Running PFLOTRAN

This problem takes a while to run, so let's get it started first.
Homogeneous permeability field version:

```
> cd $PFLOTRAN_DIR
> cd shortcourse/exercises/regional_doublet/
> pflotran -input_prefix regional_doublet
```

Running PFLOTRAN

This problem takes a while to run, so let's get it started first.
Stochastic permeability field version:

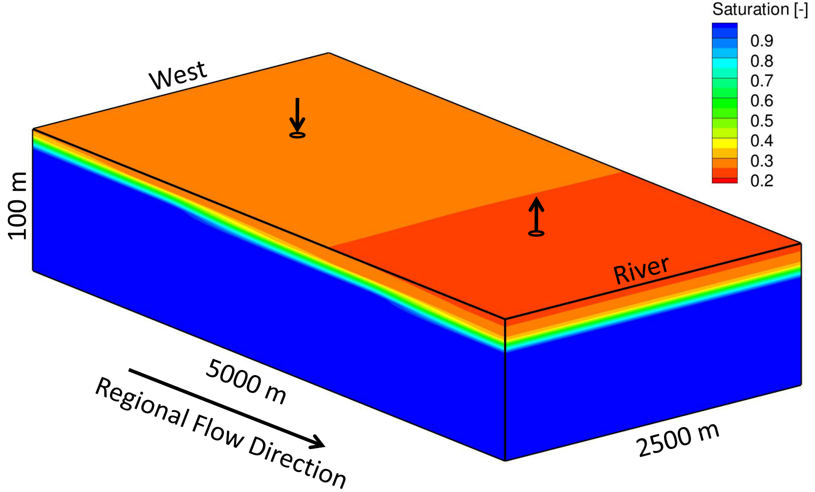
```
> cd $PFLOTRAN_DIR
> cd shortcourse/exercises/regional_doublet/
> pflotran -input_prefix stochastic_regional_doublet
 -realization_id 5
```

Description of 3D Regional Flow and Transport Scenario

The "3D Regional Flow and Transport Scenario" simulates groundwater flow and solute transport within a large kilometer-scale domain:

- Problem domain: $5000 \times 2500 \times 100$ m^3 ($x \times y \times z$)
- Grid resolution $50 \times 49.02 \times 5$ m^3 ($100\times$ $51 \times$ 20 cells)
- Maximum time step size: 0.1 y (for CFL $<=$ 1)
- Total simulation time: 10 y

3D Regional Flow and Transport Scenario Schematic



Governing Flow Equations

Continuity Equation:

$$\frac{\partial}{\partial t}\left(\varphi s \rho\right) + \boldsymbol{\nabla} \cdot \rho \mathbf{q} \;=\; Q$$

Darcy's Law:

$$\mathbf{q} \;=\; -\frac{\mathbf{k} k_r}{\mu} \boldsymbol{\nabla}\left(P - \rho g z\right)$$

- φ = porosity
- s = saturation
- ρ = liquid density
- $\mathbf{k}$ = intrinsic permeability tensor
- k_r = relative permeability
- μ = viscosity
- P = liquid pressure
- g = gravity
- z = distance in direction of gravity
- Q = source/sink

Constitutive Relations

- Capillary Pressure Relations
  - van Genuchten
    - Effective Saturation:

$$s_e = \left[1 + (\alpha |P_c|)^n\right]^{-m}$$

    - Saturation:

$$s = s_e(1 - s_r) + s_r$$

    - Relative Permeability (Mualem)

$$k_r = \sqrt{s_e}\left\{1 - \left[1 - s_e^{1/m}\right]^m\right\}^2$$

- s = saturation
- s_e = effective saturation
- s_r = residual saturation
- P_c = capillary pressure = $P_{\mathrm{atm}} - P$
- α = inverse of air entry pressure [Pa^{-1}]
- n = van Genuchten n
- m = $1 - 1/n$

Constitutive Relations [Cont.]

- Brooks-Corey
  - Effective Saturation:

$$s_e = (\alpha |P_c|)^{-\lambda}$$

  - Saturation:

$$s = s_e(1 - s_r) + s_r$$

  - Relative permeability (Burdine)

$$\begin{aligned} k_r &= (s_e)^{(2+3\lambda)/\lambda} \\ &= (\alpha |P_c|)^{-(2+3\lambda)} \end{aligned}$$

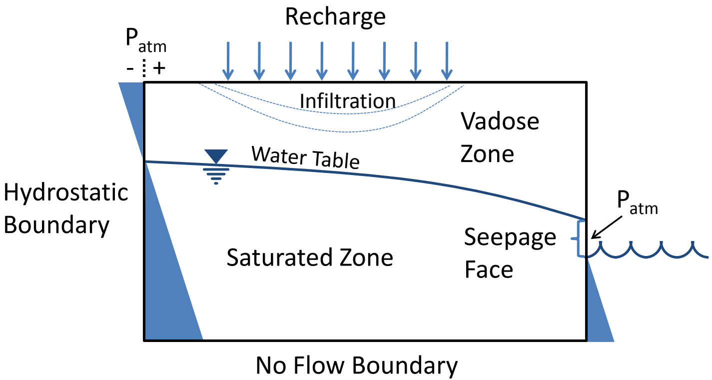
- α = inverse of air entry pressure [Pa^{-1}]
- λ = Brooks Corey function parameter λ

Flow Boundary Conditions

- Dirichlet (e.g. specified pressure)
- Neumann (e.g. specified flux)

- No Flow
- Recharge
- Hydrostatic
- Seepage Face

Flow Boundary Conditions Schematic



Flow Boundary Conditions

$$\mathbf{q} \; = \; -\frac{kk_r}{\mu}\left(\frac{P_{\text{cell}} - P_{\text{boundary}} - \rho g \mathbf{z}}{\Delta l}\right)$$

- $\mathbf{q}$ units: $\left[\frac{l^3_{\text{water}}}{l^2_{\text{bulk}} \cdot t}\right]$ where $l \; = \;$ length and $t \; = \;$ time

- No flow (Neumann) : $\mathbf{q} = 0$ or even better, no flux calculation at all
- Recharge (Neumann) : $\mathbf{q} = \mathbf{q}_0$
- Hydrostatic (Dirichlet): $P_{\text{boundary}} \; = \; f\left(P_{\text{datum}}, x, y, z, \rho\left(P, T\right)\right)$
- Seepage Face (Dirichlet) : $P_{\text{boundary}} \; = \; max\left(\text{Hydrostatic}, P_{\text{atm}}\right)$

Richards Equation - Averaging Schemes

$$\mathbf{q} = -\frac{\mathbf{k} k_r}{\mu} \boldsymbol{\nabla} \left(P - \rho g z \right)$$

- $\mathbf{k}$: inverse distance-weighted harmonic
- k_r: upwind
- μ: upwind
- ρ: arithmetic

Governing Transport Equations

$$\frac{\partial}{\partial t}\left(\varphi s \Psi_j\right) + \boldsymbol{\nabla}\cdot\boldsymbol{\Omega}_j \;=\; S_j$$

$$\boldsymbol{\Omega}_j \;=\; \left(\mathbf{q} - \varphi s \mathbf{D}\boldsymbol{\nabla}\right)\Psi_j$$

$$\begin{aligned}
\varphi &= \text{porosity;} \quad s \;=\; \text{liquid saturation}\\
\Psi_j &= \text{solute concentration for aqueous species } j\\
S_j &= \text{source/sink term for aqueous species } j\\
\boldsymbol{\Omega} &= \text{solute flux;} \quad \mathbf{q} \;=\; \text{Darcy velocity}\\
\mathbf{D} &= \text{hydrodynamic dispersion} \;=\; \mathcal{D}^* + \alpha_L|\boldsymbol{\nu}|\\
\mathcal{D}^* &= \text{species independent coefficient of diffusion}\\
\alpha_L &= \text{longitudinal dispersity}\\
\boldsymbol{\nu} &= \text{pore water velocity} \;=\; \mathbf{q}/\varphi
\end{aligned}$$

Transport Boundary Conditions

- Dirichlet (e.g. specified concentration)
- Neumann (e.g. specified mass flux)
- Zero Gradient (e.g. outflow boundary)

Transport - Averaging Schemes

$$\boldsymbol{\Omega}_j = \left(\mathbf{q} - \varphi s \mathbf{D} \boldsymbol{\nabla}\right) \Psi_j$$

- s: arithmetic
- φ: arithmetic

SIMULATION

Location of this example problem:

`$PFLOTRAN_DIR/shortcourse/exercises/regional_doublet`

```
regional_doublet.in
river_stage.txt
```

SIMULATION

- Single-phase variably saturated flow
- Conservative solute transport

```
SIMULATION
  SIMULATION_TYPE SUBSURFACE
  PROCESS_MODELS
    SUBSURFACE_FLOW flow
      MODE RICHARDS
    /
    SUBSURFACE_TRANSPORT transport
      MODE GIRT
    /
  /
END

SUBSURFACE
  ...
END_SUBSURFACE
```

GRID

- Problem domain: $5000 \times 2500 \times 100$ m ($x \times y \times z$)
- Grid resolution $50 \times 49.02 \times 5$ m

```
GRID
  TYPE structured
  NXYZ 100 51 20
  BOUNDS
    0.d0 0.d0 0.d0
    5000.d0 2500.d0 100.d0
  /
END
```

REGION I

- Delineate regions in the 3D domain for:
  - entire domain
  - west boundary face
  - east boundary face
  - top boundary face
  - well screens

```
REGION all
  COORDINATES
    0.d0     0.d0     0.d0
    5000.d0 2500.d0 100.d0
  /
END
```

REGION II

```
REGION layer2          ! layer of domain
  COORDINATES
    0.d0    0.d0    30.d0
    5000.d0 2500.d0 50.d0
  /
END

REGION Top             ! top surface
  COORDINATES
    0.d0    0.d0    100.d0
    5000.d0 2500.d0 100.d0
  /
  FACE TOP
END
```

REGION III

```
REGION Extraction_well
  COORDINATES                 ! vertical line
    3750.d0 1250.d0 20.d0
    3750.d0 1250.d0 55.d0
  /
END

REGION Obs_pt_center          ! point
  COORDINATE 2500.d0 1250.d0 60.d0
END
```

MATERIAL_PROPERTY

- Anisotropic permeability

```
MATERIAL_PROPERTY soil3
  ID 3
  POROSITY 0.25d0
  TORTUOSITY 0.5d0
  CHARACTERISTIC_CURVES cc1
  PERMEABILITY          ! diagonal permeability tensor
    PERM_X 5.d-11       !   x component
    PERM_Y 5.d-11       !   y component
    PERM_Z 5.d-12       !   z component
  /
END
```

CHARACTERISTIC_CURVES

- van Genuchten saturation function
- Mualem relative permeability

```
CHARACTERISTIC_CURVES cc1
  SATURATION_FUNCTION VAN_GENUCHTEN
    ALPHA  1.d-4
    M 0.5d0
    LIQUID_RESIDUAL_SATURATION 0.1d0
    MAX_CAPILLARY_PRESSURE 1.d8
  /
  PERMEABILITY_FUNCTION MUALEM_VG_LIQ
    M 0.5d0
    LIQUID_RESIDUAL_SATURATION 0.1d0
  /
END
```

FLUID_PROPERTY

- Assign a molecular diffusion coefficient of 10^{-9} m^2/s to all aqueous species

```
FLUID_PROPERTY
  DIFFUSION_COEFFICIENT 1.d-9    ! [m^2/s]
END
```

CHEMISTRY I

- Two tracers
- Database is not needed!

```
CHEMISTRY
  PRIMARY_SPECIES
    Tracer
    Tracer2
  /
END
```

FLOW_CONDITION I

```
FLOW_CONDITION initial
  TYPE
    PRESSURE HYDROSTATIC  ! hydrostatic condition
  /
  DATUM 0.d0 0.d0 90.d0   ! point in space
  GRADIENT
    PRESSURE -0.002 0. 0. ! gradient for pressure [m/m]
  /                       !   unless dz specified [Pa/m]
  PRESSURE 101325.d0      ! pressure at datum
END
```

FLOW_CONDITION II

```
FLOW_CONDITION river
  TYPE
    PRESSURE SEEPAGE     ! seepage face condition
  /
  INTERPOLATION LINEAR   ! dataset time interpolation
  CYCLIC                 ! cycle dataset
  DATUM FILE river_stage.txt  ! read transient datum
  PRESSURE 101325.d0          !    dataset from file
END
```

FLOW_CONDITION III

```
! Contents of river_stage.txt:
!   Note: assumes SI units

: time x y z
0.d0 5000.d0 0.d0 80.d0             ! 0 yr
7884000.d0 5000.d0 0.d0 77.d0       ! 0.25 yr
15768000.d0 5000.d0 0.d0 79.d0      ! 0.5 yr
23652000.d0 5000.d0 0.d0 79.d0      ! 0.75 yr
31536000.d0 5000.d0 0.d0 80.d0      ! 1 yr
```

FLOW_CONDITION IV

```
FLOW_CONDITION recharge
  TYPE
    FLUX NEUMANN
  /
  FLUX LIST
    TIME_UNITS yr
    DATA_UNITS cm/yr
    0.d0 25.d0
    1.d0 23.d0
    ...
    4.d0 24.d0
    5.d0 29.d0
  /
END
```

FLOW_CONDITION V

```
FLOW_CONDITION injection
  TYPE                              ! volumetric flow
    RATE SCALED_VOLUMETRIC_RATE     !   rate scaled by
  /                                 !   f(permeability)
  RATE 1.d5 m^3/day  ! flow rate 100,000 [m^3/day]
END

FLOW_CONDITION extraction
  TYPE
    RATE SCALED_VOLUMETRIC_RATE
  /
  RATE -1.d5 m^3/day  ! flow rate -100,000 [m^3/day]
END                   ! negative rate = extraction
```

TRANSPORT_CONDITION / CONSTRAINT I

- Set up three transport conditions and constraints for tracers
- Constraints embedded within transport conditions
  - Embedded constraints may not be transient

TRANSPORT_CONDITION / CONSTRAINT II

```
TRANSPORT_CONDITION initial       ! previous approach
  TYPE DIRICHLET_ZERO_GRADIENT
  CONSTRAINT_LIST          ! list of constraints
    0.d0 initial
  /
END

TRANSPORT_CONDITION initial       ! embedded approach
  TYPE DIRICHLET_ZERO_GRADIENT
  CONSTRAINT initial
    CONCENTRATIONS         ! single constraint @ time 0.
      Tracer  1.d-10 T     ! background concentration set
      Tracer2 1.d-10 T     !   to a small value, not zero
    /
  /
END
```

TRANSPORT_CONDITION / CONSTRAINT III

```
TRANSPORT_CONDITION west
  TYPE DIRICHLET_ZERO_GRADIENT
  CONSTRAINT west
    CONCENTRATIONS
      Tracer  1.d-10 T
      Tracer2 1.d0   T
    /
  /
END

TRANSPORT_CONDITION injection
  TYPE DIRICHLET_ZERO_GRADIENT
  CONSTRAINT injection
    CONCENTRATIONS
      Tracer  1.d0   T
      Tracer2 1.d-10 T
    /
  /
END
```

STRATA

- Couple material types with regions

```
STRATA
  REGION layer1
  MATERIAL soil1
END

STRATA
  REGION layer2
  MATERIAL soil2
END

...

STRATA
  REGION layer4
  MATERIAL soil4
END
```

OBSERVATION

- Couple observation points with regions in model

```
OBSERVATION  ! observation point assigned region name
  REGION Obs_pt_center   ! region name
  AT_CELL_CENTER         ! do not interpolate
  VELOCITY               ! include velocity
END

OBSERVATION
  REGION Obs_pt_west
  AT_CELL_CENTER
  VELOCITY
END

...
```

NEWTON_SOLVER

- Set converged if maximum pressure change within all cells is less than 1 Pa.

```
NEWTON_SOLVER FLOW
  ITOL_UPDATE 1.d0    ! infinity norm of update vector
END
```

INITIAL_CONDITION

- Couple the initial flow and transport conditions with region all for the initial condition

```
INITIAL_CONDITION
  FLOW_CONDITION initial
  TRANSPORT_CONDITION initial
  REGION all
END
```

BOUNDARY_CONDITION I

```
BOUNDARY_CONDITION west
  FLOW_CONDITION initial
  TRANSPORT_CONDITION west
  REGION west
END

BOUNDARY_CONDITION east
  FLOW_CONDITION river
  TRANSPORT_CONDITION initial
  REGION east
END

BOUNDARY_CONDITION top
  FLOW_CONDITION recharge
  TRANSPORT_CONDITION initial
  REGION top
END
```

SOURCE_SINK I

```
SOURCE_SINK injection_well   ! source/sink name (optional)
  FLOW_CONDITION injection       ! flow condition name
  TRANSPORT_CONDITION injection  ! tran. condition name
  REGION injection_well         ! location of source/sink
END

SOURCE_SINK extraction_well
  FLOW_CONDITION extraction
  TRANSPORT_CONDITION initial
  REGION extraction_well
END
```

TIME

- Set final simulation time to 10 years
- Set initial time step size to 1.e-2 days
- Set maximum time step size to 0.1 years

```
TIME
  FINAL_TIME 10.d0 y
  INITIAL_TIMESTEP_SIZE 1.d-2 d
  MAXIMUM_TIMESTEP_SIZE 0.1 y    ! ensures CFL ~<= 1.
END
```

OUTPUT

- Print entire solution (a snapshot) in ASCII Tecplot block formatted datapacking and binary PFLOTRAN HDF5 format compatible with ParaView and VisIt
- Specifically, we want to see the liquid pressure, saturation, material IDs, and liquid phase velocities
- Print a snapshot every 0.25 years between 0 and 2 years to see fluctuation in river stage
- Print a snapshot every year of the simulation
- Print the solution at observation points for every time step

OUTPUT

```
OUTPUT
  SNAPSHOT_FILE
    PERIODIC TIME 0.25 y between 0. y and 2. y ! specific times
    PERIODIC TIME 1. y between 0. y and 10. y  ! specific times
    FORMAT TECPLOT BLOCK  ! Tecplot BLOCK format
    FORMAT HDF5           ! PFLOTRAN HDF5 Visit format
    PRINT_COLUMN_IDS      ! Adds column ids to obs. header
    VARIABLES
      LIQUID_PRESSURE
      LIQUID_SATURATION
      MATERIAL_ID_KLUDGE_FOR_VISIT
    /
  /
  OBSERVATION_FILE
    PERIODIC TIMESTEP 1  ! observ. every step
  /
  VELOCITY_AT_CENTER     ! include velocities
END
```

CHECKPOINT/RESTART I

- Checkpointing: saving the “state” of the simulation at a point in time, from which the entire solution can be reconstructed.
  - Fault tolerance
  - Restarting from a saved initial condition
  - Checkpoint files named “pflotran-ts#.chk” where # is the time step number (e.g. pflotran-ts100.chk)
  - Checkpoint files named “pflotran-#unit.chk“ where # is the time and unit is the unit of time (e.g. pflotran-2yr.chk)
  - Restart file named “pflotran-restart.chk”
- Restart: resetting a simulation to a “state”

CHECKPOINT/RESTART II

```
SIMULATION
  SIMULATION_TYPE SUBSURFACE
  PROCESS_MODELS
    SUBSURFACE_FLOW flow
      MODE RICHARDS
    /
    ...
  /
  CHECKPOINT                      ! write a checkpoint file
    PERIODIC TIMESTEP 50          ! write it every 50 timesteps
    PERIODIC TIME 2 yr            ! write it every 2 years
  /
  RESTART restart.chk RESET_TO_TIME_ZERO
END                               ! restart simulation using
                                  ! file restart.chk
                                  ! and reset time to 0.
```

How To Run the Python Script to Plot

When the simulation is finished running, you can plot the results using the python script called regional_doublet_center_obs.py
To run the python script:

```
> python regional_doublet_center_obs.py
```