User Guide for Code to solve systems of ODEs using Runge-Kutta method On systems running Ubuntu 16.04 LTS

December 16, 2016

Abstract

This is only the guide to use our code for the purpose said in the title, for more theoretical details, please see [1] and [2]. For reference to the `Fortran` programming language, you may want to visit [3].

Contents

1 Preparation

To use our code, which was written in `Fortran`, we need the following things on a system running Ubuntu:

1. A text editor: You can use any text editor, but in this guide, we will use `gedit`, the default text editor in Ubuntu 16.04 LTS.

2. `gcc`, `gfortran` and `gnuplot`: if new versions of those were not already installed, one way to install them is to open **Terminal** and type

   ```
   sudo apt-get update
   sudo apt-get install gcc
   sudo apt-get install gfortran
   sudo apt-get install gnuplot
   ```

2 The source files

We wrote multiple source files with different purposes:

- `rkfts.f90`: `Fortran` source code for Runge-Kutta method using fixed time step

- `rkats.f90`: `Fortran` source code for Runge-Kutta method using adaptive time step

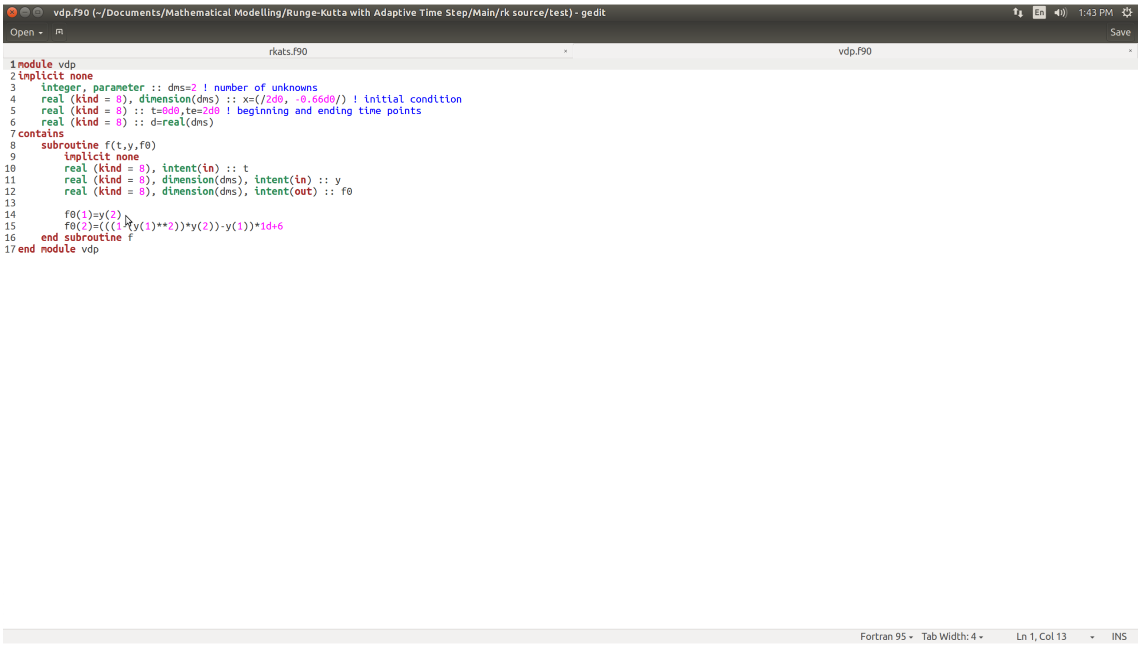
- `data_plot.plt` and `data_plot_dependency.plt` :`gnuplot` commands to plot the results

- `customf.f90`: source code for module containing the specific equation you want to solve, how to modify it will be discussed later.

- The other `*.f90`: `Fortran` source code for modules containing the example equations to solve, we included modules for: Curtiss-Hirschfelder equation, Brusselator equation, Van der Pol equation,...

3 Specifying equation by modifying the source files

As mentioned before, there are module files containing the example equations, you may want to take a look at those and [3] for reference. This section will explain about what you need to specify in the module file. For example, a module file look like this


vdp.f90 (~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive Time Step/Main/rk source/test) - gedit
1:43 PM
Open
Save
rkats.f90
vdp.f90
Fortran 95
Tab Width: 4
Ln 1, Col 13
INS

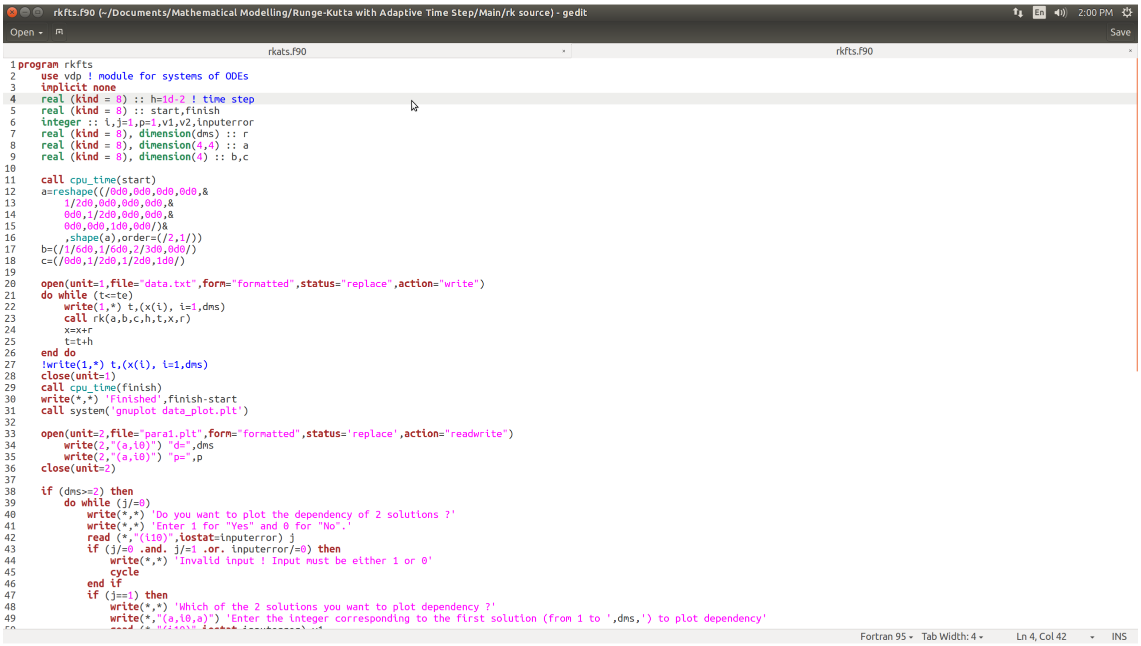
```fortran
 1 module vdp
 2 implicit none
 3     integer, parameter :: dms=2 ! number of unknowns
 4     real (kind = 8), dimension(dms) :: x=(/2d0, -0.66d0/) ! initial condition
 5     real (kind = 8) :: t=0d0,te=2d0 ! beginning and ending time points
 6     real (kind = 8) :: d=real(dms)
 7 contains
 8     subroutine f(t,y,f0)
 9         implicit none
10         real (kind = 8), intent(in) :: t
11         real (kind = 8), dimension(dms), intent(in) :: y
12         real (kind = 8), dimension(dms), intent(out) :: f0
13 
14         f0(1)=y(2)
15         f0(2)=(((1-(y(1)**2))*y(2))-y(1))*1d+6
16     end subroutine f
17 end module vdp
```

Figure 1: Module file of the Van der Pol equation

As commented in the file, line 3, 4, 4 contain the information about "number of unknowns", "initial conditions", "beginning and ending time points". The information in Figure 1 means that we are considering a equation with 2 unknown variables, the beginning and ending time points are $t_0 = 0$ and $t_e = 2$ respectively, the initial condition is $f(0, y) = (2, -0.66)$.
Where $y = y_1, y_2$ is the vector of unknown variables and

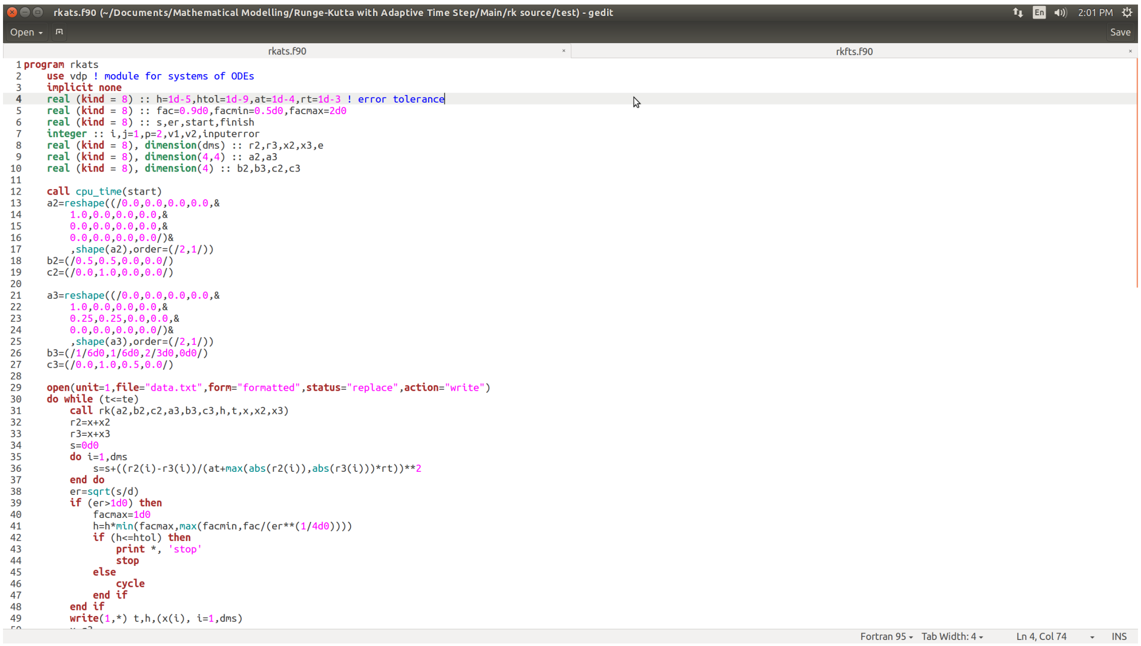
$$f(t, y) = \left[y_2(t), \frac{\left(1 - y_1(t)\right)^2 y_2(t) - y_1(t)}{10^{-6}} \right]$$

More ever, we may also need to modify the time step in `rkfts.f90` or the error tolerance in `rkats.f90`, for more details about this, refer to [1] and [2].


rkfts.f90 (~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive Time Step/Main/rk source) - gedit
2:00 PM
Open
Save
rkats.f90
rkfts.f90
Fortran 95
Tab Width: 4
Ln 4, Col 42
INS

```fortran
program rkfts
    use vdp ! module for systems of ODEs
    implicit none
    real (kind = 8) :: h=1d-2 ! time step
    real (kind = 8) :: start,finish
    integer :: i,j=1,p=1,v1,v2,inputerror
    real (kind = 8), dimension(dms) :: r
    real (kind = 8), dimension(4,4) :: a
    real (kind = 8), dimension(4) :: b,c

    call cpu_time(start)
    a=reshape((/0d0,0d0,0d0,0d0,&
        1/2d0,0d0,0d0,0d0,&
        0d0,1/2d0,0d0,0d0,&
        0d0,0d0,1d0,0d0/)&
        ,shape(a),order=(/2,1/))
    b=(/1/6d0,1/6d0,2/3d0,0d0/)
    c=(/0d0,1/2d0,1/2d0,1d0/)

    open(unit=1,file="data.txt",form="formatted",status="replace",action="write")
    do while (t<=te)
        write(1,*) t,(x(i), i=1,dms)
        call rk(a,b,c,h,t,x,r)
        x=x+r
        t=t+h
    end do
    !write(1,*) t,(x(i), i=1,dms)
    close(unit=1)
    call cpu_time(finish)
    write(*,*) 'Finished',finish-start
    call system('gnuplot data_plot.plt')

    open(unit=2,file="para1.plt",form="formatted",status='replace',action="readwrite")
        write(2,"(a,i0)") "d=",dms
        write(2,"(a,i0)") "p=",p
    close(unit=2)

    if (dms>=2) then
        do while (j/=0)
            write(*,*) 'Do you want to plot the dependency of 2 solutions ?'
            write(*,*) 'Enter 1 for "Yes" and 0 for "No".'
            read (*,"(i10)",iostat=inputerror) j
            if (j/=0 .and. j/=1 .or. inputerror/=0) then
                write(*,*) 'Invalid input ! Input must be either 1 or 0'
                cycle
            end if
            if (j==1) then
                write(*,*) 'Which of the 2 solutions you want to plot dependency ?'
                write(*,"(a,i0,a)") 'Enter the integer corresponding to the first solution (from 1 to ',dms,') to plot dependency'
```

Figure 2: rkfts.f90



rkats.f90 (~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive Time Step/Main/rk source/test) - gedit
2:01 PM
Open
Save
rkats.f90
rkfts.f90
Fortran 95
Tab Width: 4
Ln 4, Col 74
INS

```
program rkats
    use vdp ! module for systems of ODEs
    implicit none
    real (kind = 8) :: h=1d-5,htol=1d-9,at=1d-4,rt=1d-3 ! error tolerance
    real (kind = 8) :: fac=0.9d0,facmin=0.5d0,facmax=2d0
    real (kind = 8) :: s,er,start,finish
    integer :: i,j=1,p=2,v1,v2,inputerror
    real (kind = 8), dimension(dms) :: r2,r3,x2,x3,e
    real (kind = 8), dimension(4,4) :: a2,a3
    real (kind = 8), dimension(4) :: b2,b3,c2,c3

    call cpu_time(start)
    a2=reshape((/0.0,0.0,0.0,0.0,&
        1.0,0.0,0.0,0.0,&
        0.0,0.0,0.0,0.0,&
        0.0,0.0,0.0,0.0/)&
        ,shape(a2),order=(/2,1/))
    b2=(/0.5,0.5,0.0,0.0/)
    c2=(/0.0,1.0,0.0,0.0/)

    a3=reshape((/0.0,0.0,0.0,0.0,&
        1.0,0.0,0.0,0.0,&
        0.25,0.25,0.0,0.0,&
        0.0,0.0,0.0,0.0/)&
        ,shape(a3),order=(/2,1/))
    b3=(/1/6d0,1/6d0,2/3d0,0d0/)
    c3=(/0.0,1.0,0.5,0.0/)

    open(unit=1,file="data.txt",form="formatted",status="replace",action="write")
    do while (t<=te)
        call rk(a2,b2,c2,a3,b3,c3,h,t,x,x2,x3)
        r2=x+x2
        r3=x+x3
        s=0d0
        do i=1,dms
            s=s+((r2(i)-r3(i))/(at+max(abs(r2(i)),abs(r3(i)))*rt))**2
        end do
        er=sqrt(s/d)
        if (er>1d0) then
            facmax=1d0
            h=h*min(facmax,max(facmin,fac/(er**(1/4d0))))
            if (h<=htol) then
                print *, 'stop'
                stop
            else
                cycle
            end if
        end if
        write(1,*) t,h,(x(i), i=1,dms)
```

Figure 3: rkats.f90

4 Using the code

• **Step 1:** Decide which equation you want to solve and whether you want to solve it using Runge-Kutta method with fixed time step or adaptive time step. Put the file containing the module specifies that equation and the file corresponding to the method of your choice together with `data_plot.plt` and `data_plot_dependency.plt` in a same folder.

For example: You want to solve the Van der Pol equation specified in `vfp.f90` using Runge-Kutta method with adaptive time step, you need to put `rkats.f90`, `vdp.f90`, `data_plot.plt` and `data_plot_dependency.plt` in the same folder. From now on, we will use this example for sake of convenience.

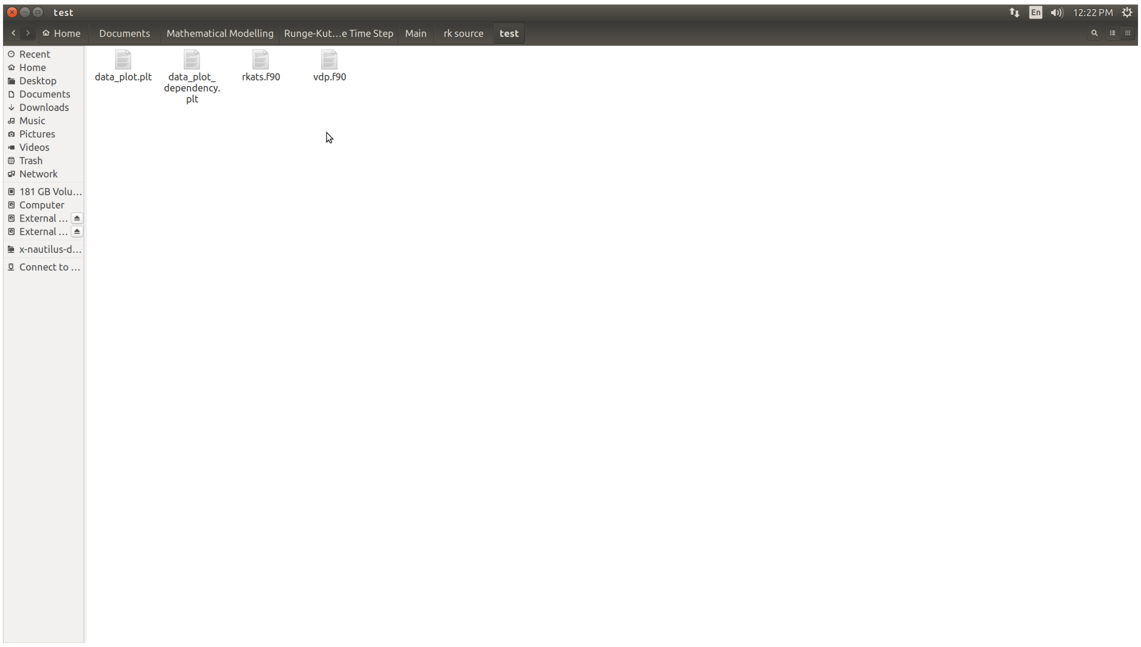


Figure 4: Put the needed files in the same folder

- **Step 2:** Open the folder in **Terminal**

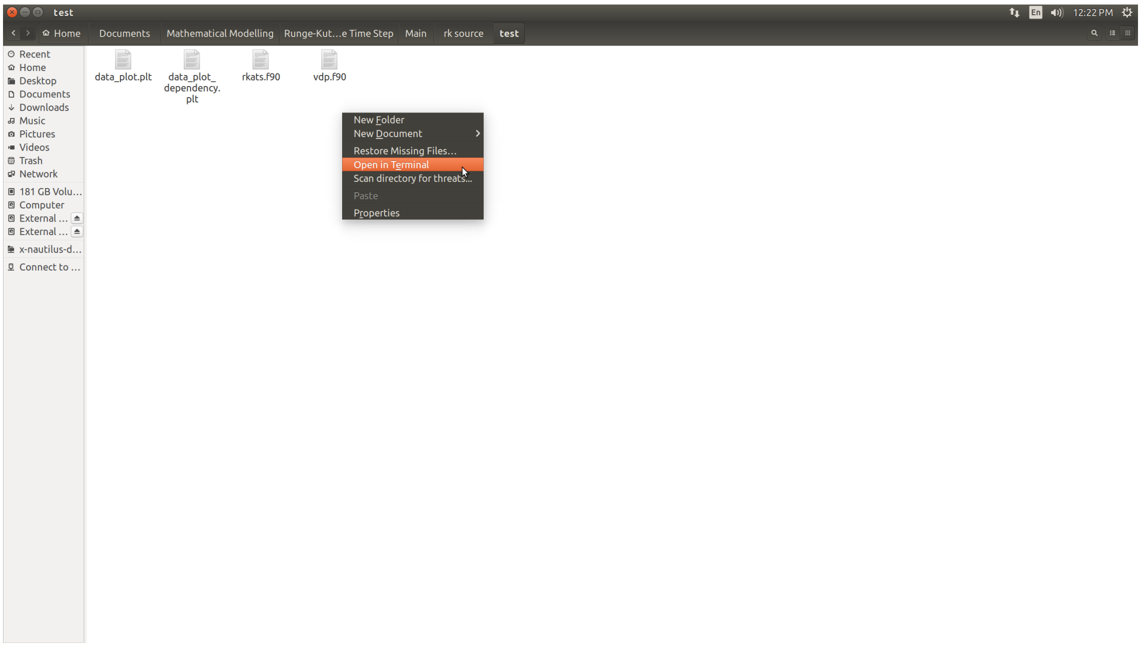
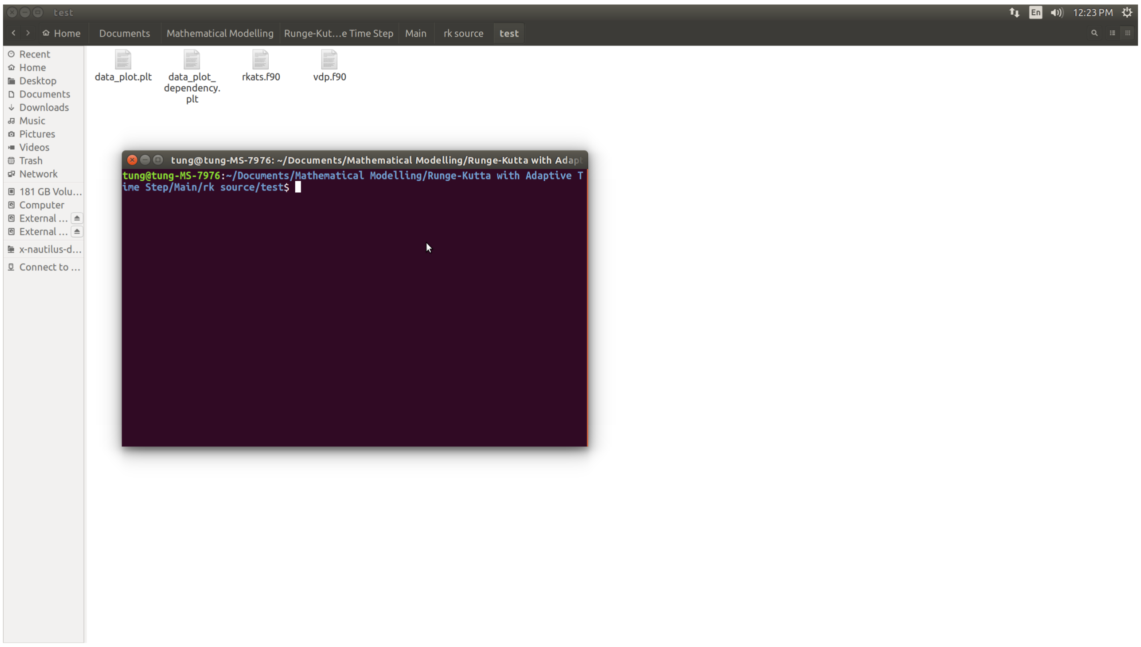


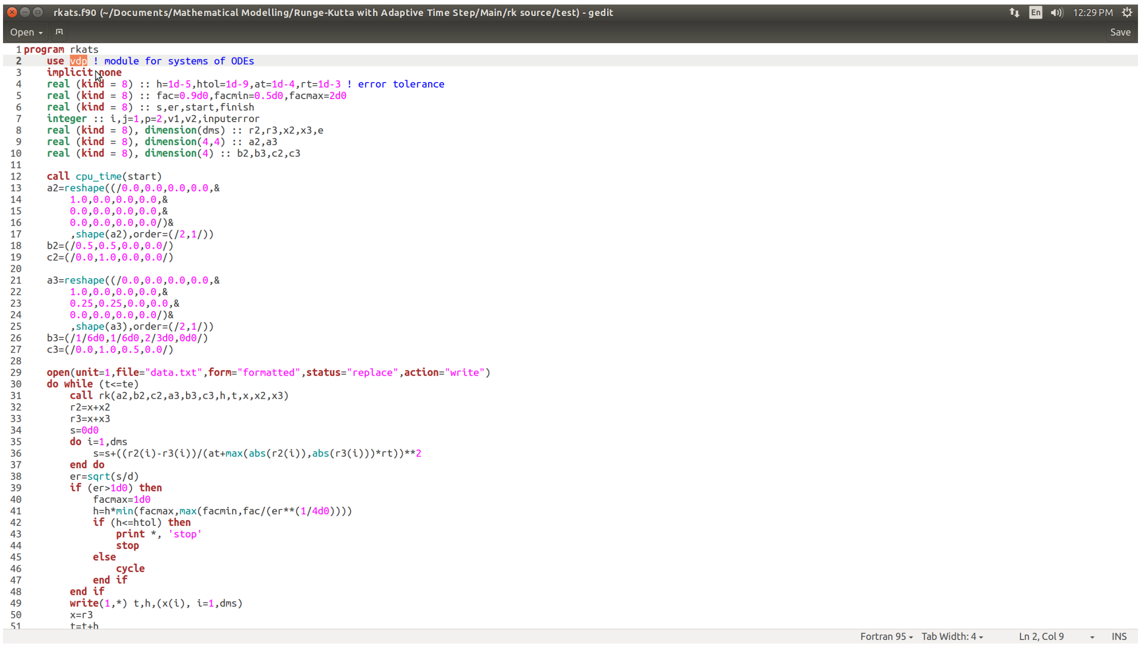
Figure 5: Right click at the empty space and select `Open in Terminal`



```
tung@tung-MS-7976: ~/Documents/Mathematical Modelling/Runge-Kutta with Adapt
tung@tung-MS-7976:~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive T
ime Step/Main/rk source/test$ 
```

Figure 6: The folder is now opened in Terminal

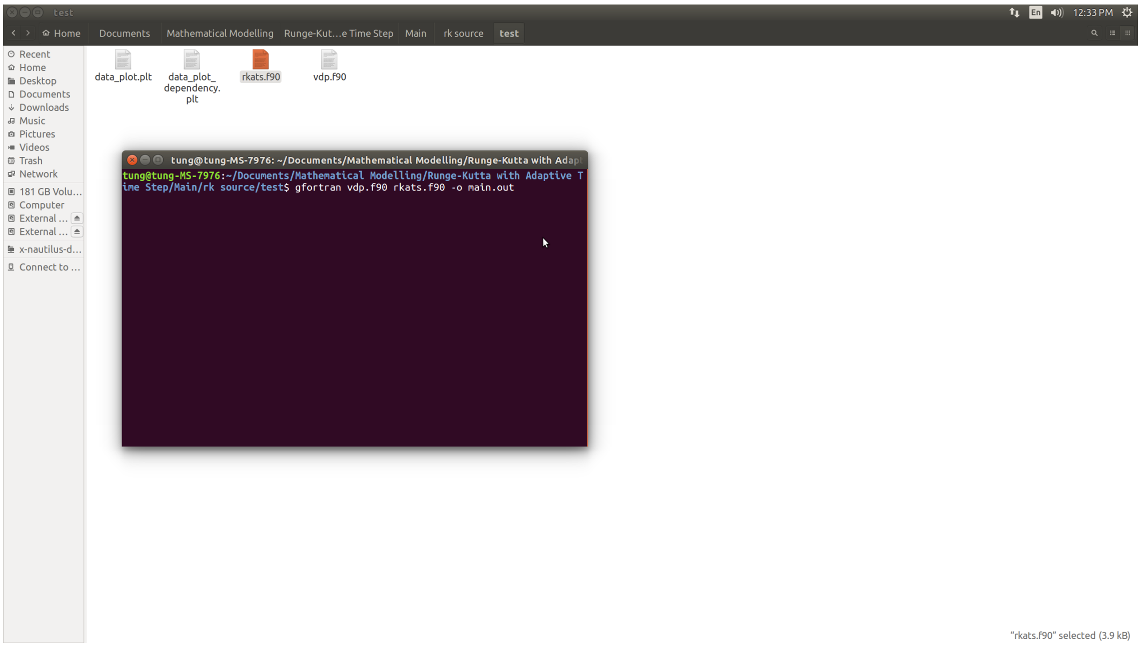
- **Step 3:** Open `rkats.f90` in a text editor and make sure that it use the module for your equation of choice (`vdp.f90` for the Van der Pol equation in this example) by modifying the second line: from `use [something]` to `use vdp`


rkats.f90 (~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive Time Step/Main/rk source/test) - gedit
Open
Save
12:29 PM
Fortran 95
Tab Width: 4
Ln 2, Col 9
INS

```fortran
program rkats
    use vdp ! module for systems of ODEs
    implicit none
    real (kind = 8) :: h=1d-5,htol=1d-9,at=1d-4,rt=1d-3 ! error tolerance
    real (kind = 8) :: fac=0.9d0,facmin=0.5d0,facmax=2d0
    real (kind = 8) :: s,er,start,finish
    integer :: i,j=1,p=2,v1,v2,inputerror
    real (kind = 8), dimension(dms) :: r2,r3,x2,x3,e
    real (kind = 8), dimension(4,4) :: a2,a3
    real (kind = 8), dimension(4) :: b2,b3,c2,c3

    call cpu_time(start)
    a2=reshape((/0.0,0.0,0.0,0.0,&
        1.0,0.0,0.0,0.0,&
        0.0,0.0,0.0,0.0,&
        0.0,0.0,0.0,0.0/)&
        ,shape(a2),order=(/2,1/))
    b2=(/0.5,0.5,0.0,0.0/)
    c2=(/0.0,1.0,0.0,0.0/)

    a3=reshape((/0.0,0.0,0.0,0.0,&
        1.0,0.0,0.0,0.0,&
        0.25,0.25,0.0,0.0,&
        0.0,0.0,0.0,0.0/)&
        ,shape(a3),order=(/2,1/))
    b3=(/1/6d0,1/6d0,2/3d0,0d0/)
    c3=(/0.0,1.0,0.5,0.0/)

    open(unit=1,file="data.txt",form="formatted",status="replace",action="write")
    do while (t<=te)
        call rk(a2,b2,c2,a3,b3,c3,h,t,x,x2,x3)
        r2=x+x2
        r3=x+x3
        s=0d0
        do i=1,dms
            s=s+((r2(i)-r3(i))/(at+max(abs(r2(i)),abs(r3(i)))*rt))**2
        end do
        er=sqrt(s/d)
        if (er>1d0) then
            facmax=1d0
            h=h*min(facmax,max(facmin,fac/(er**(1/4d0))))
            if (h<=htol) then
                print *, 'stop'
                stop
            else
                cycle
            end if
        end if
        write(1,*) t,h,(x(i), i=1,dms)
        x=r3
        t=t+h
```

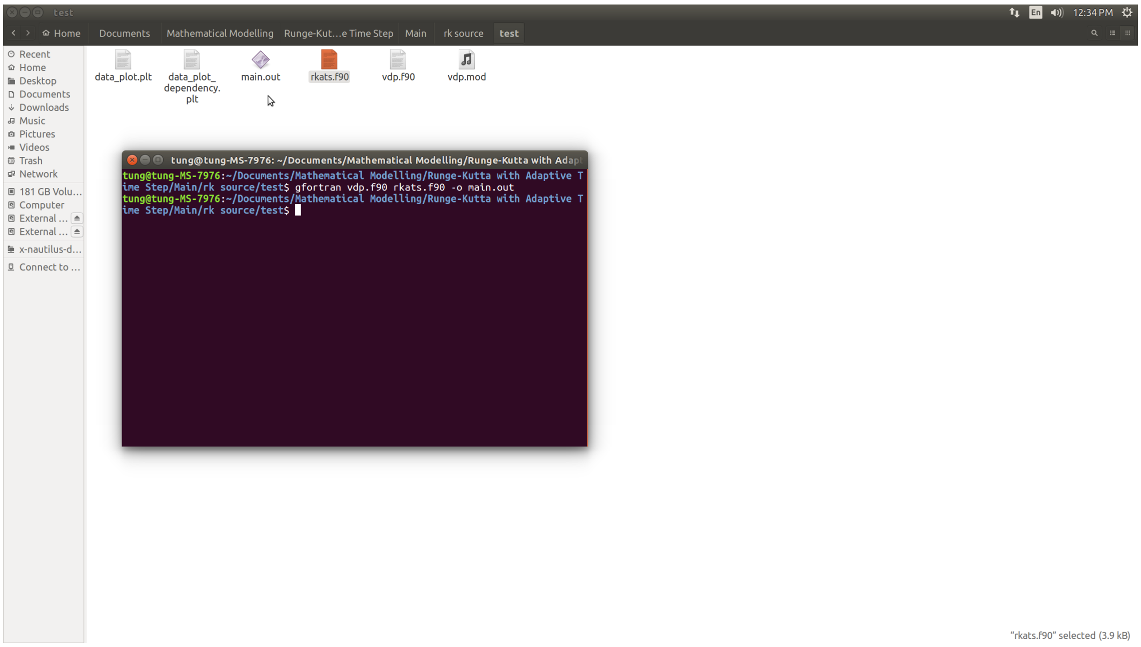
Figure 7: The result look like this

- **Step 4:** Type `gfortran vdp.f90 rkats.f90 -o main.out` to make the output file named `main.out`, of course you can choose other names as well.



```
tung@tung-MS-7976:~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive T
ime Step/Main/rk source/test$ gfortran vdp.f90 rkats.f90 -o main.out
```

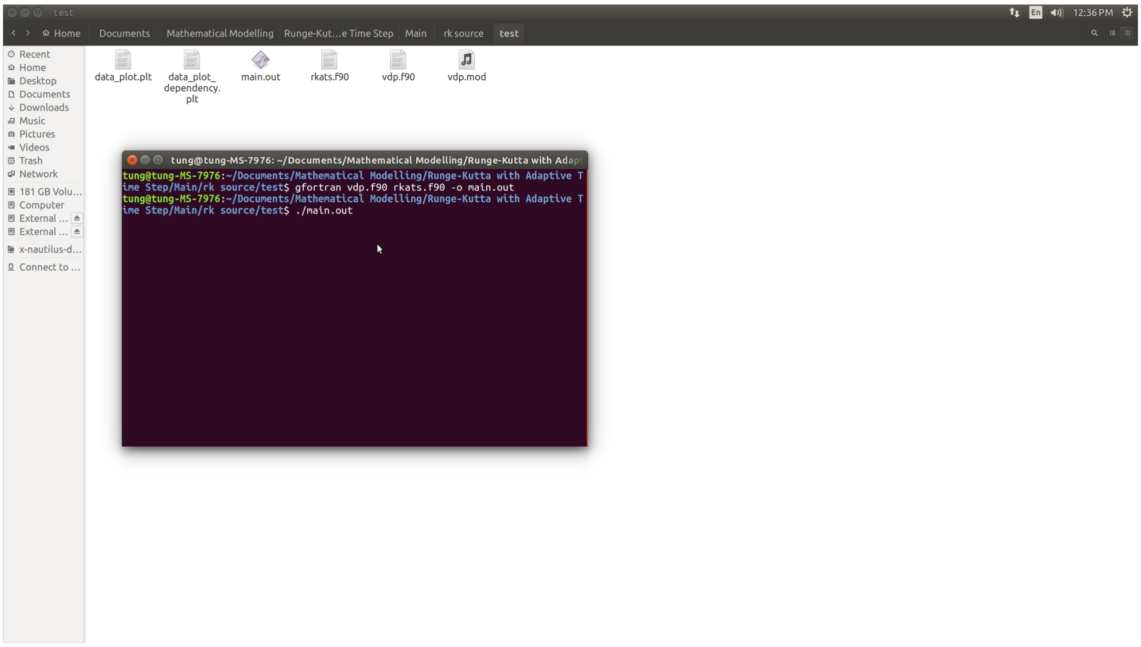
Figure 8: Typing the command in the Terminal



```
tung@tung-MS-7976:~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive T
ime Step/Main/rk source/test$ gfortran vdp.f90 rkats.f90 -o main.out
tung@tung-MS-7976:~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive T
ime Step/Main/rk source/test$ 
```

Figure 9: Completing the command will result in some new files

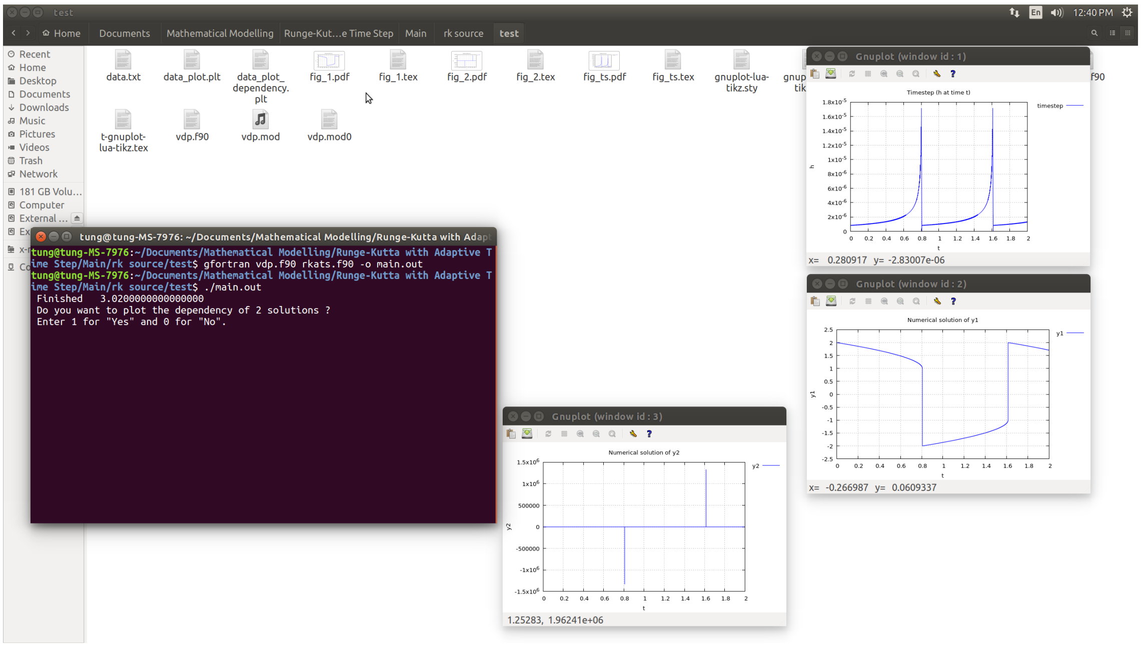
- **Step 5:** Type `./main.out` to run the file `main.out`



```
tung@tung-MS-7976:~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive T
ime Step/Main/rk source/test$ gfortran vdp.f90 rkats.f90 -o main.out
tung@tung-MS-7976:~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive T
ime Step/Main/rk source/test$ ./main.out
```

Figure 10: Typing the command in the Terminal

The command will run the program to solve the equation. The numerical result will be save into the file `data.txt` and the plots of the size of the step h at time t (only appear if you use adaptive time step method), the **solutions of the unknown variables of the equation** will appear, those plots would be saved in the same folder with the other file in the form of `*.pdf` and `*.tex` files. Additionally, several other files created by `gnuplot` are needed to compile the newly created `*.tex` files.

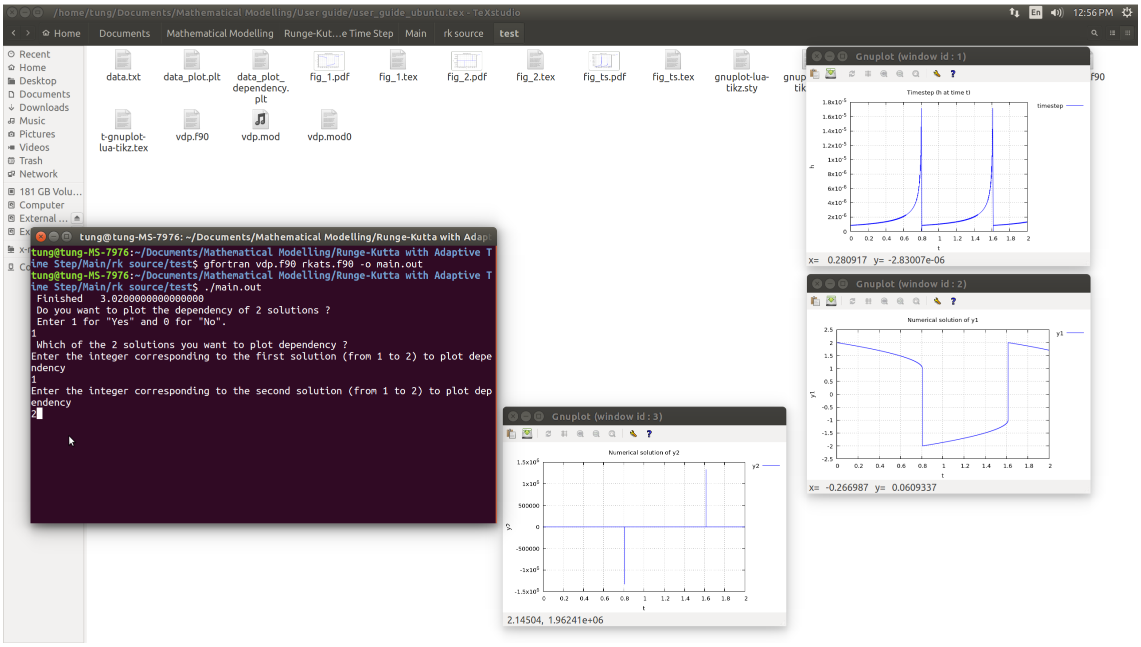


```
tung@tung-MS-7976:~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive T
ime Step/Main/rk source/test$ gfortran vdp.f90 rkats.f90 -o main.out
tung@tung-MS-7976:~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive T
ime Step/Main/rk source/test$ ./main.out
 Finished   3.0200000000000000
 Do you want to plot the dependency of 2 solutions ?
 Enter 1 for "Yes" and 0 for "No".
```

Figure 11: The result look like this

If the equation has more than one unknown variable (like in this example), the program will also ask whether if you want to plot the dependency between the solutions of those variables. This will be discussed in the next step.

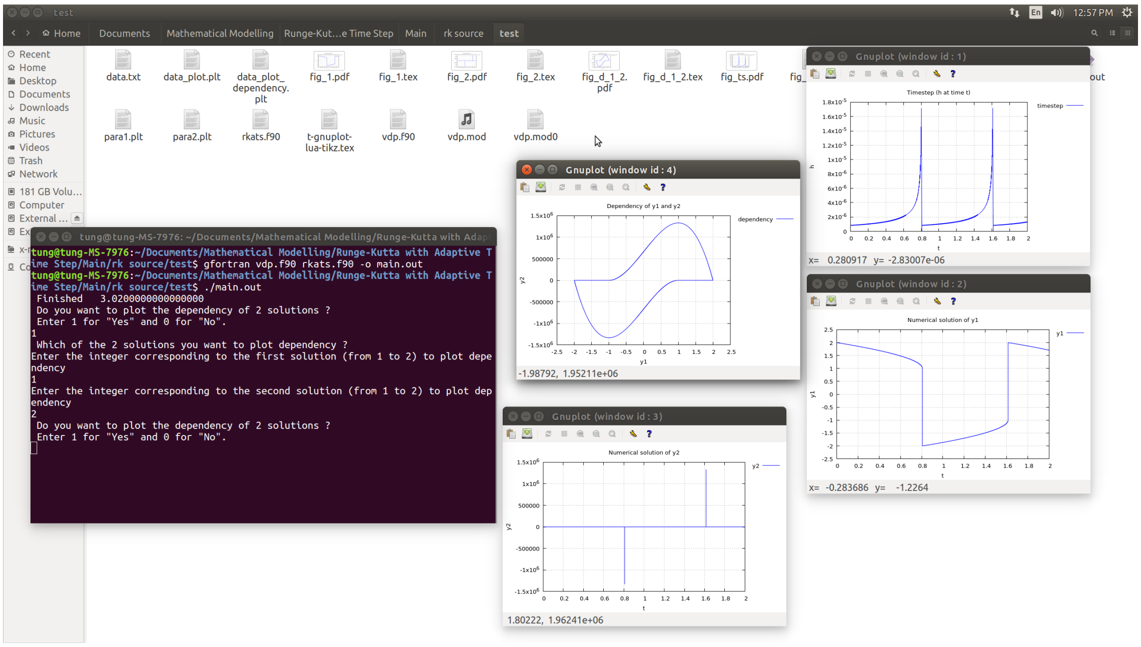
• **Step 6*:** Plot the dependency between the solutions of variables. To do this, you just need to follow the instructions in the **Terminal**. Suppose you want to plot the dependency of y_1 and y_2, type 1 in the **Terminal** to confirm your intention, then type in 1 and 2 respectively for the next 2 line.



```
tung@tung-MS-7976:~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive T
ime Step/Main/rk source/test$ gfortran vdp.f90 rkats.f90 -o main.out
tung@tung-MS-7976:~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive T
ime Step/Main/rk source/test$ ./main.out
 Finished   3.0200000000000000
 Do you want to plot the dependency of 2 solutions ?
 Enter 1 for "Yes" and 0 for "No".
1
 Which of the 2 solutions you want to plot dependency ?
Enter the integer corresponding to the first solution (from 1 to 2) to plot depe
ndency
1
Enter the integer corresponding to the second solution (from 1 to 2) to plot dep
endency
2
```

Figure 12: Typing the integers correspond to your choices in the Terminal

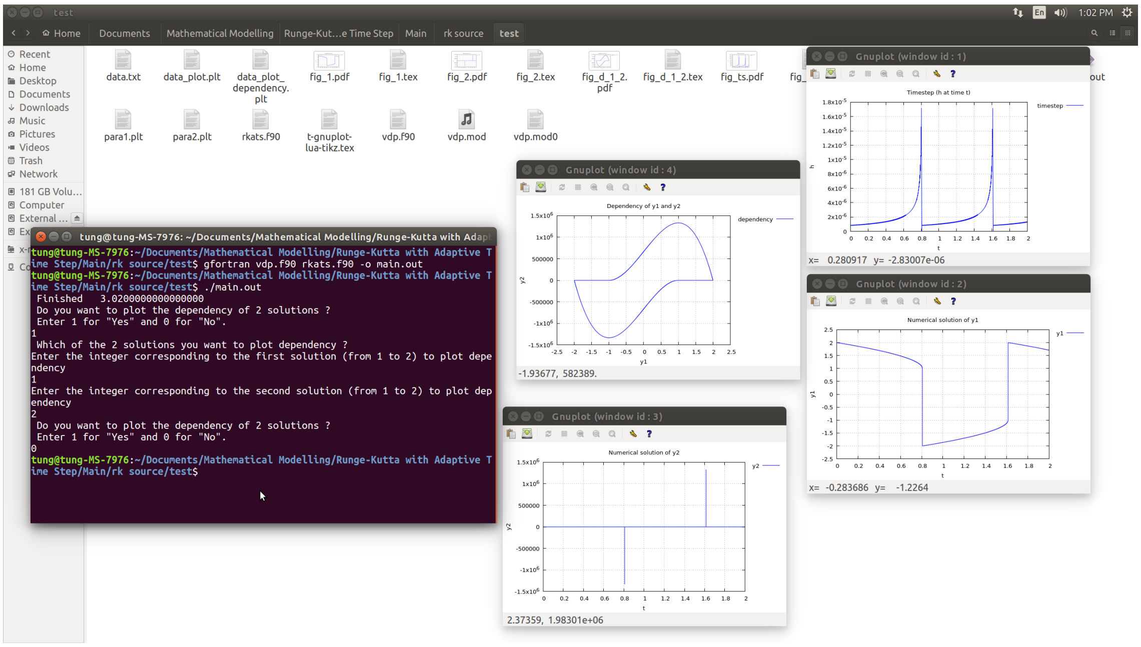
The result will be a new plot of the dependency, like before, additional files of the plot will appear.



```
tung@tung-MS-7976:~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive T
ime Step/Main/rk source/test$ gfortran vdp.f90 rkats.f90 -o main.out
tung@tung-MS-7976:~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive T
ime Step/Main/rk source/test$ ./main.out
 Finished   3.0200000000000000
 Do you want to plot the dependency of 2 solutions ?
 Enter 1 for "Yes" and 0 for "No".
1
 Which of the 2 solutions you want to plot dependency ?
Enter the integer corresponding to the first solution (from 1 to 2) to plot depe
ndency
1
Enter the integer corresponding to the second solution (from 1 to 2) to plot dep
endency
2
 Do you want to plot the dependency of 2 solutions ?
 Enter 1 for "Yes" and 0 for "No".
```

Figure 13: The result look like this

Now, if you want to continue plotting dependency (maybe if the equation you want to solve has more than 2 variables), type 1, or if you want to stop, type 0.



```
tung@tung-MS-7976:~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive T
ime Step/Main/rk source/test$ gfortran vdp.f90 rkats.f90 -o main.out
tung@tung-MS-7976:~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive T
ime Step/Main/rk source/test$ ./main.out
 Finished   3.0200000000000000
 Do you want to plot the dependency of 2 solutions ?
 Enter 1 for "Yes" and 0 for "No".
1
 Which of the 2 solutions you want to plot dependency ?
Enter the integer corresponding to the first solution (from 1 to 2) to plot depe
ndency
1
Enter the integer corresponding to the second solution (from 1 to 2) to plot dep
endency
2
 Do you want to plot the dependency of 2 solutions ?
 Enter 1 for "Yes" and 0 for "No".
0
tung@tung-MS-7976:~/Documents/Mathematical Modelling/Runge-Kutta with Adaptive T
ime Step/Main/rk source/test$
```

Figure 14: The program is stopped

References

[1] Tan Trung Nguyen, Frederique Laurent, Rodney Fox, Marc Massot. *Solution of population balance equations in applications with fine particles: mathematical modeling and numerical schemes.* Journal of Computational Physics, Elsevier, 2016, 325

[2] Nguyen Quan Ba Hong, Doan Tran Nguyen Tung, Nguyen An Thinh, *Runge Kutta methods for Ordinary Differential Equations*, 2016.

[3] `http://fortranwiki.org/fortran/show/HomePage`