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Discussions

Interactive comment on "A parallelization scheme to simulate reactive transport in the subsurface environment with OGS#IPhreeqc" *by* W. He et al.

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This paper describes a coupling between OGS software and iPHREEQC software, for reactive transport numerical modeling. OGS deals with flow, transport and heat transfer, whereas PHREEQC deals with geochemistry. The coupling is of type SNIA. Does it mean that the time discretization scheme is explicit ? Is there any condition on the timestep such as a CFL condition ? The flow and transport models can be nonlinear. How is the nonlinearity handled in OGS ? Flow and transport and heat transfer can be coupled. How is the coupling handled in OGS ?

The coupling between OGS and PHREEQC is done with files. This is probably very costly. What is the computational overhead ? Would it be possible to develop a more efficient interface between the two software ?

Parallelism is defined with Domain Decomposition in OGS. What does DDC mean ?

As many cores as domains are used in OGS. How is decomposition done ? Does it use METIS for example ? How are communications between subdomains defined ?

Geochemistry is trivially parallel, since computations in spatial elements are independent. New cores can be added for these computations, but these cores remain idle when OGS computations are done. Is this efficient ? Communications seem to be done with files. Is this efficient ? Also, it seems that global communications occur quite often. Is this scalable ?

Numerical examples are simple. In fact, 2D and 3D examples remain 1D, since the results do not depend on the (y,z) coordinates. Could real 2D or 3D examples be presented ?

In the examples, geochemistry represents most of the CPU time, so that parallelism is globally efficient. What happens if time of OGS computations becomes higher ?

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