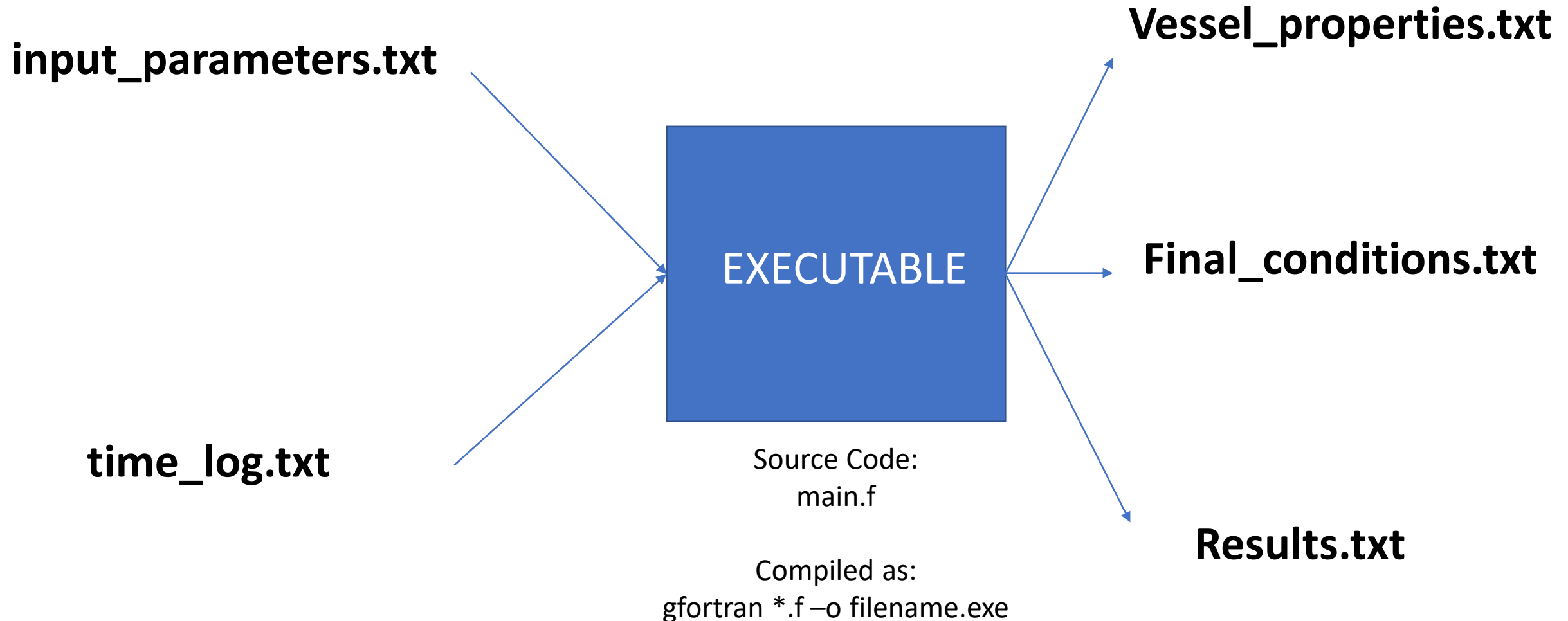# Workflow for the CryoH2Vehicle simulation framework

Make sure all FORTRAN files for REFPROP are in the same directory,
where "main.f", "input_paraemeters.txt" and "time_log.txt" are.
Also include the "fluid" folder, from REFPROP

input_parameters.txt

Vessel_properties.txt

EXECUTABLE

Final_conditions.txt

Source Code:
main.f

Compiled as:
gfortran *.f –o filename.exe

time_log.txt

Results.txt

Input_parameters.txt

100	20	400	400	144.518	10	80	80000	1550	2700	290	1862	0.333	3	0.01	0.003	50	200	0.3	40	280	100000	1	0.1	14	4	2	1	1	1	0
999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999
P0	rho_0	Pf	Pfill	Vol	s_fill	T_fill	Xrating	rhocomp	rhoalum	sigma_y	sigma_cf	Dint	SF	x0	xpump	step	Pmin	e	n	Tout	fuelec	fill	fuelcons10	fill0	fill10	iteration	Results	ResultsSC	p-o	Model_fill
[bar],	[g/L],	[bar],	[bar],	[Lit],	[J/g-K],	[K],	[meters],	[g/L],	[g/L],	[MPa],	[MPa],	[m],	[-],	[-],	[-],	[s],	[kPa],	[-],	[-],	[K],	[km/kgH2],	[mole],	[mole],	[mole],	[mole],	[-],	[-],	[-],	[-]	[-]

Input parameters:
```
          P0 = Initial pressure, (bar)
       rho_0 = Initial density, (g/L)
          Pf = Pressure vessel rating, (bar)
       Pfill = Filling pressure, (bar)
         Vol = Vessel internal volume, (liters)
      s_fill = Cryogenic vessel H2 inlet entropy, (J/g-K)
      T_fill = Cryogenic vessel H2 inlet temperature, (K)
      Xrating = Remaining range in meters when refueling is done, (meters)
     rhocomp = Composite density in vessel, (g/L)
     rhoalum = Aluminum density in vessel, (g/L)
     sigma_y = Yield stress of aluminum, (Mpa)
    sigma_cf = Failure stress (T300 carbon fiber/epoxy), (MPA)
        Dint = Inner Diameter (m)
          SF = Factor of safety against burst, (-)
          xo = Initial ortho fraction, (-)
       xpump = Ortho concentration of pumped H2 (=0.003 for pure para H2, 99.97%)
        step = Time steps size during the driving (=seconds)
        Pmin = Mimimum pressure at which hydrogen starts to be extracted at constant pressure (kpa)
           e = emissivity of 1 layer, (=0.225)
           n = number of layers, (=40)
        Tout = outside temperature, (=280 K)
      fuelec = fuel economy, meters per kg H2, (=100000)
        fill = filled mass step size, mol-g (=2.0 mol)
  fuelcons10 = Reduced fuelcons close to critical point, (= mol)
       fill0 = filled mass step size at two phases region, (=mol)
      fill10 = filled mass step size close to critical point, (= mol)
   iteration = number of iterations
     Results = (=1) to write results on file Results.txt
   ResultsSC = (=1) to write results on screen
    paraortho = !=1 to consider p-o or =0 to neglect it
  Model_fill  = != 1 Refueling with constant Cryogenic vessel H2 inlet entropy
              != 0 Refueling with constant Cryogenic vessel H2 inlet temperature
```

Depending which method is selected (constant outlet entropy or temperature fill, 1 or 0 for Model_fill), either s_fill OR T_fill will be used

Time_log.txt

```
0 0.000 2005-03-31 00:00:00 TH
1 0.000 2005-03-31 01:00:00 TH
2 0.000 2005-03-31 02:00:00 TH
3 0.000 2005-03-31 03:00:00 TH
4 0.000 2005-03-31 04:00:00 TH
5 0.000 2005-03-31 05:00:00 TH
6 0.000 2005-03-31 06:00:00 TH
7 0.000 2005-03-31 07:00:00 TH
8 0.000 2005-03-31 08:00:00 TH
9 2.025 2005-03-31 09:00:00 TH
10 2.598 2005-03-31 10:00:00 TH
11 3.065 2005-03-31 11:00:00 TH
12 12.999 2005-03-31 12:00:00 TH
13 5.110 2005-03-31 13:00:00 TH
14 3.579 2005-03-31 14:00:00 TH
15 12.035 2005-03-31 15:00:00 TH
16 5.529 2005-03-31 16:00:00 TH
17 4.491 2005-03-31 17:00:00 TH
18 3.604 2005-03-31 18:00:00 TH
19 0.000 2005-03-31 19:00:00 TH
20 0.000 2005-03-31 20:00:00 TH
21 0.000 2005-03-31 21:00:00 TH
22 0.000 2005-03-31 22:00:00 TH
23 0.000 2005-03-31 23:00:00 TH
24 0.000 2005-04-01 00:00:00 FR
25 0.000 2005-04-01 01:00:00 FR
26 0.000 2005-04-01 02:00:00 FR
27 0.000 2005-04-01 03:00:00 FR
28 0.000 2005-04-01 04:00:00 FR
29 0.000 2005-04-01 05:00:00 FR
```

```
8709 8.346 2006-03-28 21:00:00 TU
8710 0.000 2006-03-28 22:00:00 TU
8711 0.000 2006-03-28 23:00:00 TU
8712 0.000 2006-03-29 00:00:00 WE
8713 0.000 2006-03-29 01:00:00 WE
8714 0.000 2006-03-29 02:00:00 WE
8715 0.000 2006-03-29 03:00:00 WE
8716 0.000 2006-03-29 04:00:00 WE
8717 0.000 2006-03-29 05:00:00 WE
8718 0.000 2006-03-29 06:00:00 WE
8719 0.000 2006-03-29 07:00:00 WE
8720 0.000 2006-03-29 08:00:00 WE
8721 4.123 2006-03-29 09:00:00 WE
8722 1.319 2006-03-29 10:00:00 WE
8723 25.121 2006-03-29 11:00:00 WE
8724 3.182 2006-03-29 12:00:00 WE
8725 0.021 2006-03-29 13:00:00 WE
8726 0.000 2006-03-29 14:00:00 WE
8727 22.904 2006-03-29 15:00:00 WE
8728 2.580 2006-03-29 16:00:00 WE
8729 13.886 2006-03-29 17:00:00 WE
8730 6.974 2006-03-29 18:00:00 WE
8731 11.484 2006-03-29 19:00:00 WE
8732 5.473 2006-03-29 20:00:00 WE
8733 5.074 2006-03-29 21:00:00 WE
8734 0.871 2006-03-29 22:00:00 WE
8735 0.000 2006-03-29 23:00:00 WE
9999 9999
```

Hours (total)

Km driven during that hour

Date, hour of the day, day of the week
(information only, not needed to run the code)

Make sure those characters are included at end of file

Vessel_properties.txt

```
P_rating[bar] V_int[L] D_int[m] th_liner[m] th_cf[m]    Vliner[L] VcarbonFiber[L] Mliner[kg] Mcarbofiber[kg]         MassTank[kg] Py  Pwork/Py SF sigma_a[bar] sigma_h[bar] L/D        L_cyl[m] Lint[m] Lext[m] Dext[m] Vext[L] Surface_ext[m2]
  400.000000000000    144.518000000000    0.333000000000002    1.0541391396824328E-002  9.7825124445494287E-003   20.312999243081702       20.122703265979151        54.845097956320593         31.190190062267682         86.035288018588275
```

Rating, volume, Diameter, liner and composite thickness, masses of liner and composite….

Final_conditions.txt

```
#Iteration           mass(kg)   density(g/L)    pressure(bar)  temp(K)  Fill-cycles Total-kgH2 Total-used-kgH2    Total-vented-mass(kg) %Vented-mass  Average-mass-Capacity(kg)   Total-parking-time(hr) Total-driving-time-(hr) Distance(km)        Xortho(-) Ce(-
start  2.8903600000000003          20.00000000000000        100.0000000000000      113.57752419566995                 0          0                0                0                0                0                0   0   1.0000000000000000E-002  0.6526700414992907
       1  6.6998636645273706         46.360063552826439          342.51002103504339            124.50940896129495            29.000000000000000      186.37172584000001           179.67186217547263                 0      4.0317600000006E-003    2.1632895128423416E-003    7.1990250289655195
       2  3.3388821690547212         23.103573043183005          108.56389111364672            106.26728249645120            28.000000000000000      183.00671258452738           179.66783041547265                 0      0.0000000000000000           0.0000000000000000           7.3073825923045508
```

Final conditions and overall results (boil-off, average capacity…) for each iteration

Results.txt

```
iteration  K   J   I   time(hr)   distance(km)  mass(kg) density(g/L) pressure(bar)  temp(K)  u(J/g)  up(J/g)  uo(J/g)  un(J/g)  hout(J/g)  s(J/g-K)  q(-)  vented-mass(kg)  Ucomp(J)   Ualum(J)       Usteel(J) Utotal(J)     Xortho(-) Ce(-)  Qheat(W)  Qap(W)  Qpo(W)     hpo(kJ/
start     1    1    1      0   0.0000000000000000       0.0000000000000000       2.8903600000000003        20.000000000000000       100.0000000000000      113.57752419566995      621.52195520619625      615.53282843442389       1214.445
park      1    1    1      1   1.0000000000000000       0.0000000000000000       2.8903600000000003        20.000000000000000       100.23755402474087      113.85791970348245      624.00898736822785      617.90331187381935       1216.541
park      1    1    1      2   2.0000000000000000       0.0000000000000000       2.8903600000000003        20.000000000000000       100.50916023421404      114.11390114879495      626.84528894957054      620.62767036199966       1218.270
park      1    1    1      3   3.0000000000000000       0.0000000000000000       2.8903600000000003        20.000000000000000       100.77983373088558      114.36902810191995      629.67988534947142      623.34771969459632       1219.994
park      1    1    1      4   4.0000000000000000       0.0000000000000000       2.8903600000000003        20.000000000000000       101.04957483934434      114.62330056285745      632.51277335457780      626.06339025858836       1221.714
park      1    1    1      5   5.0000000000000000       0.0000000000000000       2.8903600000000003        20.000000000000000       101.31838388271561      114.87671853160745      635.34395195691161      628.77461285890536       1223.428
park      1    1    1      6   6.0000000000000000       0.0000000000000000       2.8903600000000003        20.000000000000000       101.58639063928001      115.12940407848245      638.17472629707379      631.48262805621744       1225.139
park      1    1    1      7   7.0000000000000000       0.0000000000000000       2.8903600000000003        20.000000000000000       101.85346594786402      115.38123513316995      641.00380051870275      634.18606259381647       1226.845
park      1    1    1      8   8.0000000000000000       0.0000000000000000       2.8903600000000003        20.000000000000000       102.11961012753036      115.63221169566995      643.83118050414726      636.88484850958230       1228.545
drive     1    1    1     50   9.0000000000000000       2.0249999999999999       2.8762974996274746       19.902693779511718      101.63016007212565      115.69825173473245      645.03738076158561      638.09412136175439       1229.493
drive     1    1    1     71   9.0000000000000000       2.0249999999999999       2.8701099997984119       19.859879044813876      101.41110146002373      115.72376443004495      645.53023890313716      638.58816895525399       1229.886
drive     1    1    1     50  10.000000000000000       2.5979999999999999       2.8520683326538125       19.735038767861528      100.73012831399964      115.75745583629495      646.53133428133106      639.59082270160332       1230.756
drive     1    1    1     71  10.000000000000000       2.5979999999999999       2.8441299995968237       19.680109049369797      100.42707230484473      115.76868630504495      646.93341670674658      639.99342266237704       1231.114
drive     1    1    1     50  11.000000000000000       3.0649999999999999       2.8228452768107424       19.532828276136826      99.592089204227833      115.77601052379495      647.76758512449487      640.82791107458161       1231.921
drive     1    1    1     71  11.000000000000000       3.0649999999999999       2.8134799993952360       19.468024740137810      99.221636754606607      115.77564431285745      648.09633149053457      641.15663003878728       1232.252
```

Thermodynamic states at each hour of the time_log, for each iteration…