Parallel computations in the hydrogeological code GeRa:
organization and efficiency

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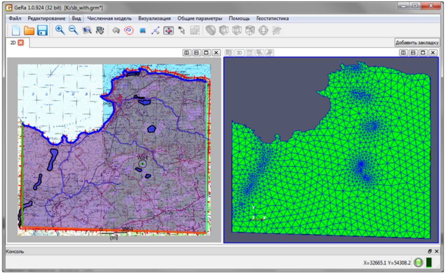
- **GeRa: organization and structure**
- Models
- Numerical experiments
- Linear solver parameters tuning

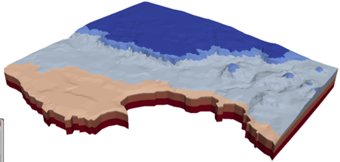
GeRa: hydro-geological modeling code

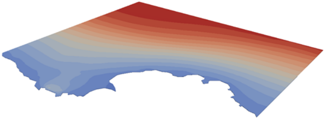
The major present-day abilities of GeRa

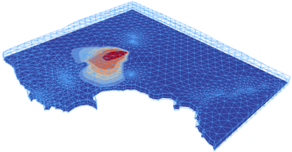
Modeling:

- geological
- groundwater flow
- transport in geological media









GeRa: major processes can be modeled

- 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.

Wednesday 13:50   I. Kapyrin — GeRa: density driven flow

GeRa: view and properties

- General user (view to interface)
- Advanced user (view to specific facilities)
- Code designer (view to structure and modules interaction)

- Interaction of modules
- Software used

150,000+ rows of C++ code

GeRa: software used

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

Most of the software is freely distributed

INMOST: http://www.inmost.org

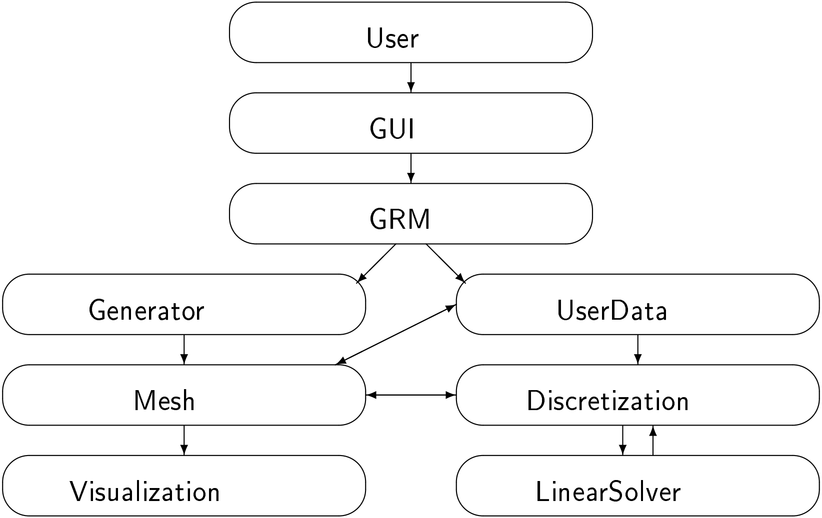
- **I**ntegrated
- **N**umerical
- **M**odelling and
- **O**bject-oriented
- **S**upercomputing
- **T**echnologies

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

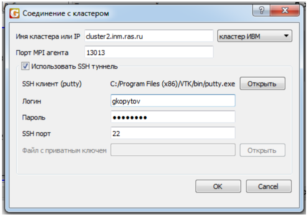
INMOST is a tool for supercomputer simulations characterized by a maximum generality of supported computational meshes, distributed data structure flexibility, cost-effectiveness, cross platform portability.

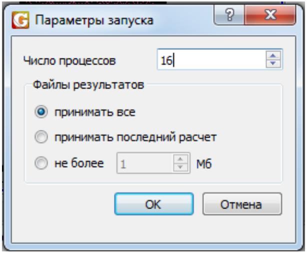
Friday 13:50 K. Terekhov — INMOST

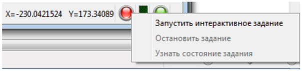
User and GeRa modules/objects

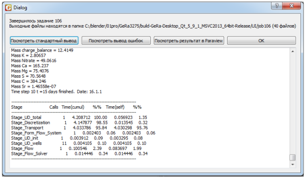


Computations on the remote cluster via GUI









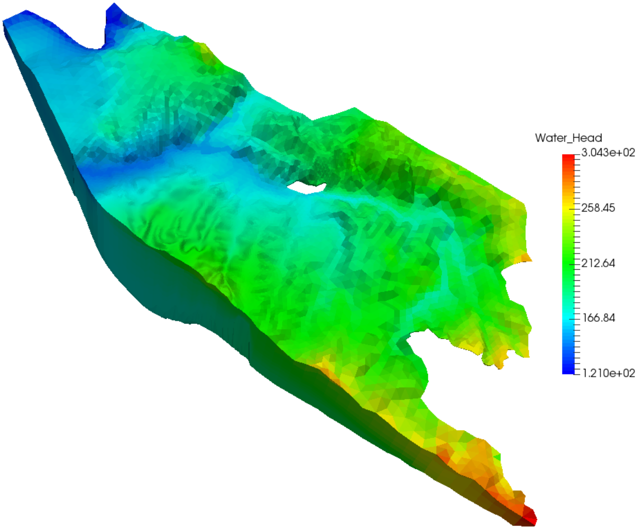
3 models description: “Severny” polygon

- **Pflow** – stationary groundwater flow in an unconfined regime
- **Ptran** – nonstationary groundwater flow and migration of radionuclides
- **Pchem** – reactive transport

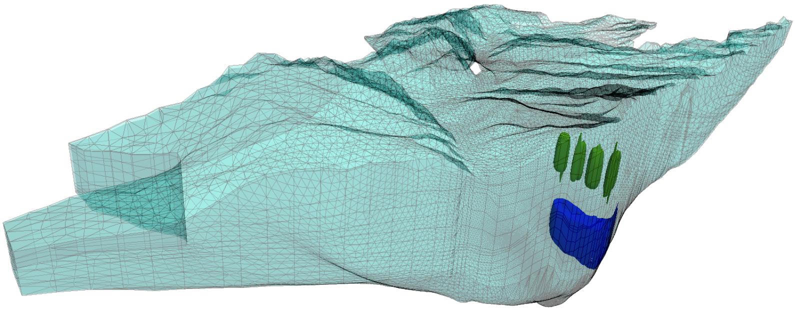
- 27 km x 27 km x 600 m
- 10 geological layers
- number of cells: 480350 for Pflow and Ptran, 26476 for Pchem

Wednesday 16:30 F. Grigoryev — “Severny” polygon: thermal processes

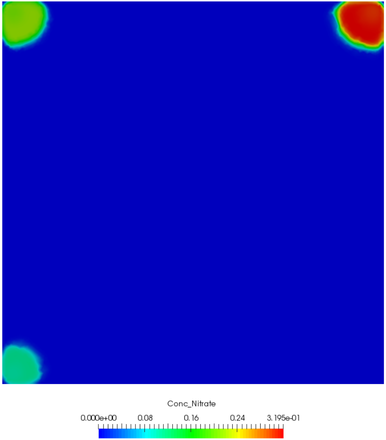
Pflow: hydraulic head

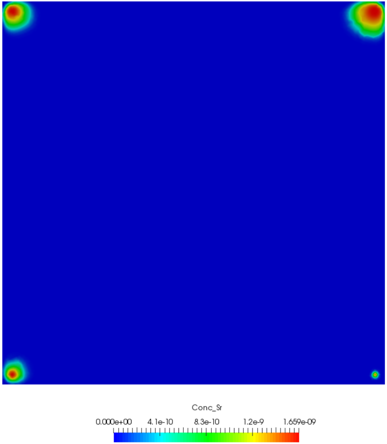


Ptran: computed halos of radioactive contamination



Pchem: NO_3-ion and Sr distribution at 300-th day





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INM RAS cluster segments

x6core:

- Compute Node Asus RS704D-E6;
- 12 cores (2x 6-cores processors Intel Xeon X5650@2.67GHz);
- RAM: 24 GB;
- OS: SUSE Linux Enterprise Server 11 SP1 (x86_64);

x8core:

- Compute Node Arbyte Alkazar+ R2Q50;
- 16 cores (2x 8-cores processors Intel Xeon X2665@2.40GHz);
- RAM: 64 GB;
- OS: SUSE Linux Enterprise Server 11 SP1 (x86_64);

x12core:

- Compute Node Arbyte Alkazar+ R2Q50;
- 24 cores (2x 12-cores processors Intel Xeon E5-2670v3@2.30GHz);
- RAM: 64 GB;
- OS: SUSE Linux Enterprise Server 11 SP3 (x86_64).

Numerical experiments

- INMOST -> PETSc linear solver
- AS($q = 3$) + ILU($k = 3$) preconditioner
- BiCGstab iterations up to relative residual 10^9 times reduction

- p – number of cores used;
- $T = T(p)$ – simulation time on p cores (in sec.);
- S_r – relative speedup on p cores with respect to run on r cores, $S_r = T(r)/T(p)$;
- $S_{p/2}$ – relative speedup on p cores with respect to run on $p/2$ cores, $S_{p/2} = T(p/2)/T(p)$.

Pflow: x12core and x6core

p	T (s)	S_1	$S_{p/2}$
1	2044.97	1.00	—
2	1086.56	1.88	1.88
4	571.91	3.57	1.89
8	324.19	6.30	1.76
16	205.35	9.95	1.57
32	140.97	14.50	1.45
64	105.25	19.42	1.33
128	46.49	43.98	2.26
192	32.16	63.58	1.44

p	T (s)	S_1	$S_{p/2}$
1	2686.60	1.00	—
2	1541.19	1.74	1.74
4	784.49	3.42	1.96
8	529.28	5.07	1.48
16	484.56	5.54	1.09
32	178.52	15.04	2.71
64	80.46	33.39	2.21
128	43.78	61.36	1.83

Ptran: x12core and x6core

p	T (s)	S_2	$S_{p/2}$
2	57027.52	1.00	—
4	30899.76	1.84	1.84
8	17928.51	3.18	1.72
16	10795.76	5.28	1.66
32	7692.88	7.41	1.40
64	4111.9	13.86	1.87
128	2065.94	27.60	1.99
192	1542.59	36.96	1.33

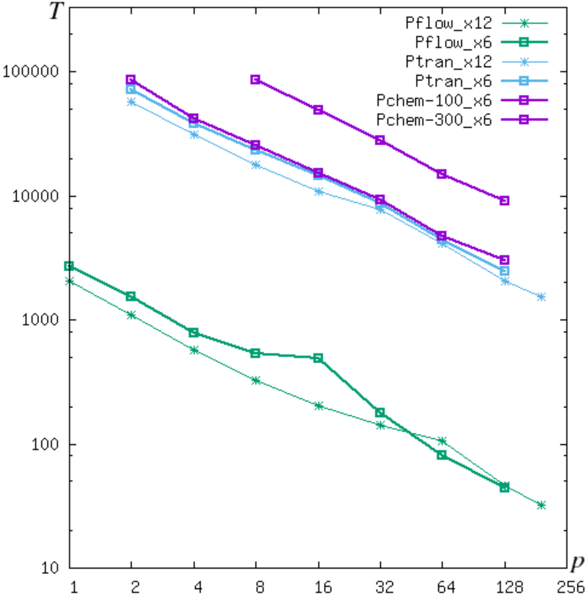
p	T (s)	S_2	$S_{p/2}$
2	72267.77	1.00	—
4	37872.65	1.90	1.90
8	23490.57	3.07	1.61
16	14593.40	4.95	1.60
32	8639.32	8.36	1.68
64	4377.29	16.50	1.97
128	2470.17	29.25	1.77

Pchem: 100 and 300 days (x6core)

p	T (s)	S_2	$S_{p/2}$
2	86215.83	1.00	—
4	41767.22	2.06	2.06
8	25631.87	3.36	1.62
16	15313.55	5.63	1.67
32	9283.06	9.28	1.64
64	4697.10	18.35	1.97
128	2982.72	28.90	1.57

p	T (s)	S_8	$S_{p/2}$
8	85080.86	1.00	—
16	48762.31	1.74	1.74
32	28159.37	3.02	1.77
64	14993.77	5.67	1.87
128	9004.06	9.44	1.60

GeRa time reduction for $p = 1, ..., 192$ cores



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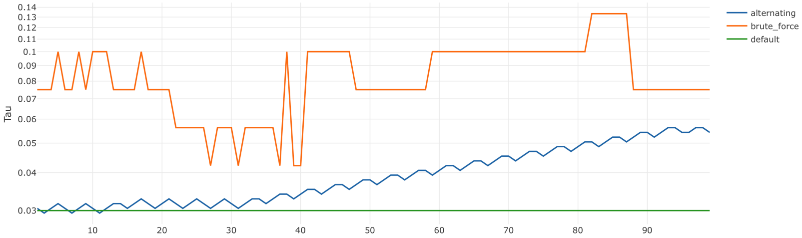
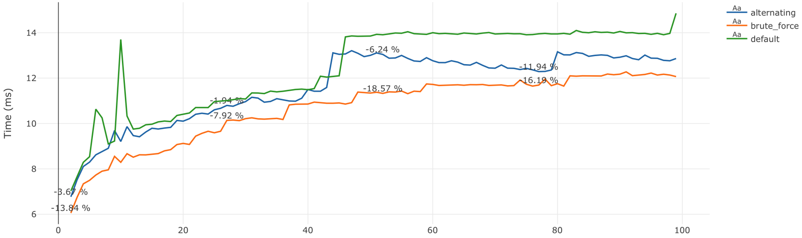
$\text{BIILU2}(\tau, q) = \text{BIILU}(q) + \text{ILU2}(\tau)$

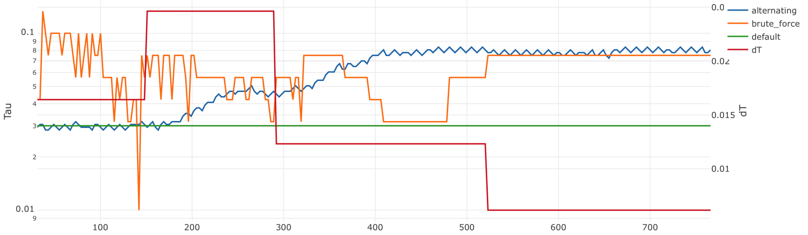
tuning of τ for $q = 1$

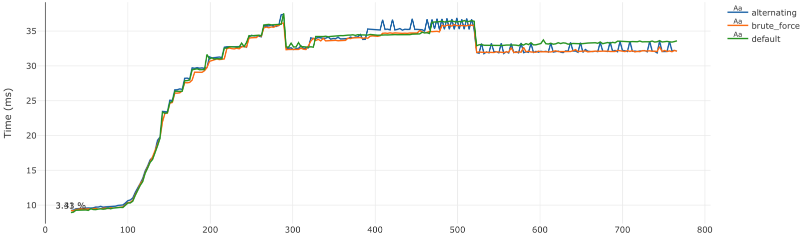
GeRa verification test t14



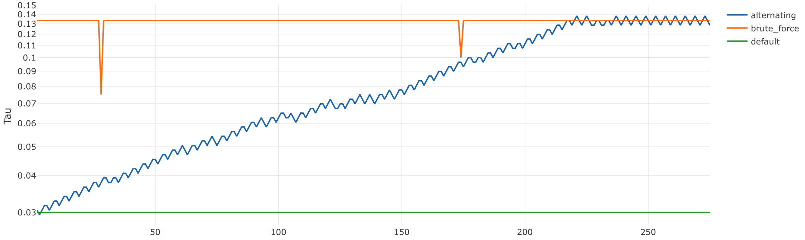


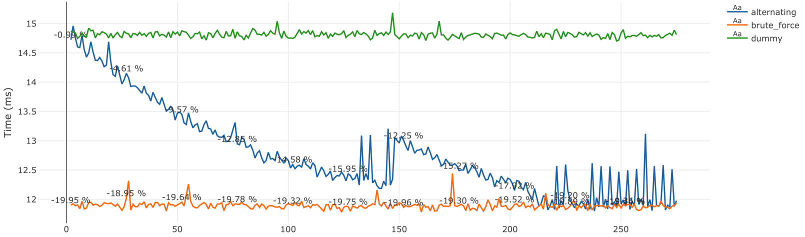
GeRa verification test t15



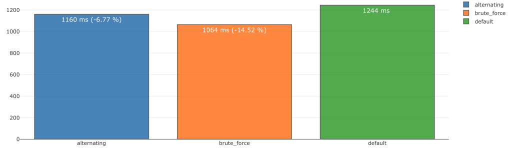


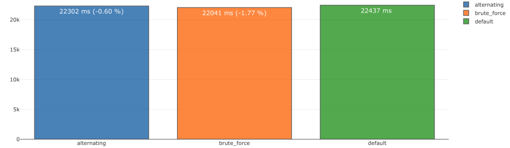
Pflow+Ptran

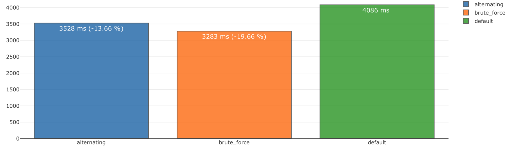

Tau
0.15
0.14
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
50
100
150
200
250
alternating
brute_force
default


Time (ms)
15
14.5
14
13.5
13
12.5
12
0
50
100
150
200
250
alternating
brute_force
dummy
-4.61 %
-12.85 %
-12.25 %
-15.27 %
-17.92 %
-19.95 %
-18.95 %
-19.64 %
-19.78 %
-19.32 %
-19.75 %
-19.96 %
-19.30 %
-19.52 %
-19.20 %

Cumulative time for t14, t15, and Pflow+Ptran







Conclusions

- GeRa reasonable scalability up to 192 cores
- about 50% efficiency for 128 cores
- maximal speedup is for chemical interactions
- monotone time reduction with number of cores increased
- linear solver parameter tuning can be performed automatically