A Test Bed for Modelling the Liberation of Silica from Feldspar Using Parallel Computing Techniques

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Outline

- Introduce the problem
- Describe a sequential algorithm
- Parallel approaches
- Results
- A parallel workbench
- Conclusions
- Future work

Experimental data

ref. R. Wollast, “Kinetics of the alteration of K-feldspar in buffered solutions at low temperature”, Geochimica Acta, 1967

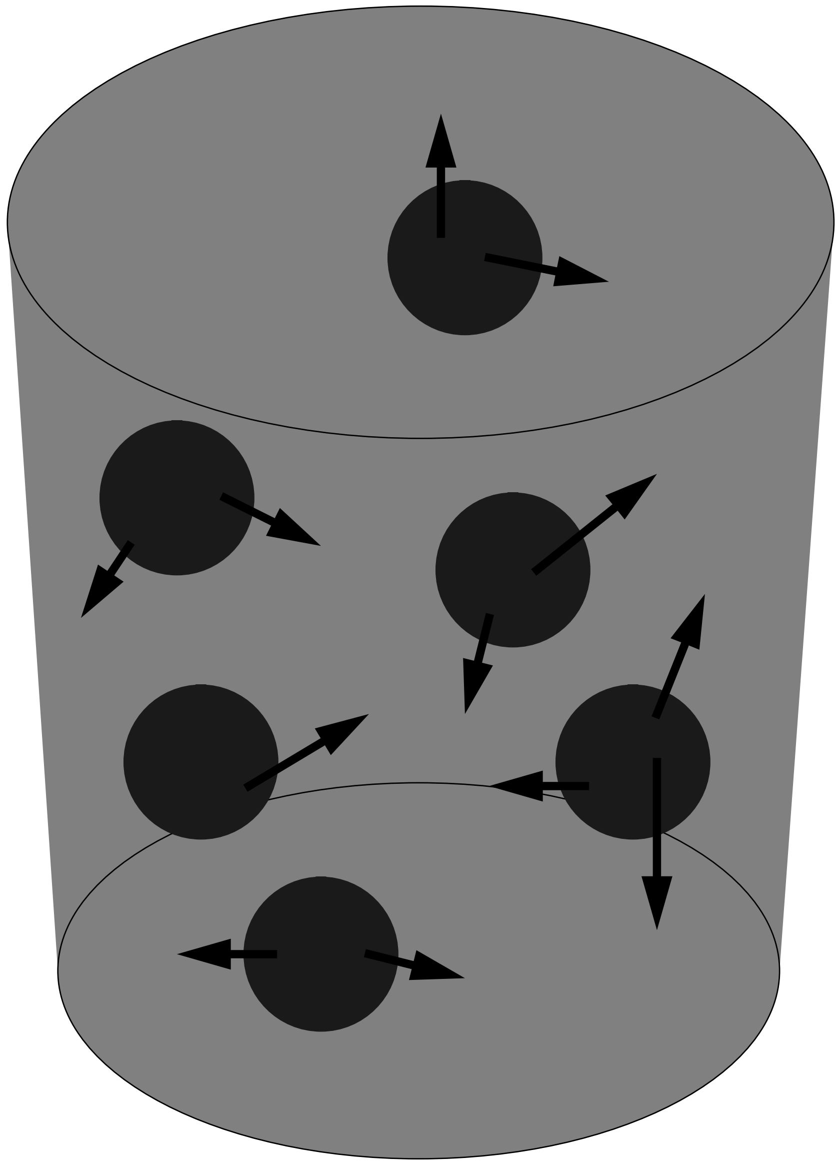
The high power offered by clustered computing allows

a large quantity of events to be simulated

and

avoids the need to set up analytic expressions

Feldspar Particles



Sequential Approach

1. Initialise 0 particles released at time 0
2. Calculate time from now to release of next particle, as:

    random number * factor related to pH * cubed particles already released

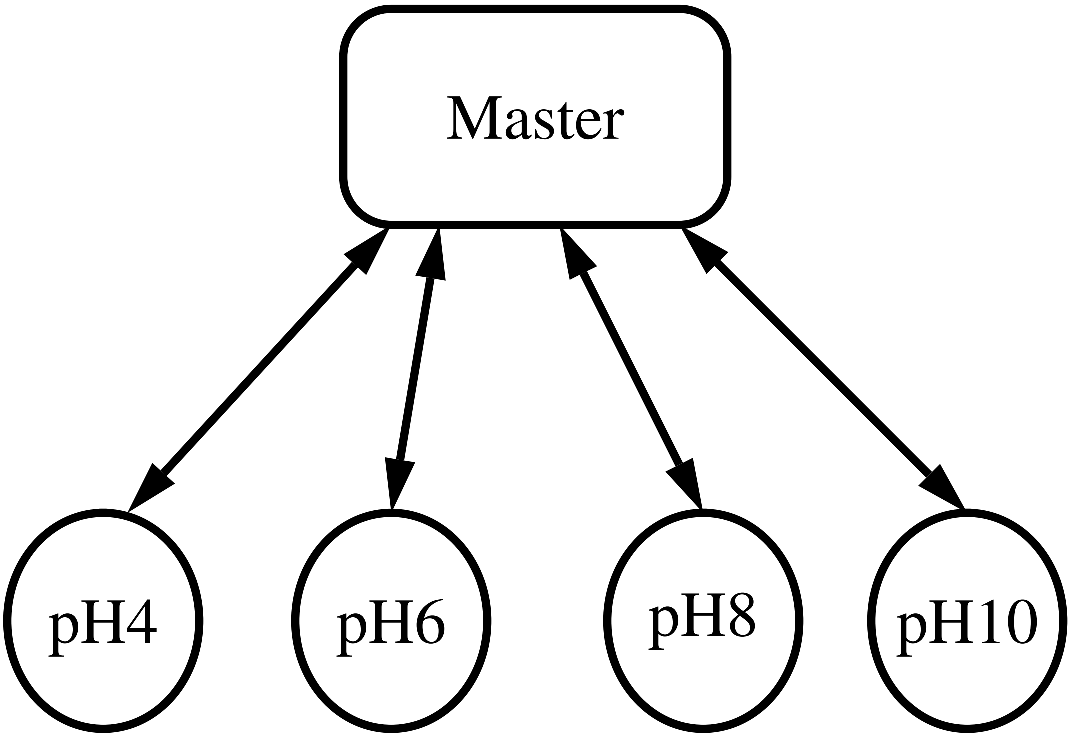
3. Repeat 2. until sufficient particles released.

Repeat for different sets of random numbers[1].

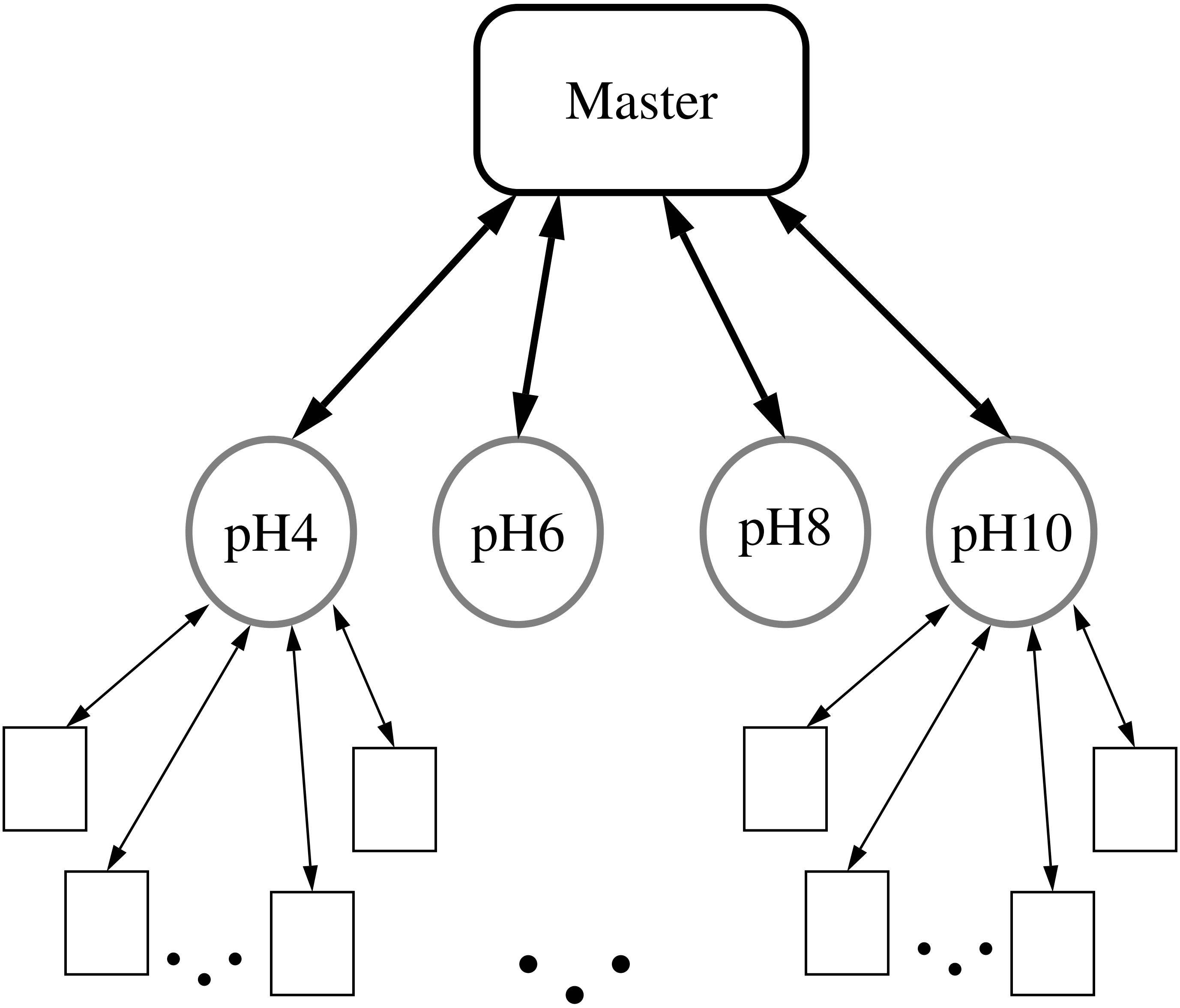
Repeat for each required pH value.

1. to ensure correct behaviour.

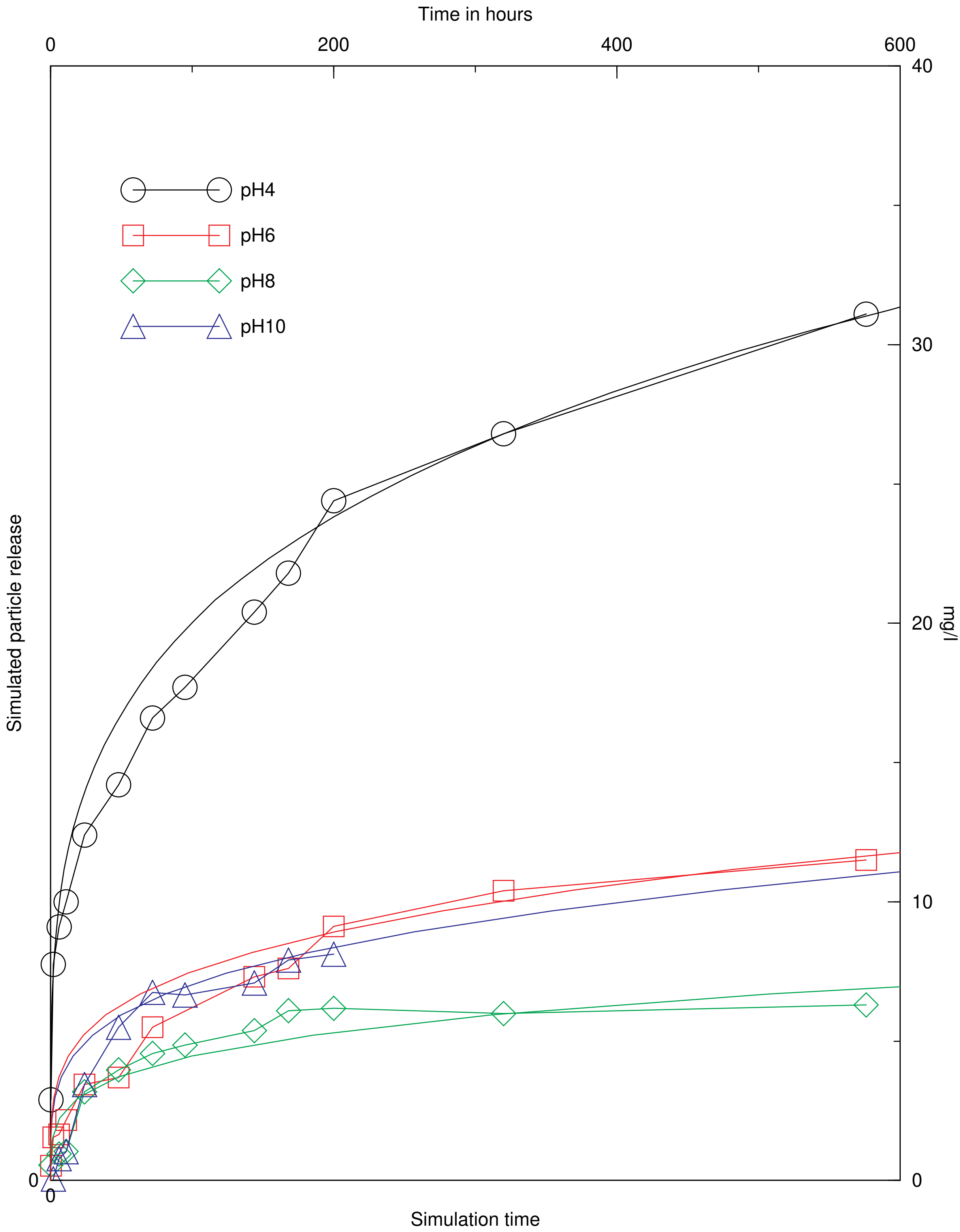
Parallel Approach



Improved Parallel Approach



Results

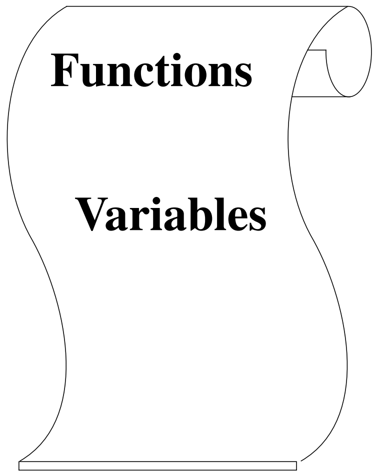

Time in hours
0
200
400
600
40
30
20
10
0
pH4
pH6
pH8
pH10
Simulated particle release
mg/l
0
0
Simulation time

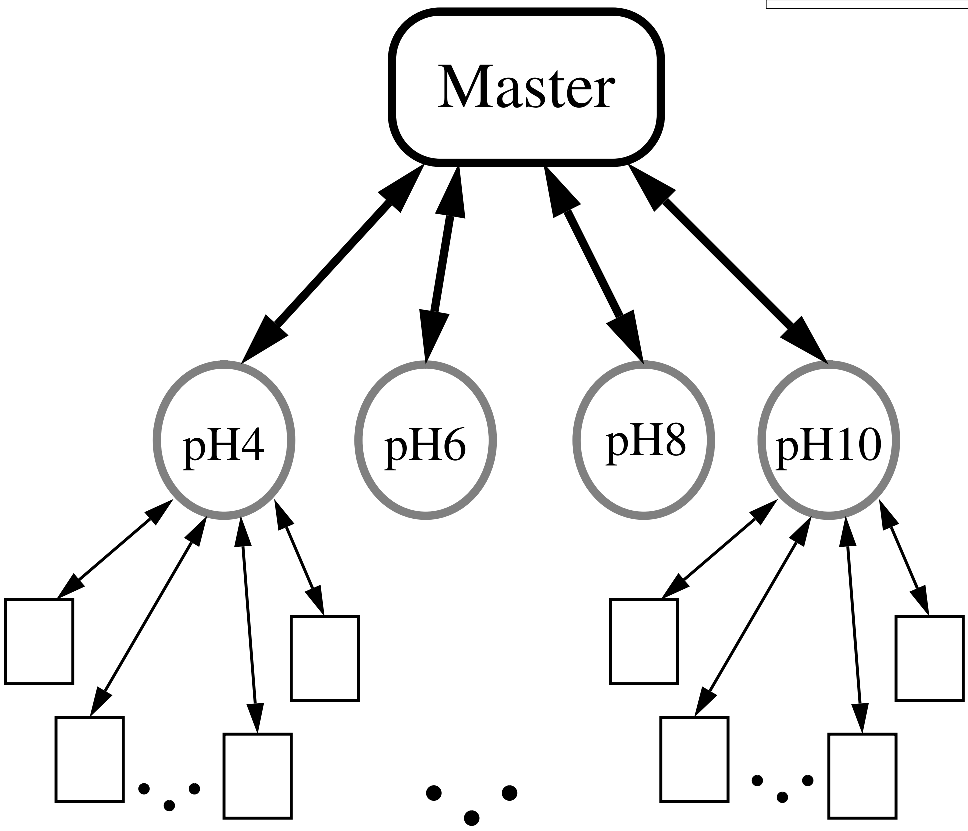
Shortcomings in the results

Not a perfect match, other factors need to be taken in to account:

- Temperature
- Granularity of feldspar
- Amount in solution
- Effect of residual layer

A Parallel Workbench





Conclusions

The use of PVM on a cluster of workstations has enabled us to develop a test bed for the simulation of the actions of particles.

We can:

- easily adjust variables and functions used
- recompile and execute
- compare our simulated results with experimental data.

Future

We intend to apply our approach to other chemical systems and extend it to more complex systems, such as the liberation of silica in sea water.