PFLOTRAN

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PFLOTRAN: Recent Developments Facilitating Massively-Parallel Reactive Biogeochemical Transport

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What is PFLOTRAN?

PFLOTRAN is an open source and freely-accessible code for massively-parallel subsurface simulation. The code is written in Fortran 2003/2008 and founded upon parallel MPI-based PETSc data structures and solvers with HDF5 I/O.

PFLOTRAN Subsurface Process Models:

- Multiphase Flow
- Thermal Convection/Conduction
- Geomechanics
- Hydrogeophysics
  - Coupled to E4D (Johnson et al., 2010)
- Multicomponent Solute Transport
- Biogeochemical Reaction
  - Aqueous speciation
  - Mineral precipitation-dissolution
  - Sorption (surface complexation, ion exchange, isotherm-based)
  - Radioactive decay and ingrowth
  - Microbially-mediated (Monod-based with inhibition)
  - Custom user-defined kinetics:

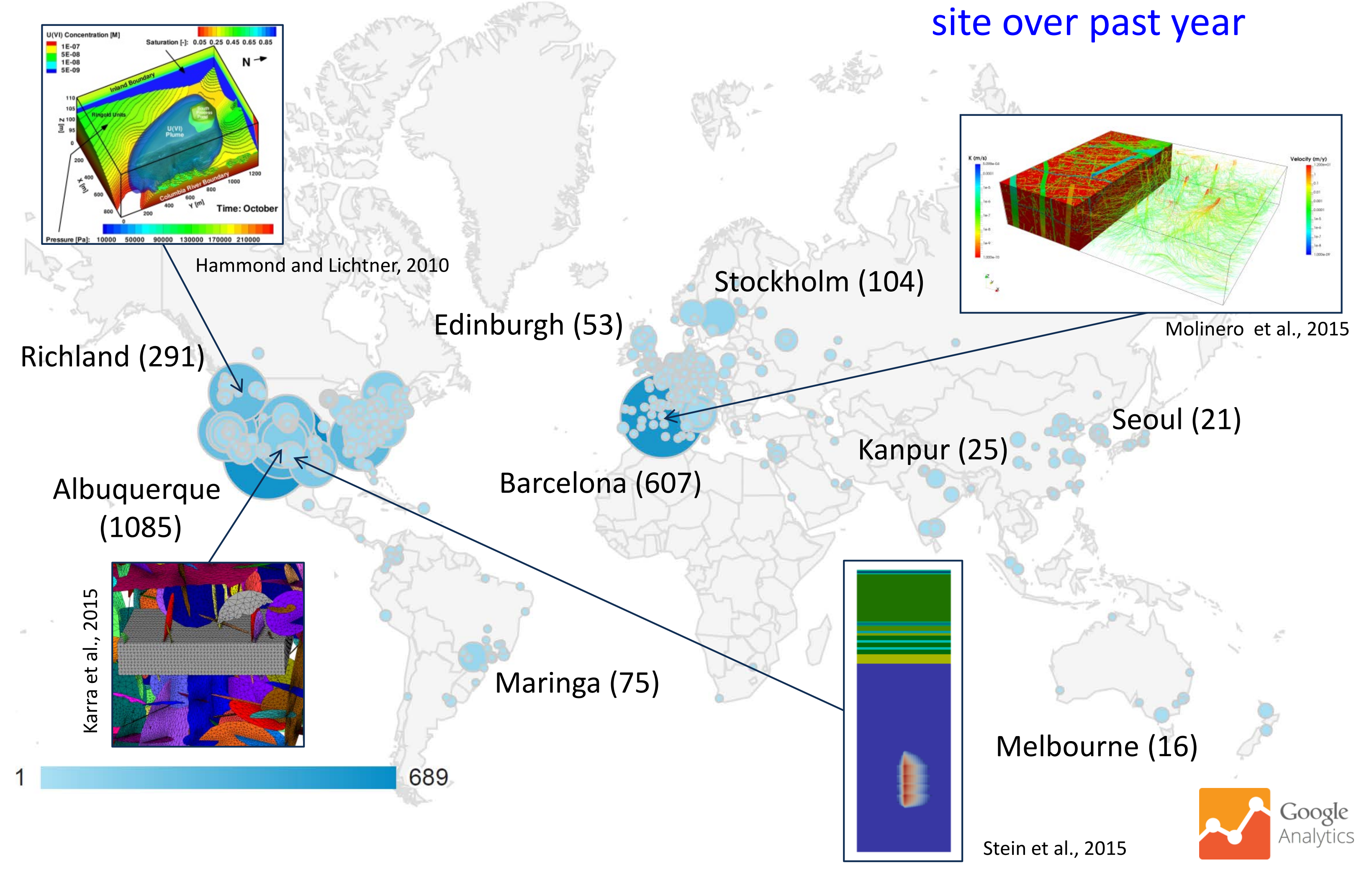
Reaction Sandbox

PFLOTRAN Support Infrastructure

PFLOTRAN website: www.pflotran.org
Distributed source code revision control: Mercurial
Public code repository: Bitbucket (www.bitbucket.org/pflotran/pflotran-dev)
User support: pflotran-users@googlegroups.com, pflotran-dev@googlegroups.com
Automated building and testing: Buildbot (pflotran.lbl.gov/pbbot/waterfall)

Who is using PFLOTRAN?

Hits on PFLOTRAN Bitbucket site over past year



What is the PFLOTRAN Reaction Sandbox?

Many PFLOTRAN users have asked for a means of implementing custom kinetic rate expressions for chemistry. The reaction sandbox fulfills this purpose by isolating PFLOTRAN's chemistry and providing a simplified reaction framework within which the researcher may quickly implement a kinetic reaction without completely learning/understanding PFLOTRAN's reaction process model. The reaction sandbox also serves as a tool for testing kinetic reactions prior to acceptance and integration within the code.

How do I use the Reaction Sandbox?

Copy and rename the source file reaction_sandbox_example.F90 and follow the enumerated instructions in the comments within. In short, one must:

- Rename the module, reaction class, and module procedures.
- Add variables to the reaction class as needed.
- Populate module procedures with code that creates, reads, initializes, evaluates, and destroys the reaction class. Note that only the procedures that create and evaluate the reaction are required, and these can be hardwired (e.g. see the Simple Reaction Sandbox to right).
- Add the new reaction class to the reaction sandbox's linked list.

Reaction Sandbox Class (to be modified by the user)

```
type, public, extends(reaction_sandbox_base_type) :: &
                                        reaction_sandbox_xxx_type
  ! Add class parameters here
  class(reaction_sandbox_base_type), pointer :: next
contains
  ! Map procedures here
  procedure, public :: ReadInput => XXXRead
  procedure, public :: Setup => XXXSetup
  procedure, public :: Evaluate => XXXReact
  procedure, public :: Destroy => XXXDestroy
end type reaction_sandbox_base_type
```

Reaction Sandbox Linked List (not modified by the user)

```
cur_reaction => rxn_sandbox_list
do
  if (.not.associated(cur_reaction)) exit
  call cur_reaction%Evaluate(Residual,Jacobian,state_variables)
  cur_reaction => cur_reaction%next
enddo
```

Want to try a Simple Reaction Sandbox?

1. Clone the PFLOTRAN code repository from Bitbucket.
2. Create a new reaction network within subroutine SimpleReact() in $PFLOTRAN_DIR/src/pflotran/reaction_sandbox_simple.F90.

Available Species:

Aqueous : `Aaq, Baq, Caq, Daq, Eaq, Faq`
Immobile: `Xim Yim`

Example Rate Expressions:

Rate = k [mol/L-sec] * L_water	! 0th Order
Rate = k [1/sec] * Aaq * L_water	! 1st Order
Rate = k [L/mol-sec] * Aaq * Baq * L_water	! 2nd Order
Rate = k [mol/L-sec] * Aaq/(K_Aaq + Aaq) * L_water	
Rate = k [mol-m^3 bulk/L-mol_biomass-sec] * Xim * L_water * Aaq/(K_Aaq + Aaq) * Baq/(K_Baq + Baq)	
Rate = (k [1/sec] * Aaq – kr [1/sec] * Caq) * L_water	

Assumed Units: Aqueous species [mol/L], Immobile species [mol/m^3 bulk volume], Rate constant k [reaction-dependent], Rate [mol/sec], K_Xxx [mol/L], L_water [L]

3. Run a 1D column experiment: $PFLOTRAN_DIR/example_problems/reaction_sandbox_simple/pflotran.in
   a. Set concentrations within the *Initial* and *Inlet* constraints.
   b. Run PFLOTRAN: $PFLOTRAN_DIR/src/pflotran/pflotran
   c. Plot the results in Excel or matplotlib (reaction_sandbox_simple.py).

References

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