A `barite`-based benchmark for FGCS interpolation paper

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1 Description

- `barite_fgcs_2.R`: POET input script with circular "crystals" on a 200x200 nodes grid
- α: isotropic 10^{-5} m^2/s outside of the crystals, 10^{-7} inside
- 200 iterations, dt = 1000
- `barite_fgcs_2.pqi`: PHREEQC input, 4 SOLUTIONS (basically the same as in `barite` benchmark):
  1. Equilibrium with Celestite, no mineral $Rightarrow$
  2. Equilibrium with Celestite, KINETICS Celestite (1 mol) and Barite (0 mol)
  3. Injection of 0.1 BaCl2 from NW corner
  4. Injection of 0.2 BaCl2 from SE corner
- `db_barite.dat`: PHREEQC database containing the kinetic expressions for barite and celestite, stripped down from `phreeqc.dat`

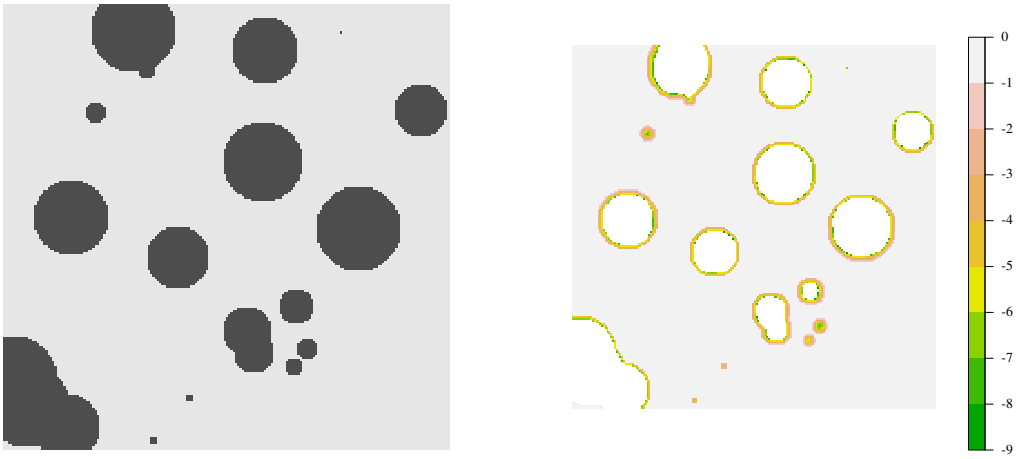

Figure 1: **Left:** Initial distribution of Celestite "crystals". **Right:** precipitated Barite

2 Interpolation

Using the following parametrization:

```
dht_species <- c("H"          = 7,
                 "O"          = 7,
                 "Ba"         = 7,
                 "Cl"         = 7,
                 "S(6)"       = 7,
                 "Sr"         = 7,
                 "Barite"     = 4,
                 "Celestite"  = 4)

pht_species <- c("Ba"         = 4,
                 "Cl"         = 3,
                 "S(6)"       = 3,
                 "Sr"         = 3,
                 "Barite"     = 2,
                 "Celestite"  = 2 )
```

Runtime goes from 1800 to 600 s (21 CPUs) but there are "suspect" errors especially in O and H, where "suspect" means some values appear to be multiplied by 2:

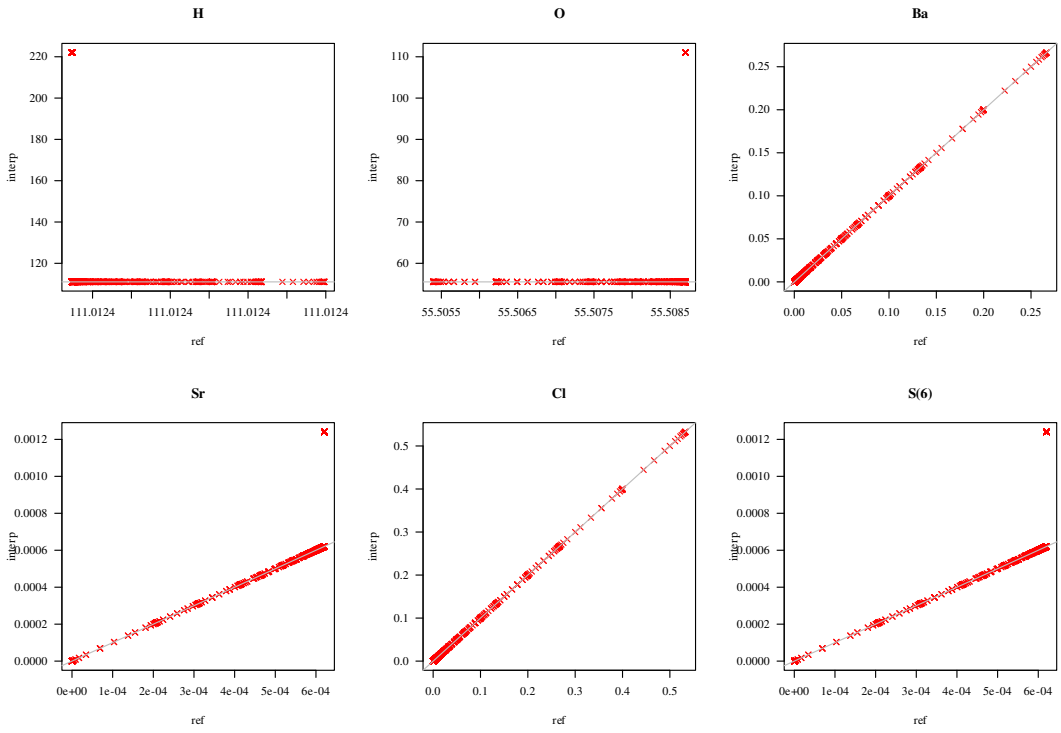

Figure 2: Scatterplots reference vs interpolated after 1 coupling iteration