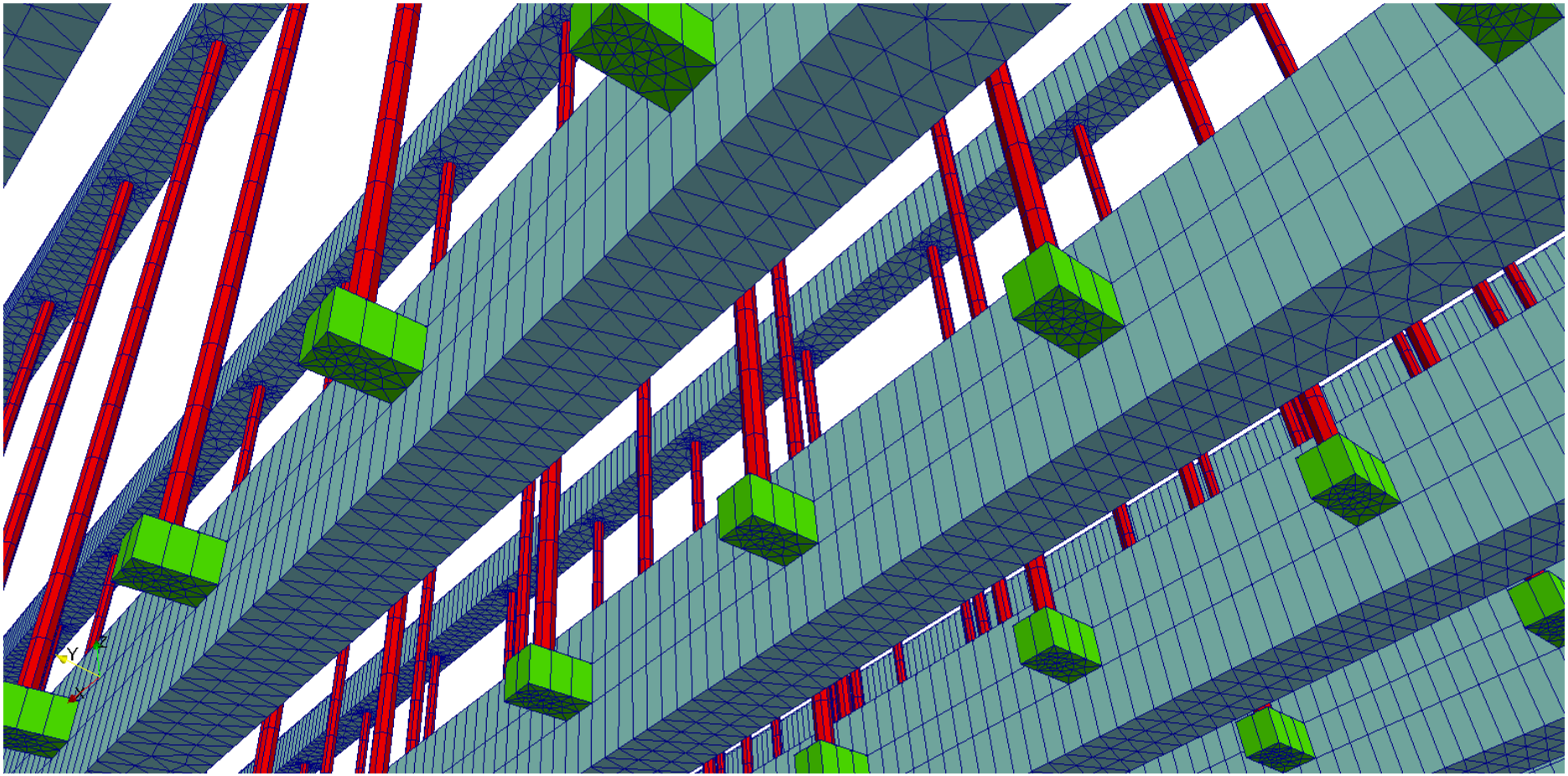



- nonstationary groundwater flow and migration of radionuclides
- reactive transport
- boundary condition of rainfall recharge
- four layers with different thickness
- different hydraulic conductivities (from $10^{-1}$ to $10^{-4}$ m/day)
- number of cells: $>10^7$

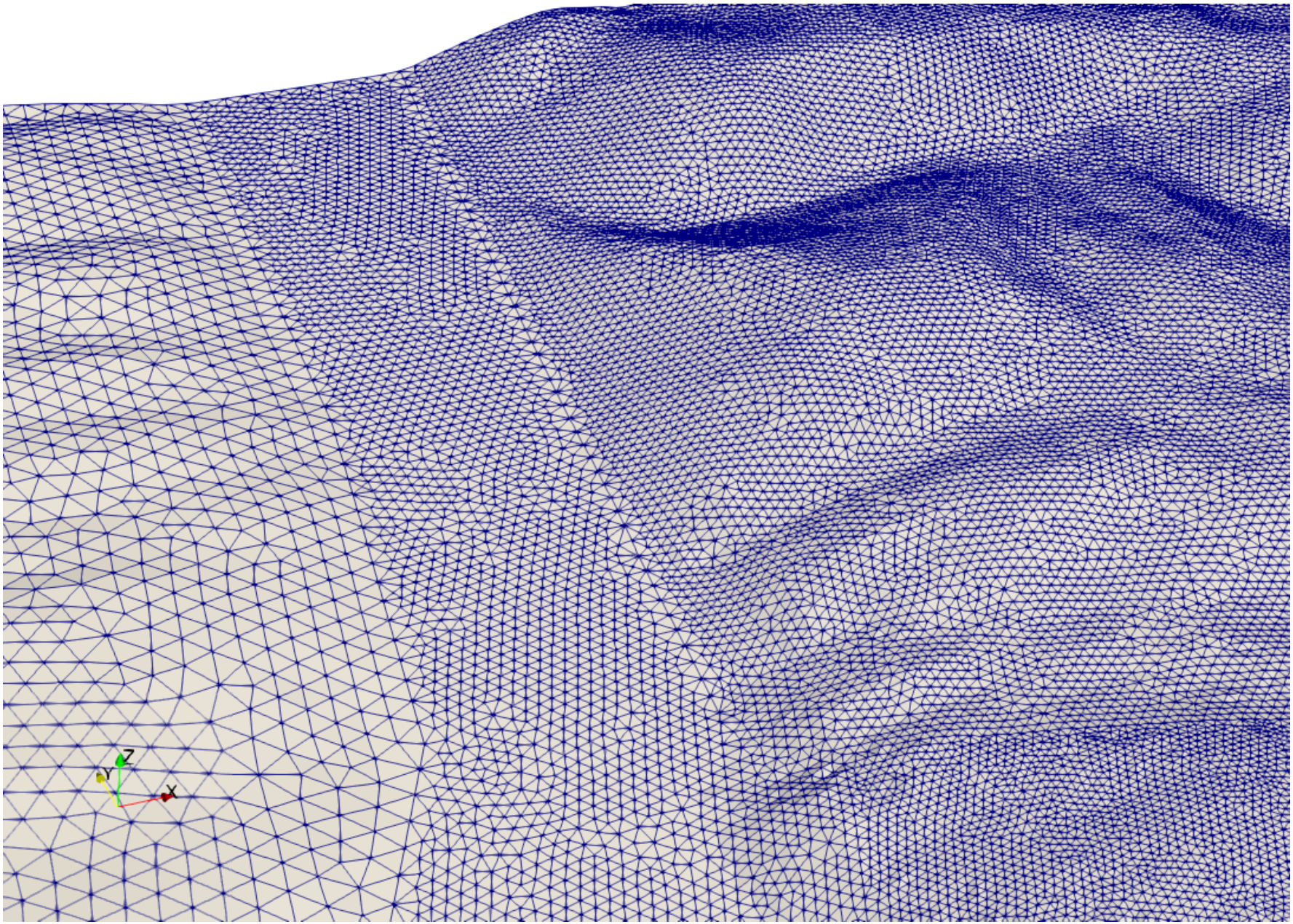
# Prismatic grid of the upper horizon



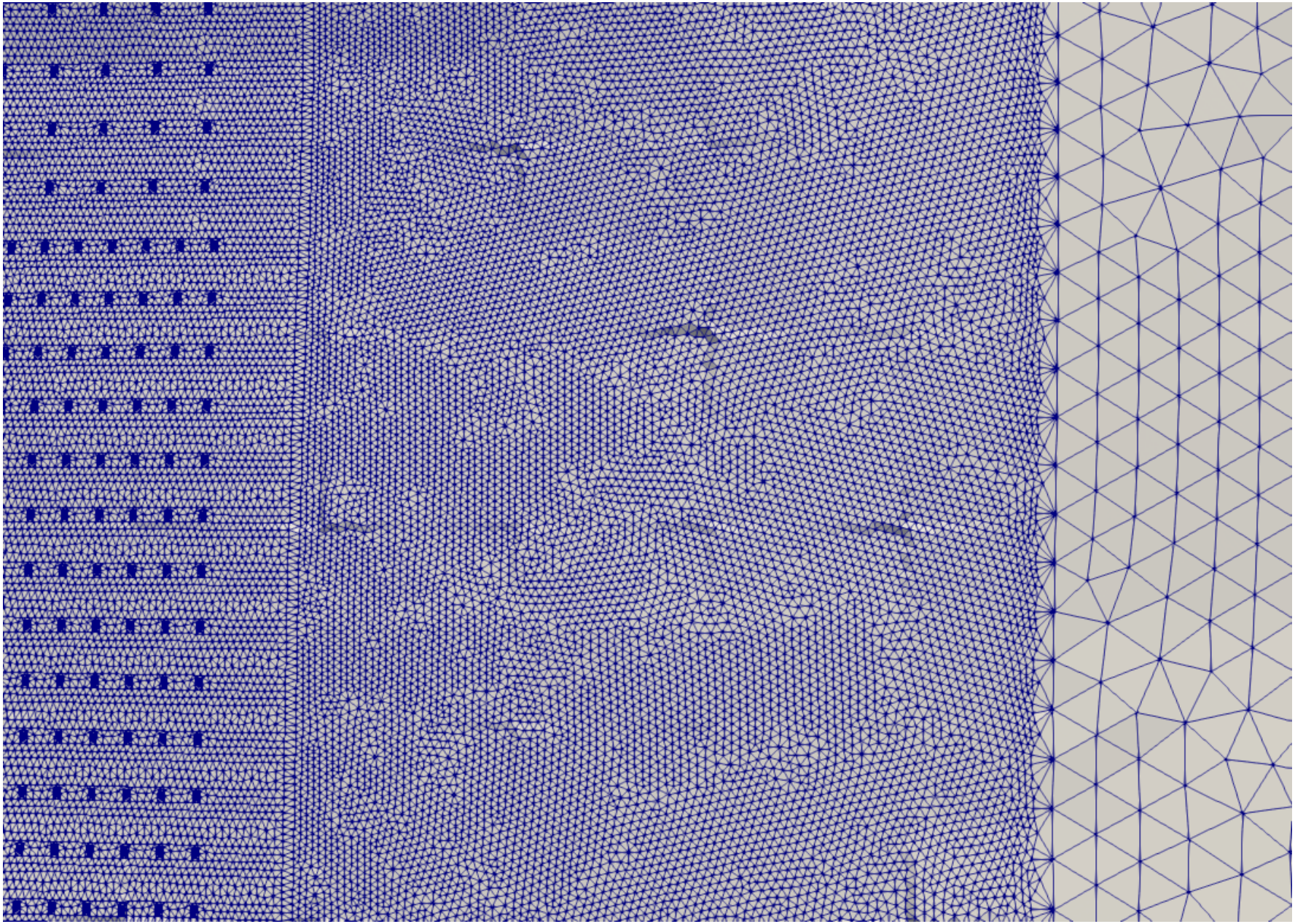
# Prismatic grid of the lower horizon



# Fragment of the computational mesh (near river)



# Fragment of the computational mesh (near wells)



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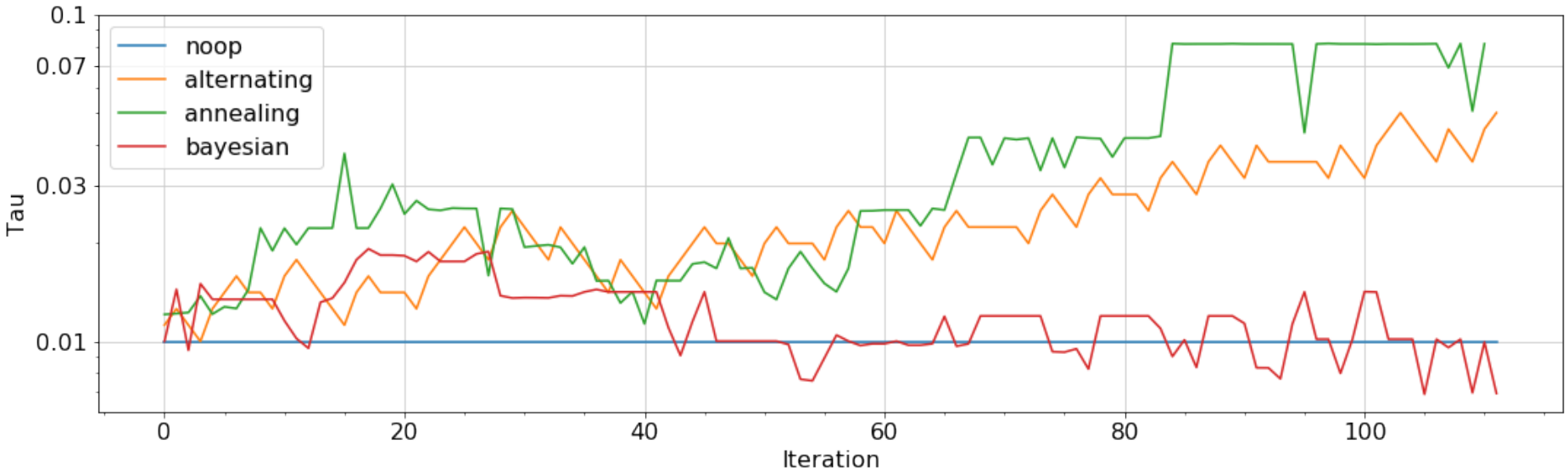
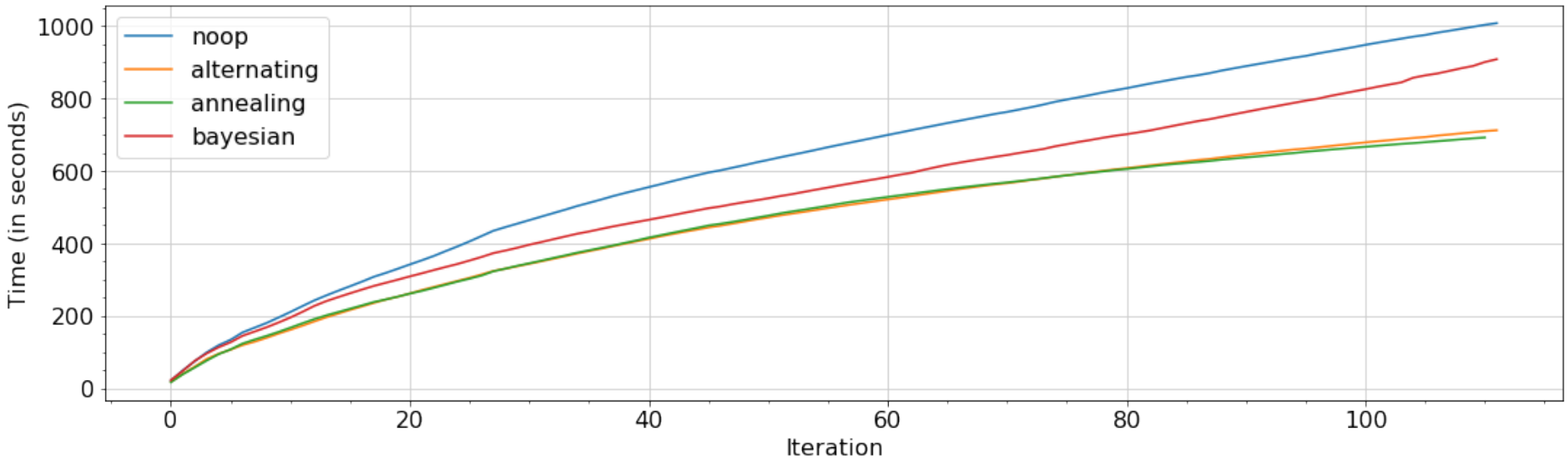
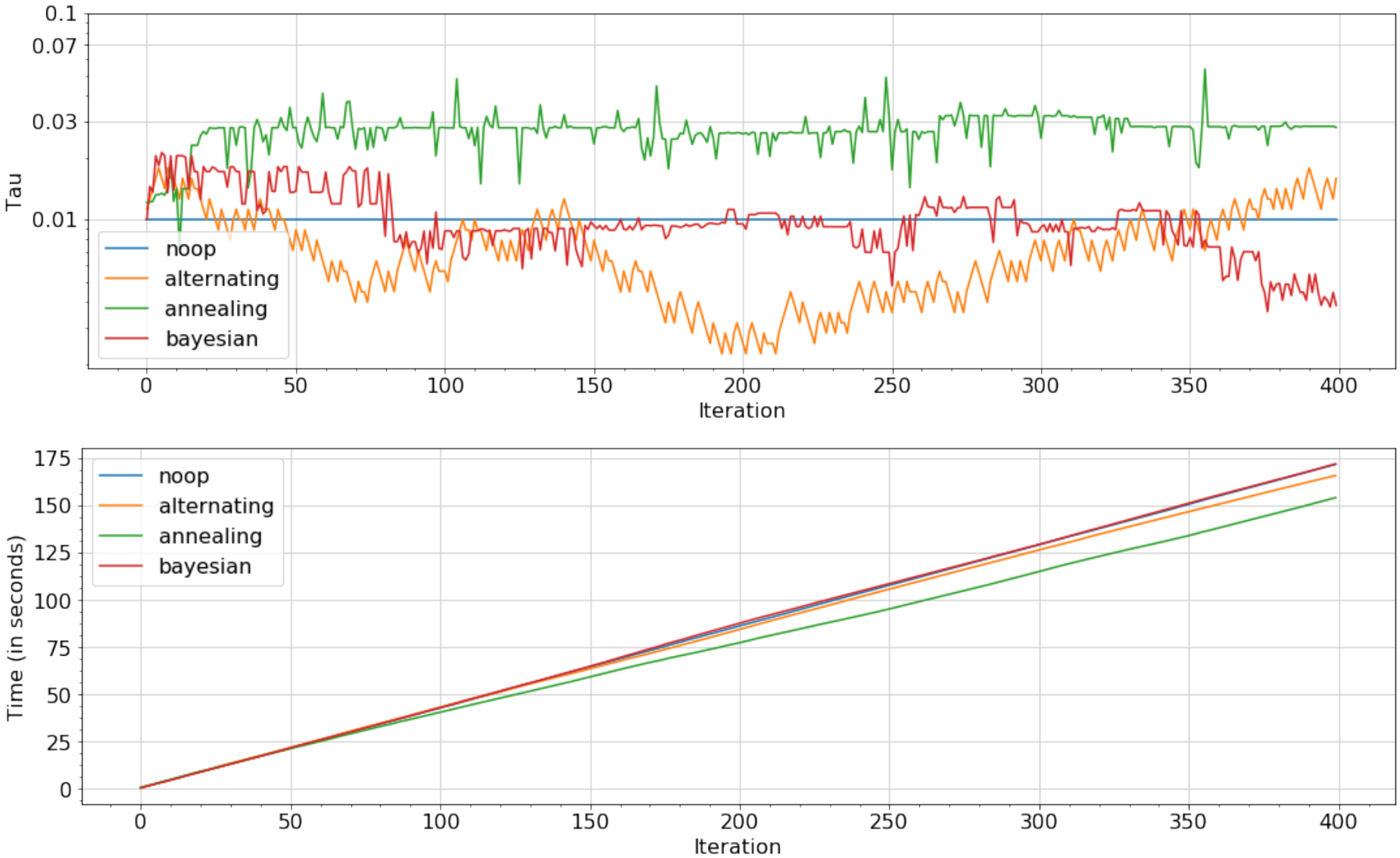
# [gw]: Optimization on $\tau$ for the GW flow modeling

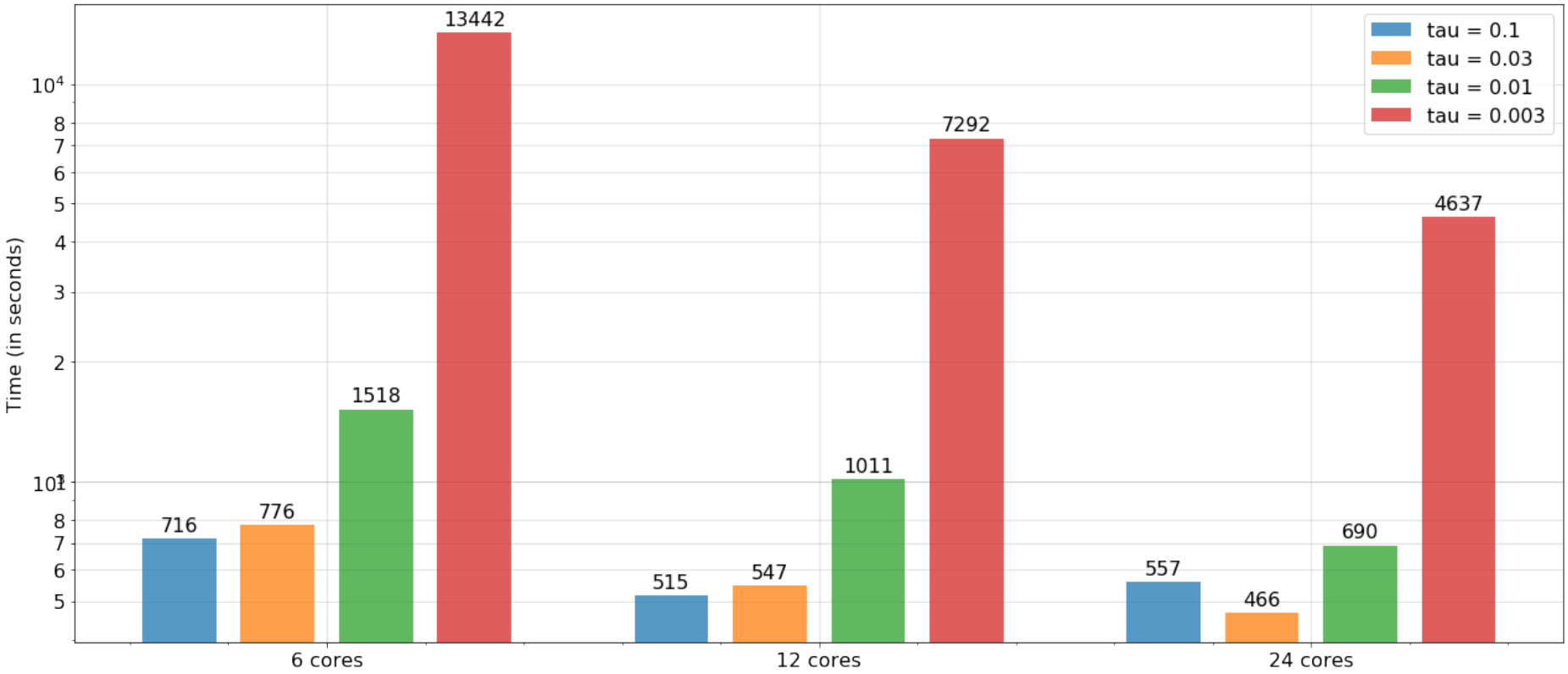


# [tr]: Optimization on $\tau$ for the transport process



# Solution time on 6, 12, 24 cores for different fixed values of $\tau$



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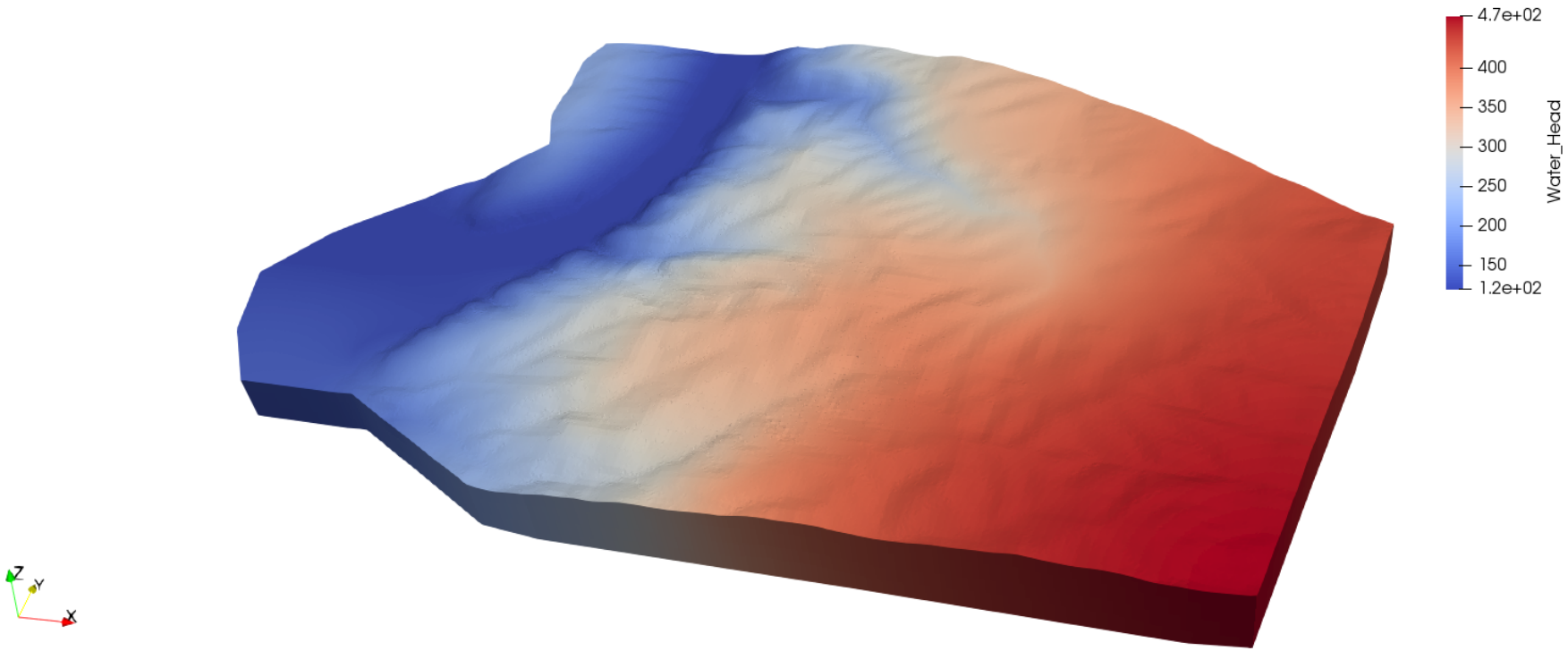
# Calculation results on the INM RAS cluster

| $p$ | $T_{\mathrm{gw}}$ | $S_{\mathrm{gw}}$ | $T_{\mathrm{tr}}$ | $S_{\mathrm{tr}}$ | $T_{\mathrm{total}}$ | $S_{\mathrm{total}}$ |
|---|---|---|---|---|---|---|
| 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 |

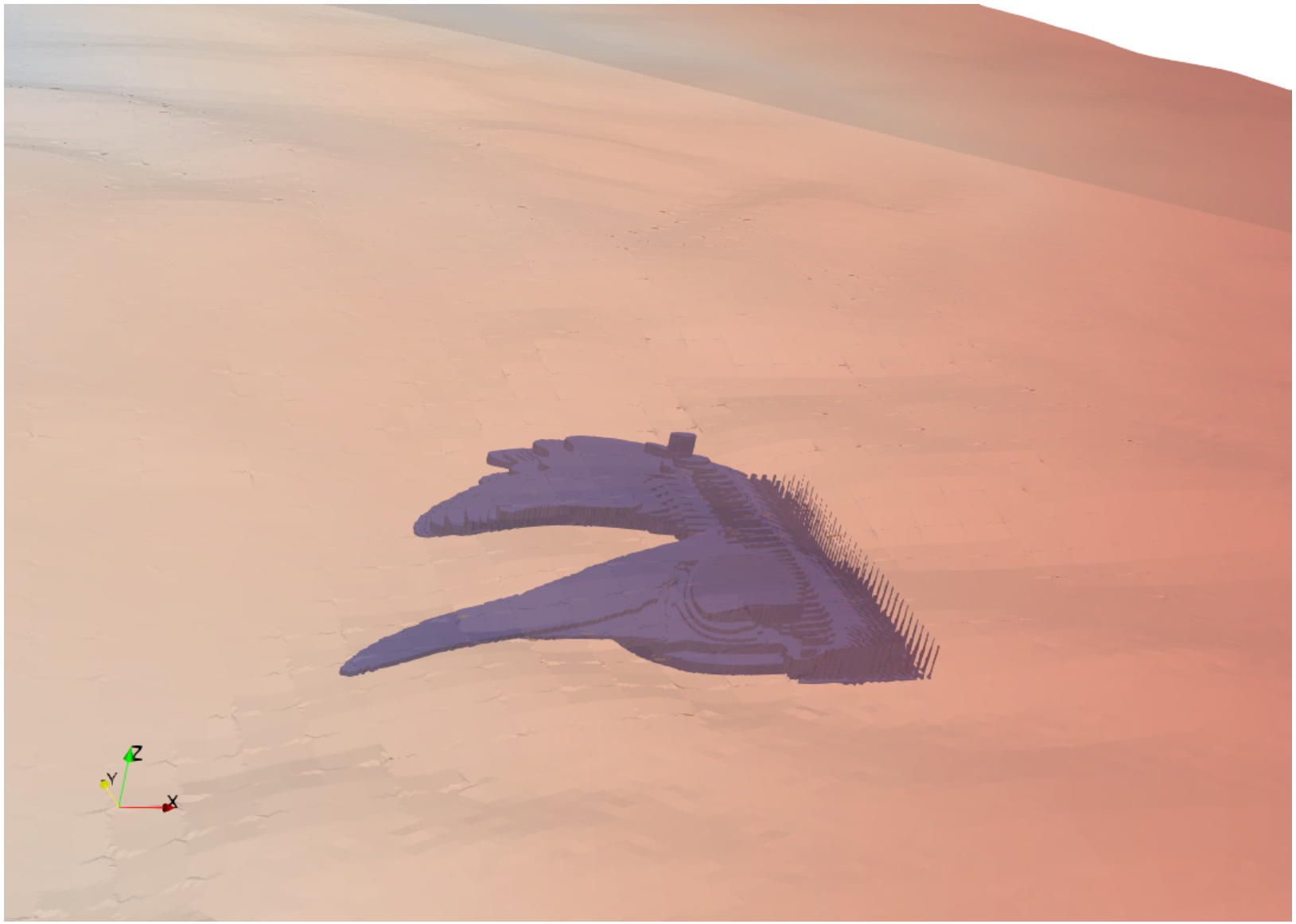
- $p$ – number of cores used
- $T = T(p)$ – simulation time on $p$ cores (in sec.)
- $S$ – relative speedup wrt. to run on 3 cores, $S = T(3)/T(p)$

- INMOST $\rightarrow$ BIILU2$(\tau, q)$ linear solver
- $\tau^*_{\mathrm{gw}} = 0.01$, $q^*_{\mathrm{gw}} = 3$ and $\tau^*_{\mathrm{tr}} = 0.02$, $q^*_{\mathrm{tr}} = 2$
- 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