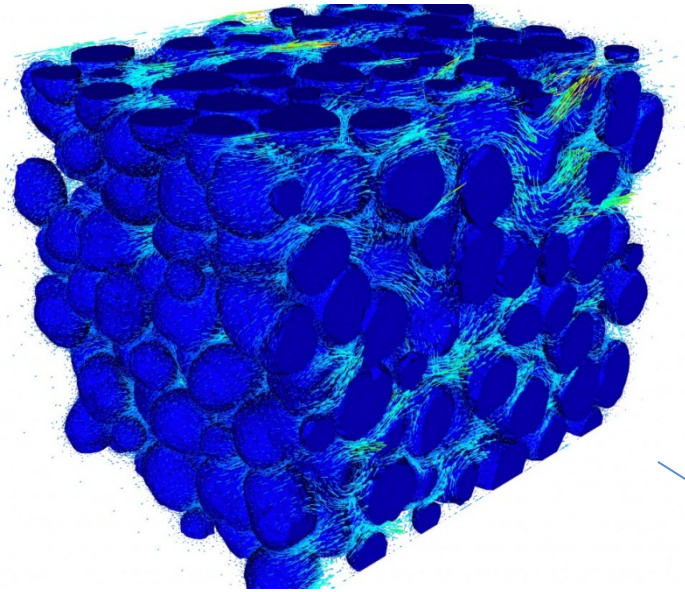
Extending the capability of TOUGHREACT simulator using parallel computing

Application to environmental problems

What is TOUGHREACT ?

Coupled Process in porous media simulator, developed in Lawrence Berkley Lab.



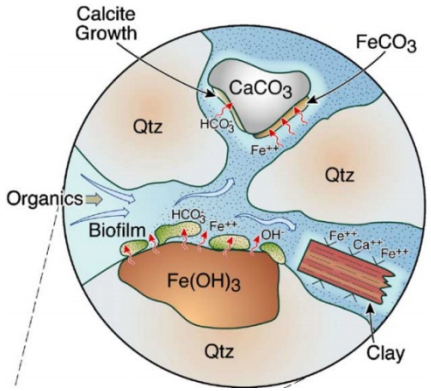
Multi-phase flow

+

Solute transport

+

Geochemical reaction



BERKELEY LAB

Motivation of the work

Lab code constraints:

- Developed for testing the model
- Running on workstation or laptop
- Numerical model can not scaling (8000 discrete grids limited)

Engineering requirements:

- Carrying the simulation of site-scale model involved complex processes
- Improve the speed in numerical solving .

Method

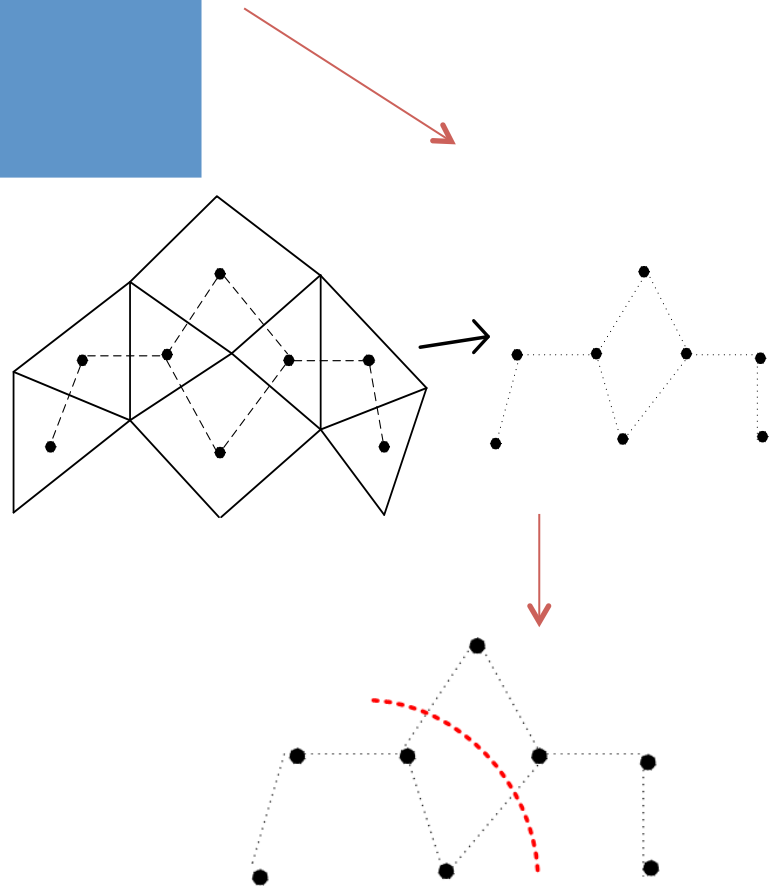
- Redevelop the software package using parallel computing schema.
- Domain Decomposition.
- Communication between divided subdomains(MPI)

Domain Partition

```
ELEME
A11 1       10.2000E+000.4000E+00      0.1000E+000.5000E+00-.5000E+00
A11 2       10.2000E+000.4000E+00      0.3000E+000.5000E+00-.5000E+00
A11 3       10.2000E+000.4000E+00      0.5000E+000.5000E+00-.5000E+00
A11 4       10.2000E+000.4000E+00      0.7000E+000.5000E+00-.5000E+00
CONNE
A11 1A11 2          10.1000E+000.1000E+000.1000E+01
A11 2A11 3          10.1000E+000.1000E+000.1000E+01
A11 3A11 4          10.1000E+000.1000E+000.1000E+01
```

Multi-level Graph Partition:

Metis



Parallel Linear Solver

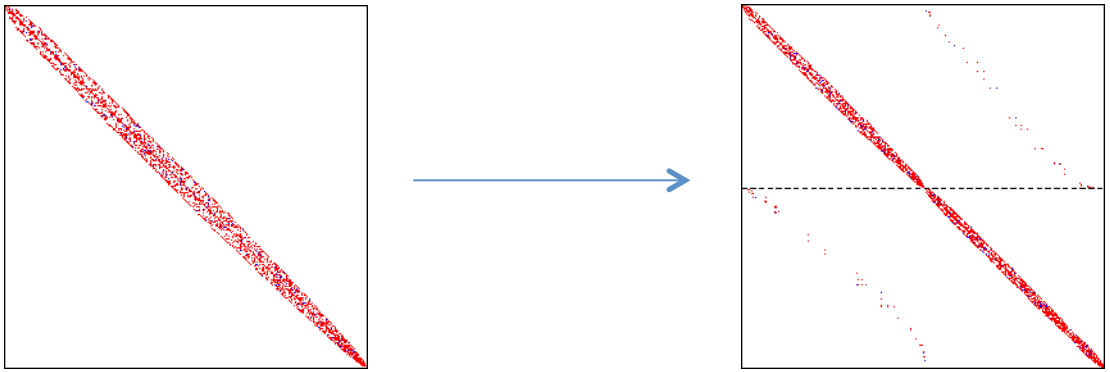
$$\sum_i \frac{\partial R_n^{\kappa,k+1}}{\partial x_i}\Big|_p \left(x_{i,p+1} - x_{i,p}\right) = R^{\kappa,k+1}\left(x_{i,p}\right)$$

$$\begin{bmatrix} a_{11} & a_{12} & & & & & & \\ a_{21} & a_{22} & a_{23} & & & & & \\ & a_{32} & a_{33} & a_{34} & & & & \\ & & a_{43} & a_{44} & a_{45} & & & \\ & & & a_{54} & a_{55} & a_{56} & & \\ & & & & a_{65} & a_{66} & a_{67} & \\ & & & & & a_{76} & a_{77} & a_{78} \\ & & & & & & a_{87} & a_{88} \end{bmatrix} \bullet \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \\ b_7 \\ b_8 \end{bmatrix}$$

proc. 1
proc. 2
proc. 3
proc. 4

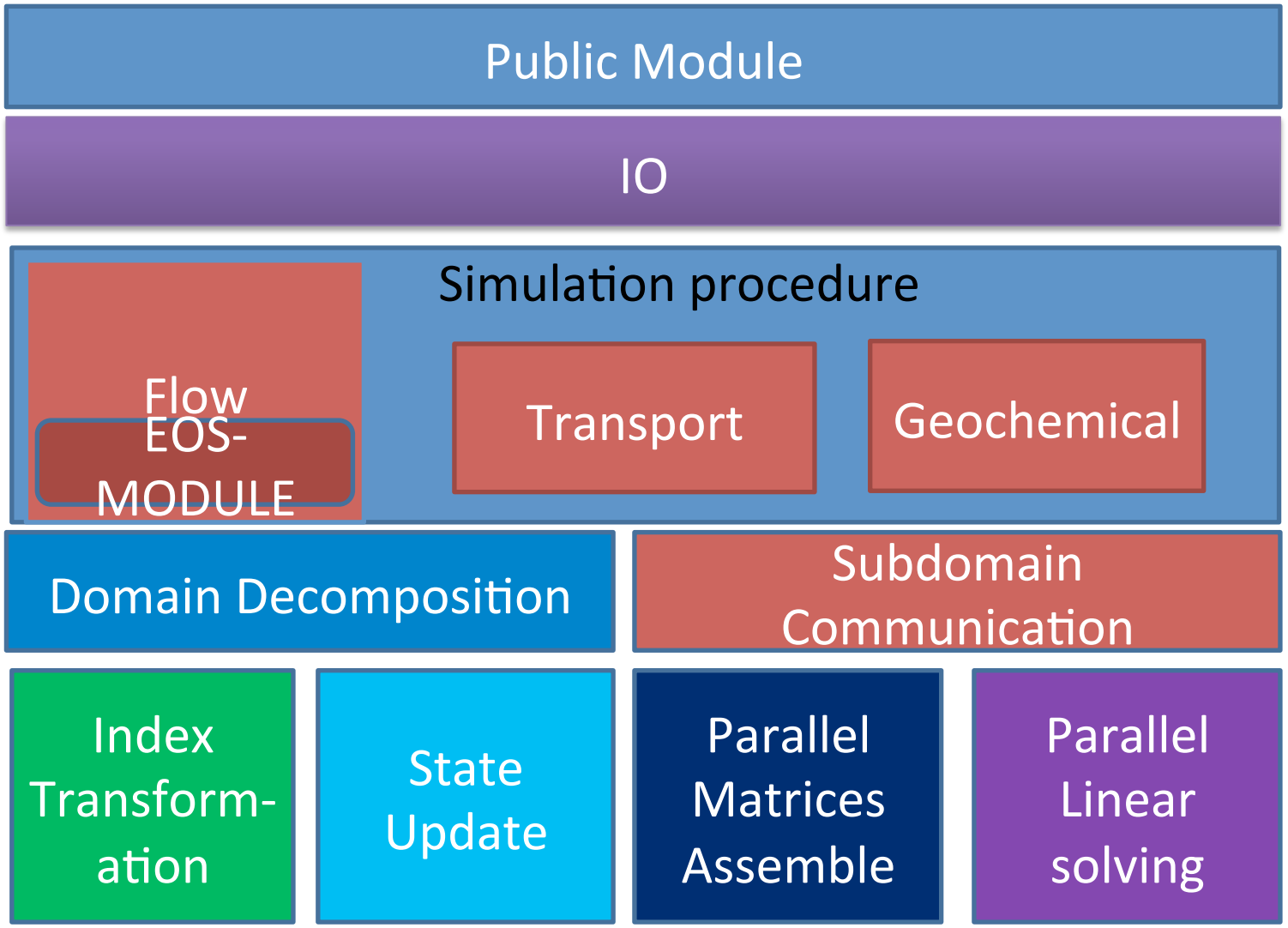
Large Sparse Linear System iterative solving

Aztec

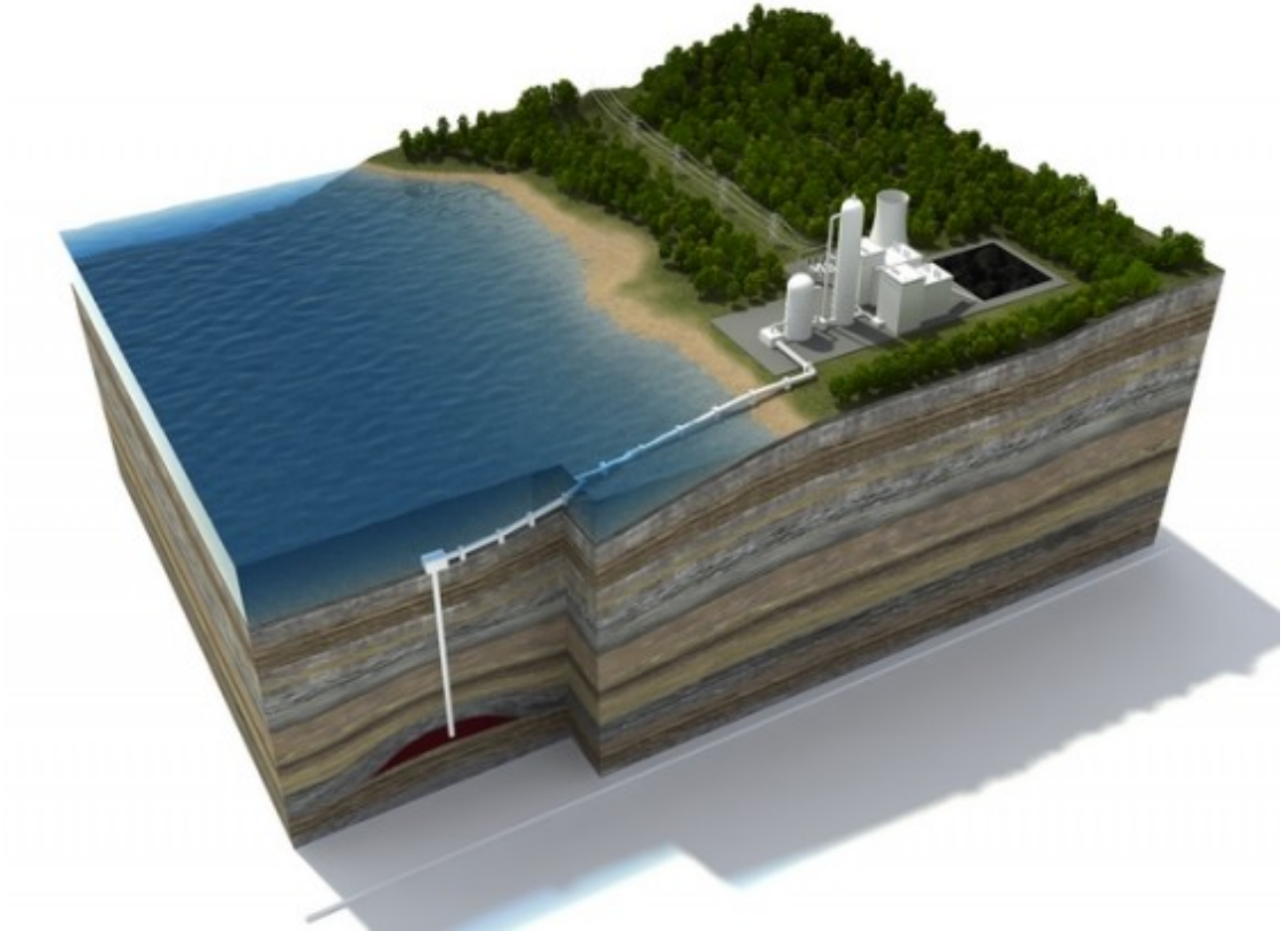


Sandia National Laboratories

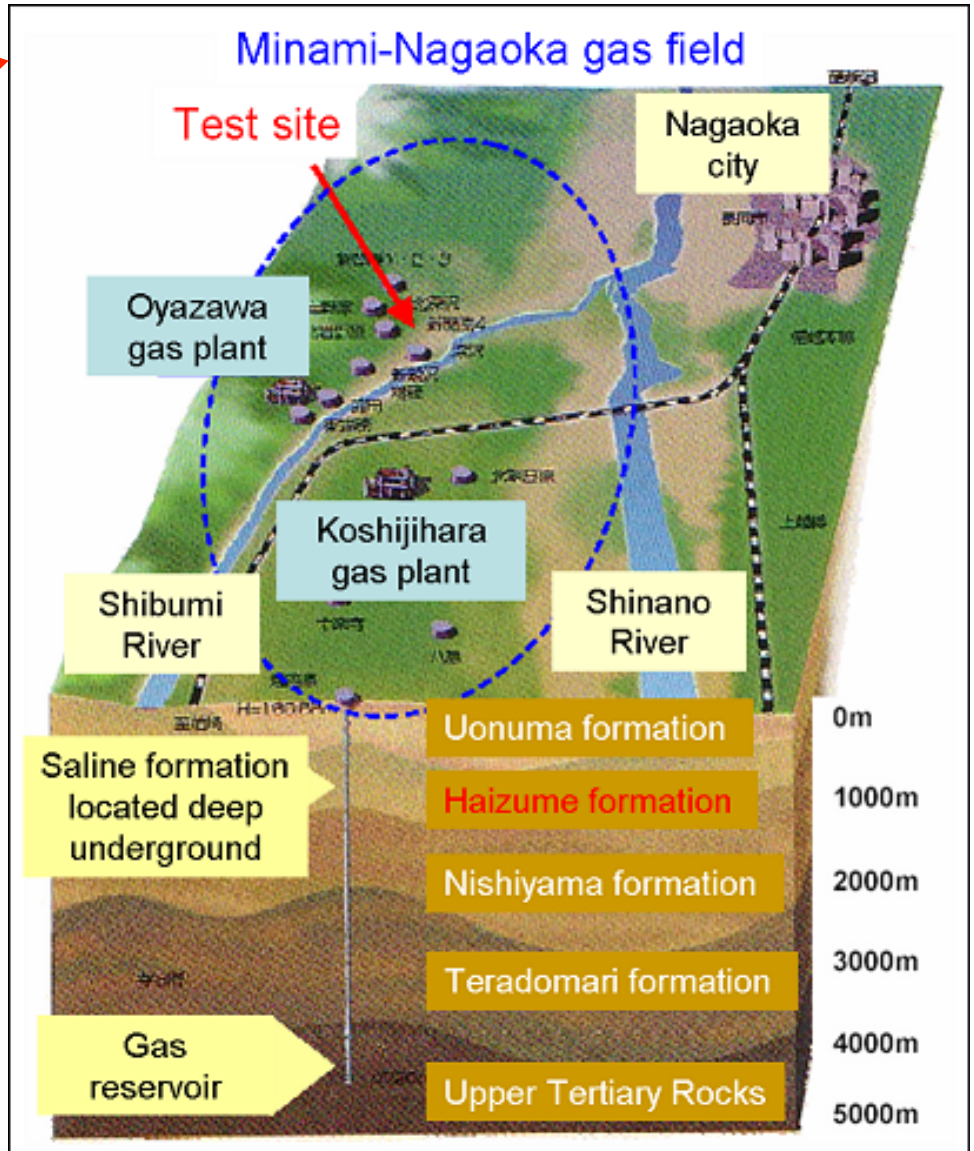
Module organization

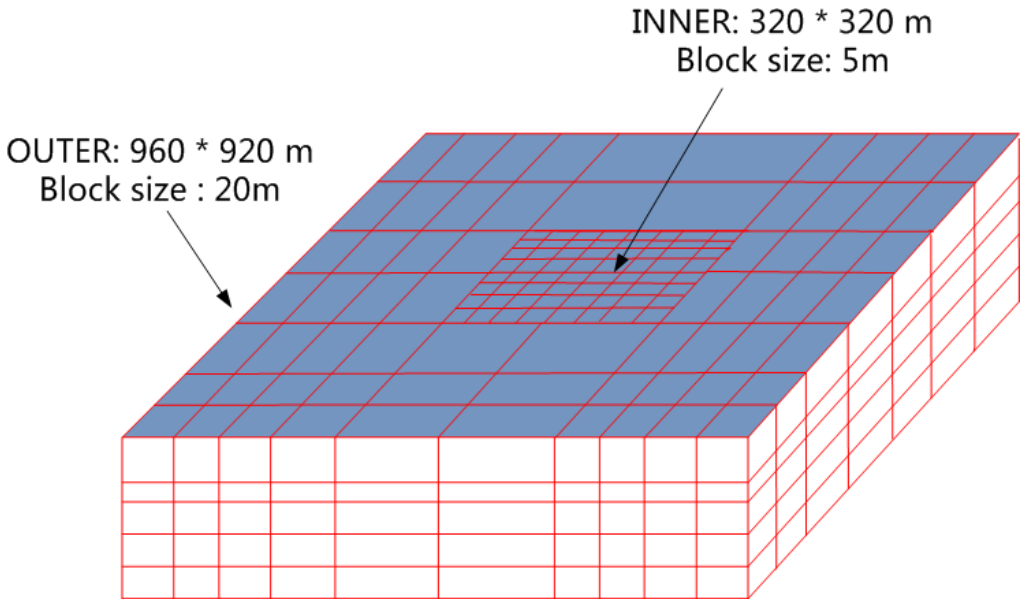


Application: Carbon dioxide sequestration



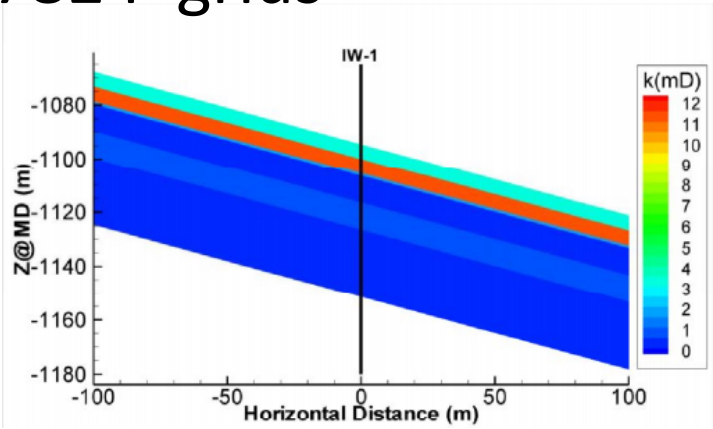

Nagaoka
Tokyo
Osaka
0
200km


Minami-Nagaoka gas field
Test site
Nagaoka city
Oyazawa gas plant
Koshijihara gas plant
Shibumi River
Shinano River
Uonuma formation
Haizume formation
Nishiyama formation
Teradomari formation
Upper Tertiary Rocks
Saline formation located deep underground
Gas reservoir
0m
1000m
2000m
3000m
4000m
5000m



Fine grid model:

Total : 37824 grids

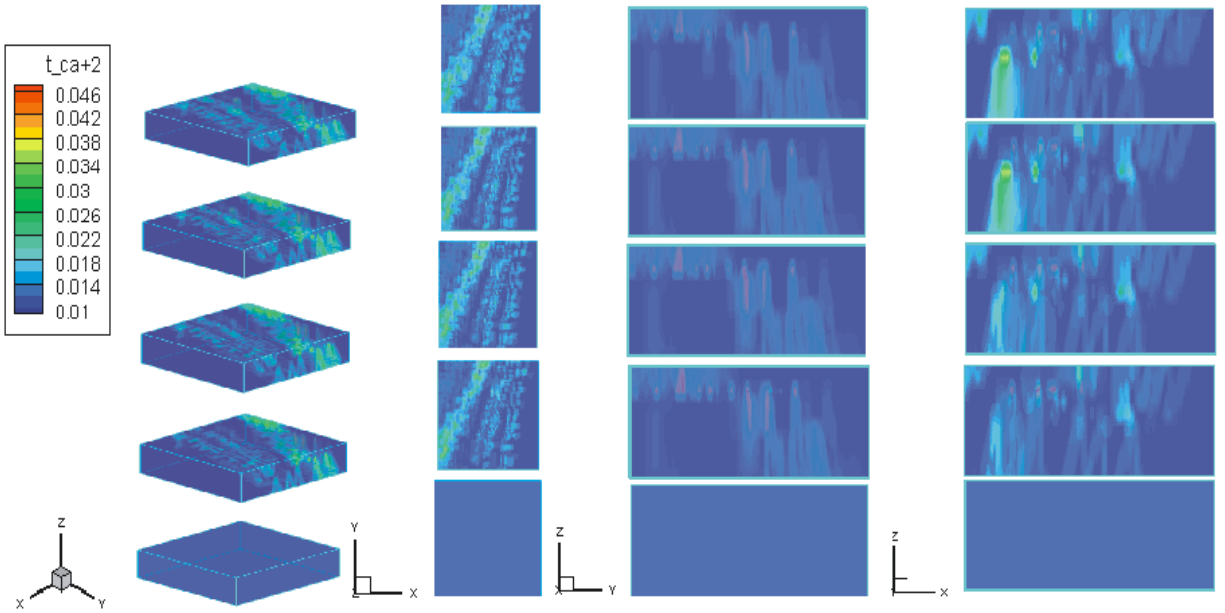


Hydrogeological parameters for the model.

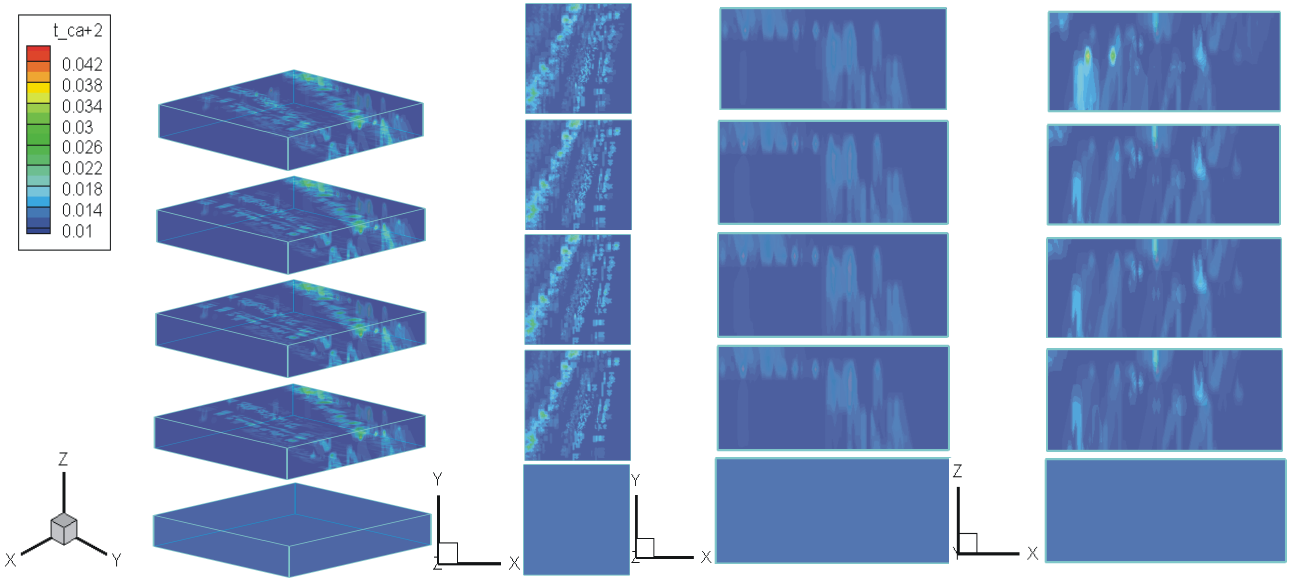
Layer name	Thickness (m)	Porosity (%)	Permeability (mD)
Zone 2 upper	5.5	22.5	2.92
Zone 2 middle	5.5	22.5	10.44
Zone 2 lower	1.0	22.5	1.486
Zone 3 upper	10.0	20.4	0.33
Zone 3 lower	10.0	20.4	0.33
Zones 4 and 5	25.0	23.4	0.46

Mid-term behavior prediction

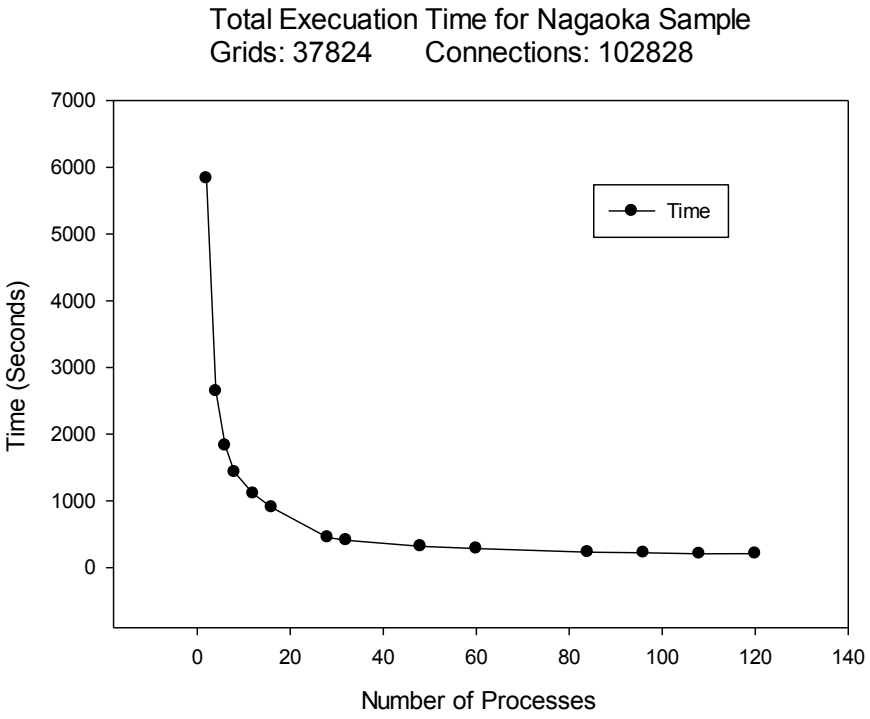
Serial computing

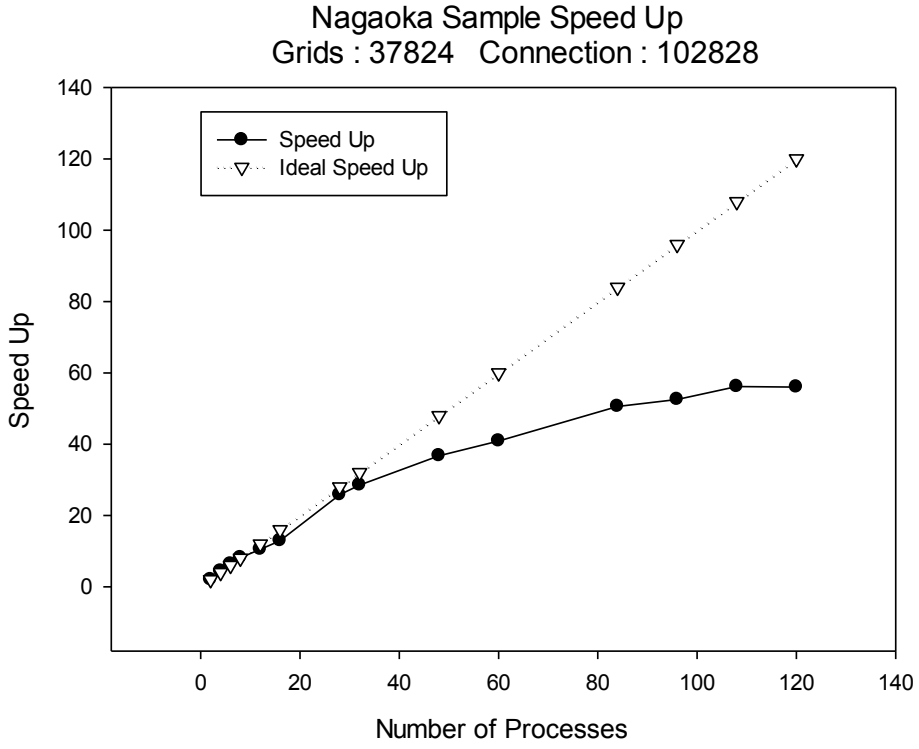


Parallel Computing



Runtime Statistics





What we've gained from work

- A new software package running on parallel computing facility (Cluster …)
- Speed up (20 X – 40 X in test case)
- Simulation model scaling up (100,000 grids have been tested)

Thanks for your attention !