

We can write this simply in matrix notation as

$$\frac{d}{dt} [N(t)] = [A(t)] [N(t)].$$

We can integrate this analytically as

$$[N(t)] = [N(0)] \exp \left\{ \int_0^t [A(t')] dt' \right\}.$$

We can make an assumption that we take the matrix inside the integrate at time t if it does not rapidly change. Therefore, the final equation is

$$[N(t)] = [N(0)] \exp \{ [A(t)] t \}.$$

The exponential term on the right hand side is known as the *matrix exponential*. There are many ways to approximate this. In this Fortran implementation we use a dense Pade approximation available in the external solver package *EXPOFIT*. We can discretize the system for any time step, k , as

$$[N^k] = [N^{k-1}] \exp \{ [A^k] dt^{k-1} \}.$$

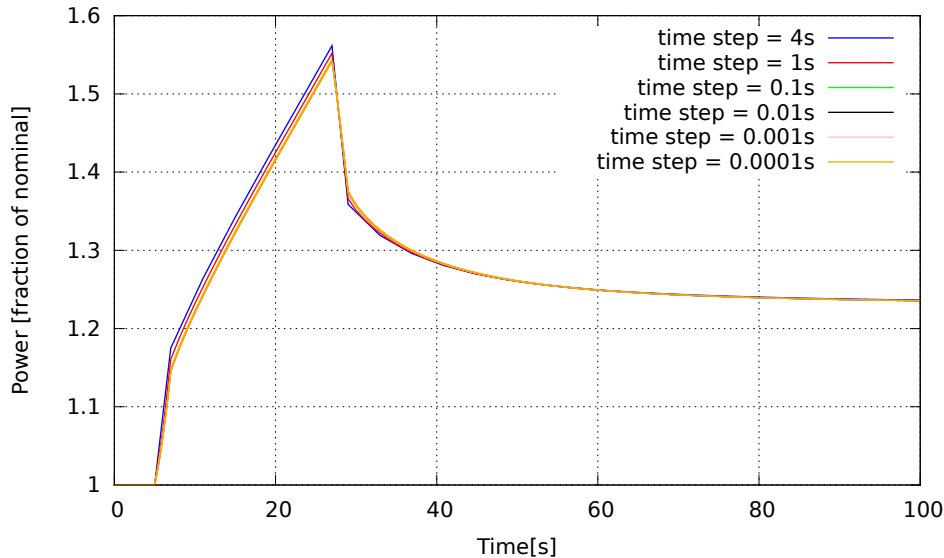
The source code to the main point kinetics is listed in the Appendix.

Part B

From the output of the code, the total value of beta and pnl is:

$$\beta = \quad \Lambda = .$$

The output of a point kinetics run can be viewed in the Appendix. Figure __ below shows fraction power vs. time during the transient for different time steps.



Source Code

Point Kinetics Main Physics Solver

```
!=====!  
! MODULE: global  
!  
!> @author Bryan Herman  
!>  
!> @brief Contains all of the global variables  
!=====!  
module physics  
  
!-module options  
  
    implicit none  
    private  
    public :: run_kinetics  
  
contains  
  
!=====!  
! RUN_KINETICS  
!=====!  
  
    subroutine run_kinetics()  
  
!-----external references  
  
        use constants,    only: NUM_PRECS  
        use expokit,      only: dense_pade  
        use global,       only: pke  
        use output,       only: header  
  
!-----local variables  
  
        integer :: i ! loop counter  
        real(8) :: dt ! local time step  
  
!-----begin execution  
  
        ! print header for run  
        call header("POINT KINETICS SIMULATION", level=1)  
  
        ! set up coefficient matrix  
        call setup_coefmat()
```

```

! set up initial conditions
call set_init()

! begin loop through time steps
do i = 1, sum(pke % nt)

    ! compute exponential matrix
    call set_reactivity(i,dt)

    ! solve matrix exponential
    call dense_pade(pke % coef, NUM_PRECS + 1, dt, pke % expm)

    ! get new vector
    pke % N(:,i+1) = matmul(pke % expm, pke % N(:,i))

end do

end subroutine run_kinetics

```

```

! SETUP_COEFMAT

```

```

subroutine setup_coefmat()

!——external references

    use constants,    only: beta, NUM_PRECS, lambda, pnl
    use global,       only: pke

!——local variables

    integer :: i ! loop counter

!——begin execution

    ! set up coefficient matrix manually for time 0
    pke % coef(1,1) = (pke % rho(1)*sum(beta) - sum(beta))/pnl

    ! begin loop around rest of matrix
    do i = 2, NUM_PRECS + 1

        ! set row 1
        pke % coef(1,i) = lambda(i - 1)

        ! set diagonal
        pke % coef(i,i) = -lambda(i - 1)
    
```

```

        ! set column 1
        pke % coef(i,1) = beta(i-1) / pnl

    end do

end subroutine setup_coefmat

=====
! SET_INIT
=====

subroutine set_init()

!——external references

    use constants,    only: ONE, beta, lambda, pnl, NUM_PRECS
    use global,       only: pke

!——local variables

    integer :: i ! loop counter

!——begin execution

    ! set power at 1.0
    pke % N(1,1) = ONE

    ! loop through precursors
    do i = 1, NUM_PRECS

        ! set initial value
        pke % N(i+1,1) = beta(i)/(pnl*lambda(i)) * pke % N(1,1)

    end do

end subroutine set_init

=====
! SET_REACTIVITY
=====

subroutine set_reactivity(i,dt)

!——external references

    use constants,    only: beta, pnl

```

```

    use global,      only: pke

!-----arguments

    integer :: i      ! current time step
    real(8) :: dt      ! current dt

!-----local variables

    integer :: idx ! interpolation index

!-----begin execution

    ! check if index should be moved in input vectors
    if (i > sum(pke % nt(1:pke % idx))) pke % idx = pke % idx + 1
    idx = pke % idx

    ! compute current time
    dt = pke % dt(idx)
    pke % time(i+1) = pke % time(i) + dt

    ! interpolate on reactivity
    pke % react(i) = pke % rho(idx) + ((pke % rho(idx+1) - pke % rho(idx)) / &
                                         (pke % t(idx + 1) - pke % t(idx))) * &
                                         (pke % time(i+1) - pke % t(idx))

    ! set values in coefficient matrix
    pke % coef(1,1) = (pke % react(i)*sum(beta) - sum(beta))/pnl

end subroutine

end module physics

```

Inverse Point Kinetics Main Physics Solver

```

module physics

!-----module options

    implicit none
    private
    public :: run_invkinetics

contains

!-----

```

```
! RUN_INVKINETICS
```

```
!
```

```
subroutine run_invkinetics()
```

```
!—external references
```

```
use constants,    only: NUM_PRECS, pnl, beta, lambda
use global,       only: ipke, total_time
use output,       only: header
```

```
!—local variables
```

```
integer :: i          ! loop counter
real(8) :: dt          ! local time step
real(8) :: avgpowers ! avg. power between timesteps
```

```
!—begin execution
```

```
! print header for run
```

```
call header("POINT KINETICS SIMULATION", level=1)
```

```
! set initial precursors
```

```
ipke % N(1,1) = ipke % power(1)
```

```
ipke % N(2:NUM_PRECS+1,1) = beta/(pnl*lambda) * ipke % N(1,1)
```

```
! begin loop through time steps
```

```
do i = 1, sum(ipke % nt)
```

```
! compute exponential matrix
```

```
call set_power(i,dt)
```

```
! compute average power
```

```
avgpowers = (ipke % N(1,i) + ipke % N(1,i+1)) / 2.0_8
```

```
! solve for precursors
```

```
ipke %N(2:NUM_PRECS+1,i+1) = ipke % N(2:NUM_PRECS+1,i)*exp(-lambda*dt) + &
beta/(lambda*pnl)*(avgpowers - avgpowers*exp(-lambda*dt))
```

```
! solve for reactivity
```

```
ipke % react(i+1) = pnl/(ipke % N(1,i+1)) *                                &
((ipke % N(1,i+1) - ipke % N(1,i))/dt) +                                &
sum(beta) - pnl/ipke % N(1,i+1) *                                       &
sum(lambda*ipke %N(2:NUM_PRECS+1,i+1))
```

```
! change to dollars
```

```
ipke % react(i+1) = ipke % react(i+1)/sum(beta)
```

```

    end do

end subroutine run_invkinetics

=====
! SET_POWER
=====

subroutine set_power(i,dt)

!——external references

    use constants,    only: beta, pnl
    use global,       only: ipke

!——arguments

    integer :: i      ! current time step
    real(8) :: dt     ! current dt

!——local variables

    integer :: idx ! interpolation index

!——begin execution

    ! check if index should be moved in input vectors
    if (i > sum(ipke % nt(1:ipke % idx))) ipke % idx = ipke % idx + 1
    idx = ipke % idx

    ! compute current time
    dt = ipke % dt(idx)
    ipke % time(i+1) = ipke % time(i) + dt

    ! interpolate on power
    ipke % N(1,i+1) = ((ipke % power(idx+1) - ipke % power(idx)) / &
        (ipke % t(idx + 1) - ipke % t(idx))) * &
        (ipke % time(i+1) - ipke % t(idx)) + &
        ipke % power(idx)

end subroutine set_power

end module physics

```