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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 and 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:

PFLOTRAN Support Infrastructure

PFLOTRAN website: www.pflotran.org

Distributed source code revision control: Mercurial

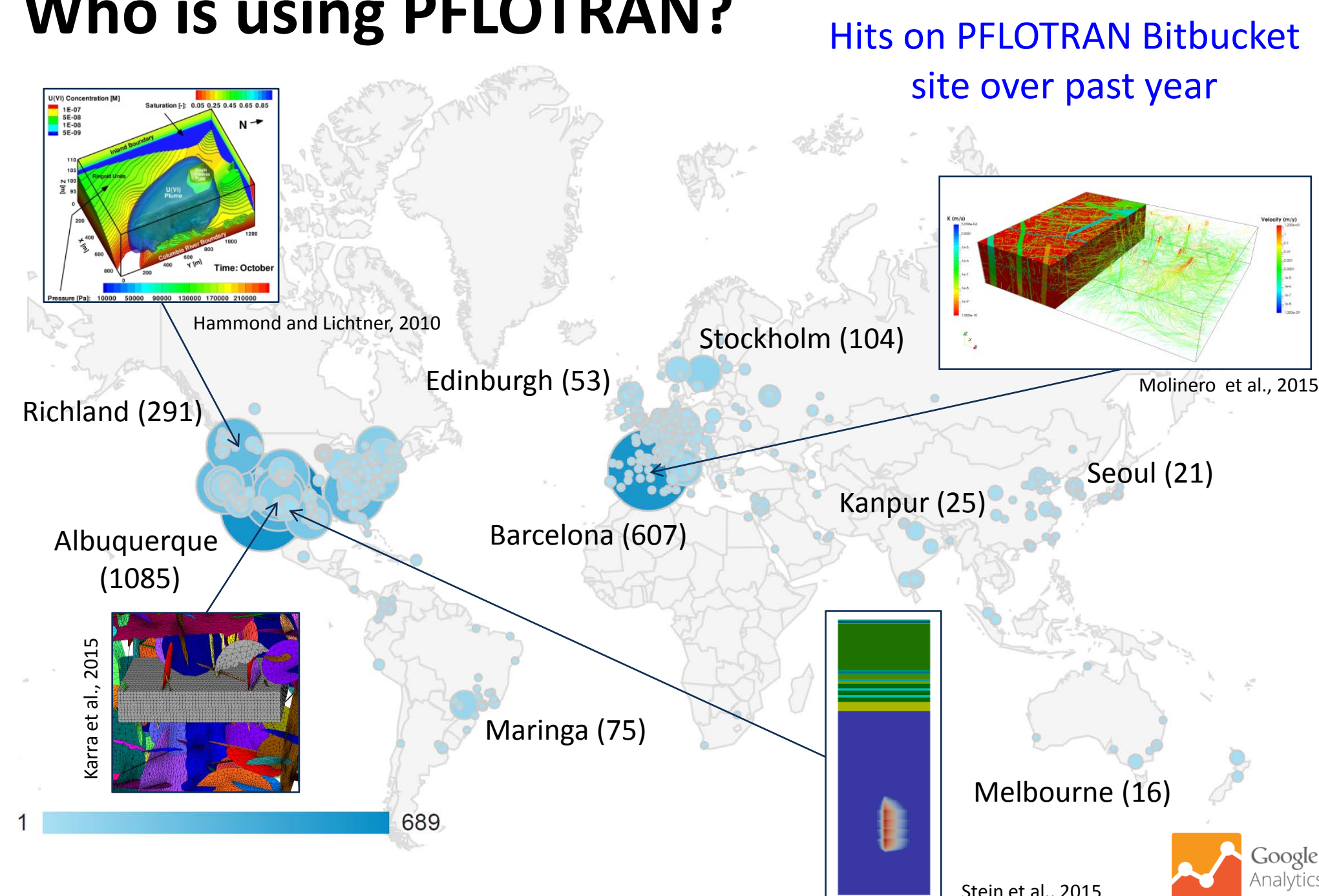
Public code repository: Bitbucket (www.bitbucket.org/pflotran/pflotran-dev)

User support: pflotran-users@googlegroups.com, pflotran-dev@googlegroups.com

Automated building and testing: Buildbot (pflotran.lbl.gov/pbbot/waterfall)

Reaction Sandbox

Who is using PFLOTRAN?



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

Potential 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/mol_biomass-sec] * Xim * volume *
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/m³ bulk volume], Rate constant k [reaction-dependent], Rate [mol/sec], K_Xxx [mol/L], L_water [L], volume [m³]

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

References

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