Parallel efficiency of hydrogeological simulations in GeRa

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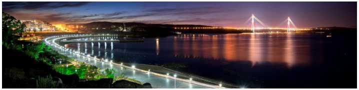


The Fourth German–Russian Workshop on
Numerical Methods and Mathematical Modelling in Geophysical and Biomedical Sciences
October 7-9, 2019, Vladivostok

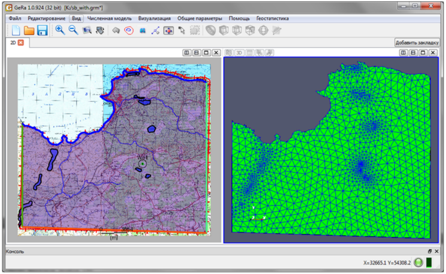
- **GeRa: modules and structure**
- Deep geological disposal
- Linear solver parameters tuning
- Numerical experiments

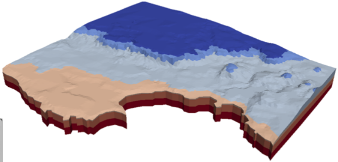
GeRa (Geomigration of Radionuclides): hydro-geological modelling code

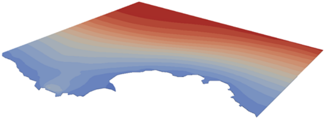
The major present-day abilities of GeRa

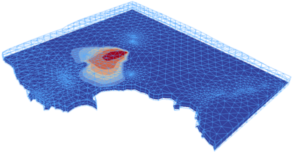
Modeling:

- geological
- groundwater flow
- transport in geological media









GeRa: announcement on Ge-Ru workshop

- Oct. 7, 14:25 — Igor Konshin
  Parallel efficiency

- Oct. 7, 15:15 — Fedor Grigoriev
  Some aspects of flow modelling

- Oct. 7, 16:10 — Konstantin Novikov
  Coupled surface–subsurface flow model

- Oct. 8, 10:10 — Ivan Kapyrin (Multiscale workshop)
  Reactive transport
- Oct. 8, 16:10 — Ivan Kapyrin
  Safety assessment problems

- Oct. 9, 10:35 — Denis Anuprienko
  Numerical solution of steady-state nonlinear groundwater flow equation

GeRa: 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**;
- **Surface water** flow (rainfall, rivers, lakes, drains, ...);
- Coupled **surface–subsurface** water flow;
- **Two-phase** flow.

(see ⊡ F.Grigoriev, K.Novikov, I.Kapyrin, D.Anuprienko)

GeRa: software used

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

Most of the software is freely distributed

GeRa = 150,000+ rows of C++ code written by 20+ code developers

The first version of the code (GeRa / V1) was certified by the Russian regulatory authority (Rostechnadzor) in 2018 for use in nuclear facilities safety assessment and transferred to a number of organizations in the nuclear industry under license agreements

INMOST: http://www.INMOST.org

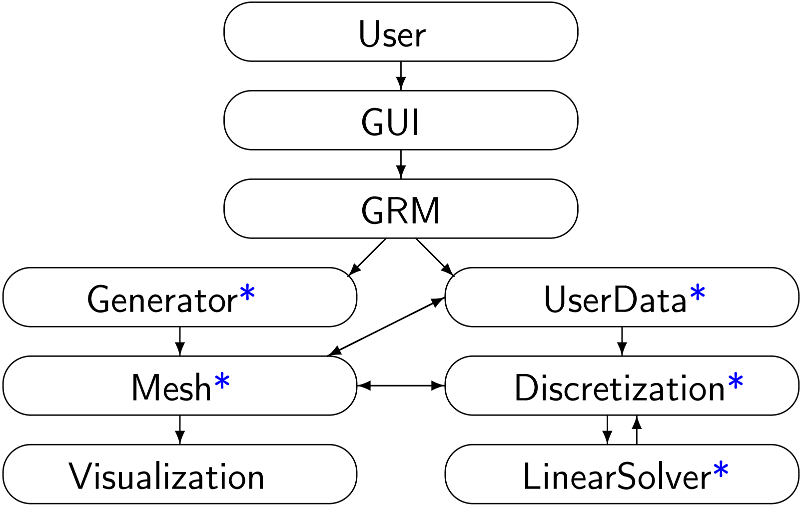
- **I**ntegrated
- **N**umerical
- **M**odelling and
- **O**bject-oriented
- **S**upercomputing
- **T**echnologies

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

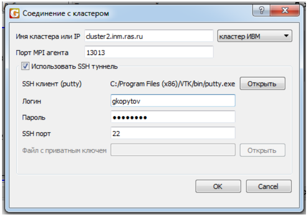
INMOST is a tool for supercomputer simulations characterized by a maximum generality of supported computational meshes, distributed data structure flexibility, *cost efficiency*, cross platform portability.

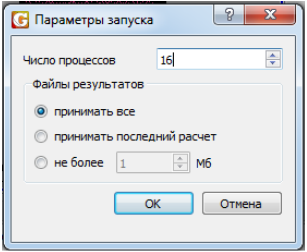
INMOST technology is implemented and used in more than 10 projects in Russia, the USA, Netherlands, Qatar...

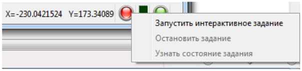
User ⟶ GeRa modules/objects (* INMOST based)

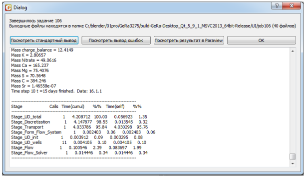


GeRa: GUI for // run on remote Linux cluster









- connect to remote cluster
- specified the number of PEs
- // run
- view the results

- GeRa: modules and structure
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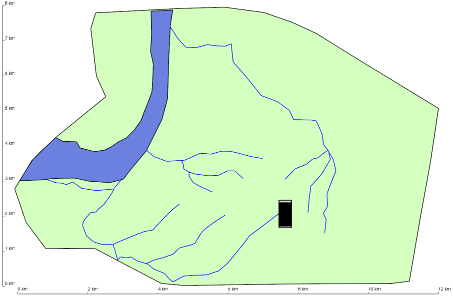
Model: Yeniseisky site

(see ⊡ F.Grigoriev)

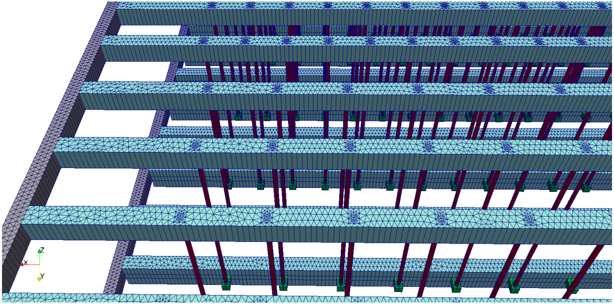


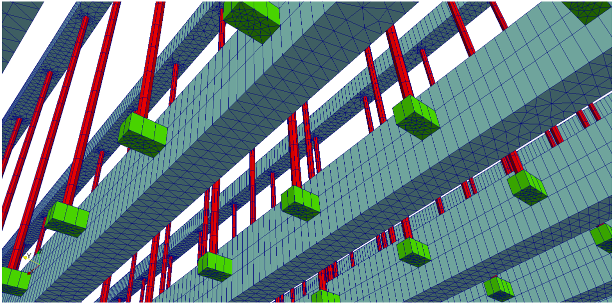
- nonstationary groundwater flow and migration of radionuclides
- reactive transport (see ⊡ I.Kapyrin)
- boundary condition of rainfall recharge
- different hydraulic conductivities (from 10^{-1} to 10^{-4} m/day)
- four layers with different thickness
- *complicated geometry*
- *number of cells:* $>10^7$

Computational prismatic mesh fragments

Upper level ⇒

* Transport tunnels
* Disposal cells

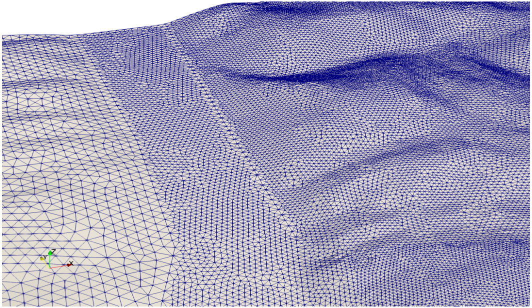




⇐ Lower level

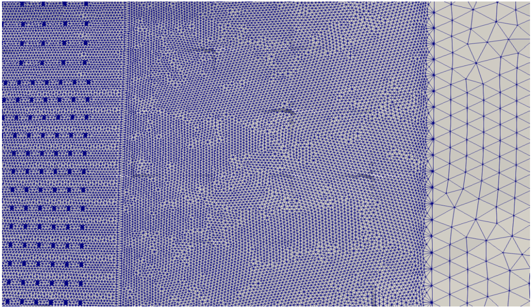
* Drilling chambers
* Disposal cells

Computational surface mesh fragments



$\Leftarrow$ The area of the far field with Yenisey river

The connection between far and near field meshes $\Rightarrow$



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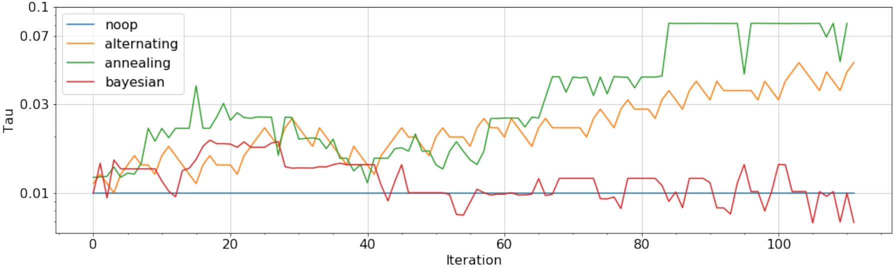
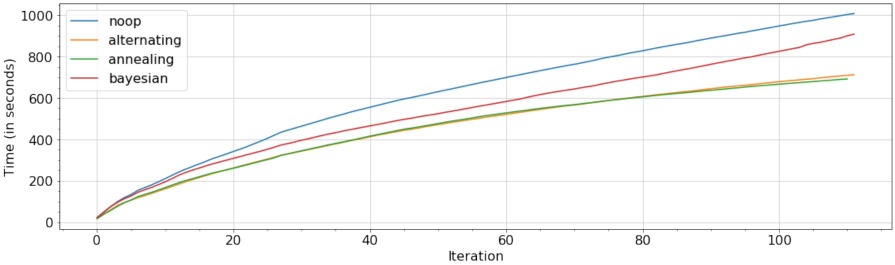
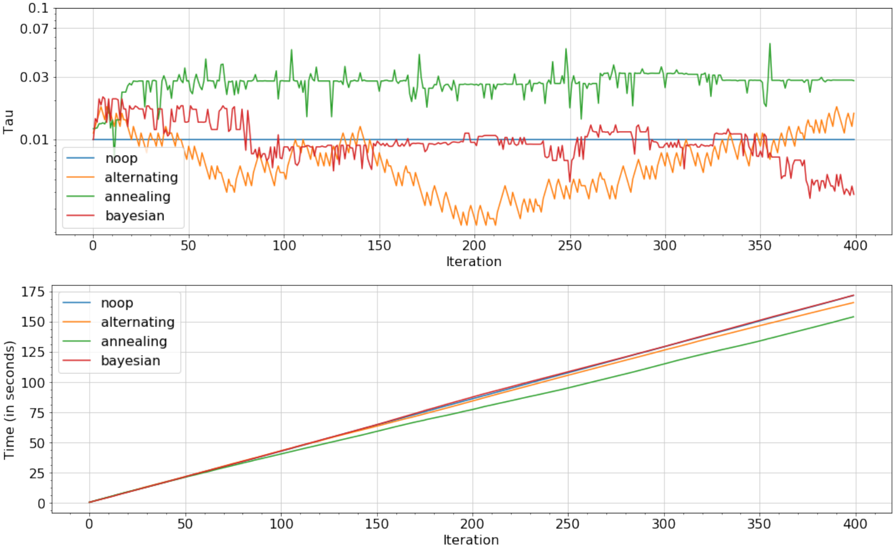
[gw]: Optimization on τ for the GW flow modelling

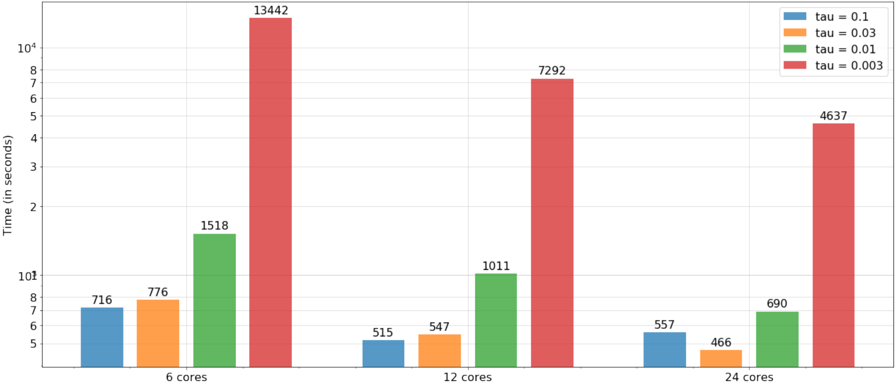




[tr]: Optimization on τ for the transport process



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



Different optimal values of τ: importance of automatic tuning

- GeRa: modules and structure
- Deep geological disposal
- Linear solver parameters tuning
- **Numerical experiments**

[gw]+[tr]: // runs on INM RAS cluster

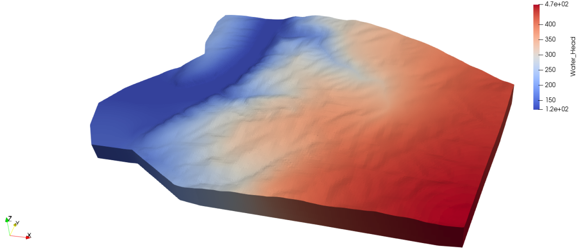
p	T_{gw}	S_{gw}	T_{tr}	S_{tr}	T_{total}	S_{total}
3	2995.2	1.00	3478.9	1.00	6474.1	1.00
6	2102.4	1.42	2213.7	1.57	4316.1	1.50
12	1570.4	1.90	1376.2	2.52	2946.6	2.19
24	807.9	3.70	737.2	4.71	1545.1	4.19
48	388.9	7.70	478.6	7.26	867.5	7.46
96	330.1	9.70	302.0	11.51	632.1	10.24
192	159.3	18.80	226.3	15.37	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 $\rightarrow$ BIILU2(τ, 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

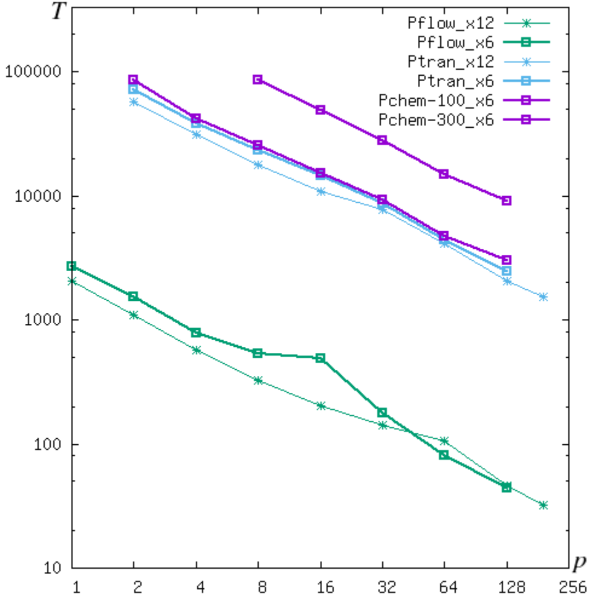
[gw]+[tr]: Computational results

Calculated GW head ⇒

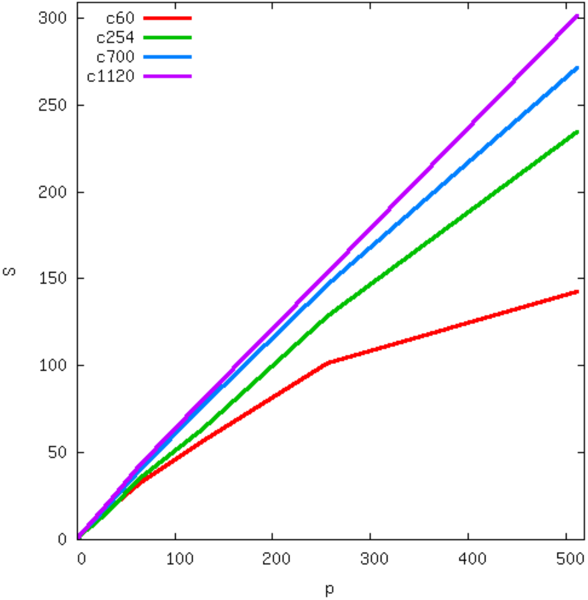


⇐ Predicted pollution plume with a relative concentration above $5 \cdot 10^{-6}$ at 8000 years

GeRa: Time reduction for other (gw, tr, chemical) problems



GeRa: Speedup for set of chemical problems by dimension



Summary

- The scalability was demonstrated up to 192 (and 512) cores;
- Linear solver parameters tuning can be performed automatically;
- The use of a fine ($> 10^7$ cells) mesh allow to obtain a more detailed prediction for safety assessment.

Thank you!

Danke!

Спасибо!

谢谢啦