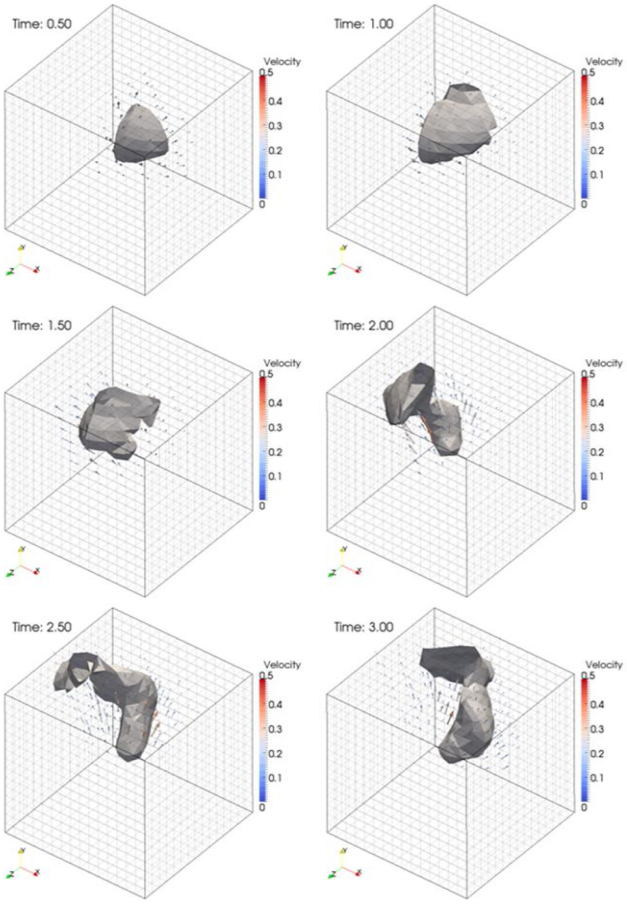
Tutorial: Point Source Spiral

This tutorial illustrates a transient gas/solids point source. In general, point source operating conditions (e.g., directional preference, mass flow rate, etc.) are constant. However, a point source can be made to vary in time by over-writing the corresponding keywords. The transient point source behavior outlined in this tutorial can be disabled by setting `CALL_USR=.FALSE.` in the mfix.dat file.

General simulation overview:

A point source injects gas and solids into the center of a cube with pressure outlets on all sides. User-defined functions are employed to change the directional preference of the point source with respect to time. This results in a gas/solids spiral emanating from the center of the domain.

- units, SI
- one solids phase
  - diameter, 285µm
  - density, 1101 kg/m^3
  - composition: Fixed Carbon (Char) and Coal Ash (Ash)
- gas properties:
  - compressible
  - composition: Nitrogen (N_2)
- pressure outlet - all boundaries
  - pressure: 1 atm
  - temperature 300K
- operating pressure: 1 atm
- geometry
  - 30cm width, 30cm height, 30cm depth
  - 3,375 computational cells



Simulation results: The contour represents solids bulk density (ROP_s) with a value of 0.3kg/m^3. Solids velocity vector field in (m/sec).

Geometry specification (mfix.dat):

The domain is decomposed into 15 partitions in the x-axial direction, 15 partitions in the y-axial direction, and 15 partitions in the z-axial direction for a total of 3,375 computational cells. The uniform cell dimensions are 2cm x 2cm x 2cm in width, height, and depth, respectively.

```
COORDINATES = 'cartesian'

XLENGTH = 0.30   IMAX = 15  ! Width
ZLENGTH = 0.30   KMAX = 15  ! Depth
YLENGTH = 0.30   JMAX = 15  ! Height
```

Phase composition specification (mfix.dat):

This case does not contain chemical reactions or phase changes. Therefore, it is not necessary to solve the species transport equations. However, the species equations have been included to illustrate the capabilities of mass point sources.

The gas phase is comprised of two species, `NMAX_g = 2`. The thermo-chemical database name and an alias are given for each species. Note that both gas phase species are nitrogen (N2) and reference the same species in the thermo-chemical database. This species aliases are uniquely identified as required.

```
NMAX_g(1) = 2

SPECIES_g(1) = 'N2'   SPECIES_ALIAS_g(1) = 'N2_1'
SPECIES_g(2) = 'N2'   SPECIES_ALIAS_g(2) = 'N2_2'
```

The solids phase composition is defined similarly.

```
NMAX_s(1) = 2

SPECIES_s(1,1) = 'Fixed Carbon'  SPECIES_ALIAS_s(1,1) = 'Char'
SPECIES_s(1,2) = 'Coal Ash'      SPECIES_ALIAS_s(1,2) = 'Ash'
```

Initial condition specification (mfix.dat):

This simulation contains one initial condition. The entire domain contains only gas which is comprised of the first gas phase species, N2_1, at 300K.

```
IC_X_w(1) =   0.00
IC_X_e(1) =   0.30
IC_Z_b(1) =   0.00
IC_Z_t(1) =   0.30
IC_Y_s(1) =   0.00
IC_Y_n(1) =   0.30

IC_EP_g(1) =   1.0

IC_T_g(1) =  300.00    ! (K)
IC_P_g(1) =  101.325d3 ! (Pa)

IC_U_g(1) =    0.0     ! (m/sec)
IC_V_g(1) =    0.0     ! (m/sec)
IC_W_g(1) =    0.0     ! (m/sec)

IC_X_g(1,1) =  1.00    ! N2
```

Boundary condition specification (mfix.dat):

This simulation contains six boundary conditions whereby all sides of the cube are defined as pressure outlets.

```
!                    west    south   east    nrth    btm     top
  BC_X_w(1)    =     0.00    0.00    0.30    0.00    0.00    0.00     ! (m)
  BC_X_e(1)    =     0.00    0.30    0.30    0.30    0.30    0.30     ! (m)
  BC_Y_s(1)    =     0.00    0.00    0.00    0.30    0.00    0.00     ! (m)
  BC_Y_n(1)    =     0.30    0.00    0.30    0.30    0.30    0.30     ! (m)
  BC_Z_b(1)    =     0.00    0.00    0.00    0.00    0.00    0.30     ! (m)
  BC_Z_t(1)    =     0.30    0.30    0.30    0.30    0.00    0.30     ! (m)

  BC_TYPE(1)   =  6*'PO'

  BC_P_g(1)    =  6*101.325d3 ! (Pa)
  BC_T_g(1)    =  6*300.00    ! (K)
  BC_T_s(1,1)  =  6*300.00    ! (K)
```

Point source specification (mfix.dat):

A point source is defined at the center of the domain. The physical coordinates (e.g., `PS_X_w`, `PS_X_e`) identify the point source location. However, the cell indices (e.g., `PS_I_w`, `PS_I_e`) could have been used to define the point source's location. The mass flow rate of for the gas and solids are given along with velocity vectors to assign a directional preference. Finally, the temperature and composition of the gas and solids are given since the energy and species equations are solved.

```
  PS_X_w(1)           =    0.15       ! (m)
  PS_X_e(1)           =    0.15       ! (m)
  PS_Y_s(1)           =    0.15       ! (m)
  PS_Y_n(1)           =    0.15       ! (m)
  PS_Z_b(1)           =    0.15       ! (m)
  PS_Z_t(1)           =    0.15       ! (m)

  PS_MASSFLOW_g(1)    =    8.0469d-5  ! (kg/sec)
  PS_U_g(1)           =    0.15       ! (m/sec)
  PS_V_g(1)           =    0.00       ! (m/sec)
  PS_W_g(1)           =    0.00       ! (m/sec)
  PS_T_g(1)           =  315.00       ! (K)
  PS_X_g(1,1)         =    0.00       ! N2_1
  PS_X_g(1,2)         =    1.00       ! N2_2

  PS_MASSFLOW_s(1,1)  =    8.2575d-4  ! (kg/sec)
  PS_U_s(1,1)         =    0.15       ! (m/sec)
  PS_V_s(1,1)         =    0.00       ! (m/sec)
  PS_W_s(1,1)         =    0.00       ! (m/sec)
  PS_T_s(1,1)         =  315.0        ! (K)
  PS_X_s(1,1,1)       =    0.00       ! Char
  PS_X_s(1,1,2)       =    1.00       ! Ash
```

Transient point source specification (usr1.f):

The transient behavior of the point source is defined such that the directional preference vector makes one revolution about the Y axis over a three second period. The subroutine `usr1.f` is selected for making transient adjustments because it is called at the start of each time step.

This and all other user-defined subroutines (i.e., `usr0`, `usr1`, and `usr2`) are invoked at run time by including the keyword `CALL_USR` in the mfix.dat file. The transient point source behavior can be disabled by setting this keyword to 'false'.

```
CALL_USR = .TRUE.
```

A copy of `usr1.f` is located in the run directory. All modifications to usr1.f are isolated to the local copy. When `make_mfix` is invoked, a backup copy of the original `usr1.f` in the model is created and the local file contain in the run directory is used to update the MFIX executable.

The desired rotational behavior of the point source is achieved by modifying the direction preference vector with respect to time. The direction preference specified in the `mifx.dat` file is converted into a unit vector and magnitude as part of the point source preprocessing. The unit vector is stored in the same variable as the user input (e.g., `PS_U_g`). **It is imperative that you understand the runtime usage of any variable before making any changes.**

UDF Overview (usr1.f)

The top of `subroutine usr1` lists five modules which provide access to several global variables. The `usr` module is included in the default `usr1.f` file and provides access to user-defined variables. This tutorial does not require new global variables and therefore this module is not needed.

```
      use ps
      use constant
      use run
      use physprop
      use usr
```

The desired transient behavior is achieved by calculating the X and Z components of the directional preference vector. First, the UDF calculates the radial position with respect to the simulation time, `TIME`. The global variables `TIME` and `Pi` are contain within the `RUN` and `CONSTANT` modules, respectively. The radial position is calculated such that the point source makes one rotation about the y-axis over three seconds.

```
      lRad = 2.0d0*Pi*(lTime/3.0d0)

      lV = (0.12d0/0.15d0)
      lU = (0.09d0/0.15d0)*cos(lRad)
      lW = (0.09d0/0.15d0)*sin(lRad)
```

The u and w gas phase velocity components have a maximum amplitude of 0.09m/sec, and the v velocity component has a fixed amplitude of 0.12m/sec. This gives the point source a dominant flow in the y-axial direction while rotating in the XZ plane. **The velocity components are normalized to remain consistent with the point source implementation.** Finally, the time-dependent values are assigned to the gas and solids phases. The variable `MMAX` used in a loop over the solids phases is found in the `PHYSPROP` module.

```
      PS_V_g(1) = lV
      PS_U_g(1) = lU
      PS_W_g(1) = lW

       do M=1,MMAX
          PS_V_s(1,M) = lV
          PS_U_s(1,M) = lU
          PS_W_s(1,M) = lW
       enddo
```

The MFIX executable should be (re)built from the directory containing the `usr1.f` and `mfix.dat` files. Detailed instructions on building MFIX are provided in the MFIX Readme. A serial run of this simulation takes approximately 20 minutes on a 2X Quad Core Intel Xeon E5440 2.83GHz processor.

An animation of the solids spiral pattern is available at the following URL:
https://mfix.netl.doe.gov/results.php#point_source_spiral

The MFIX Readme is available at the following URL:
https://mfix.netl.doe.gov/documentation/Readme.pdf