An informal introduction to NEKNEK

model set-up tutorial

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References/ reading material

[1] MITTAL, K., DUTTA, S., & FISCHER, P. (2019). Nonconforming Schwarz-spectral element methods for incompressible flow. *Computers & Fluids*, *191*, 104237.

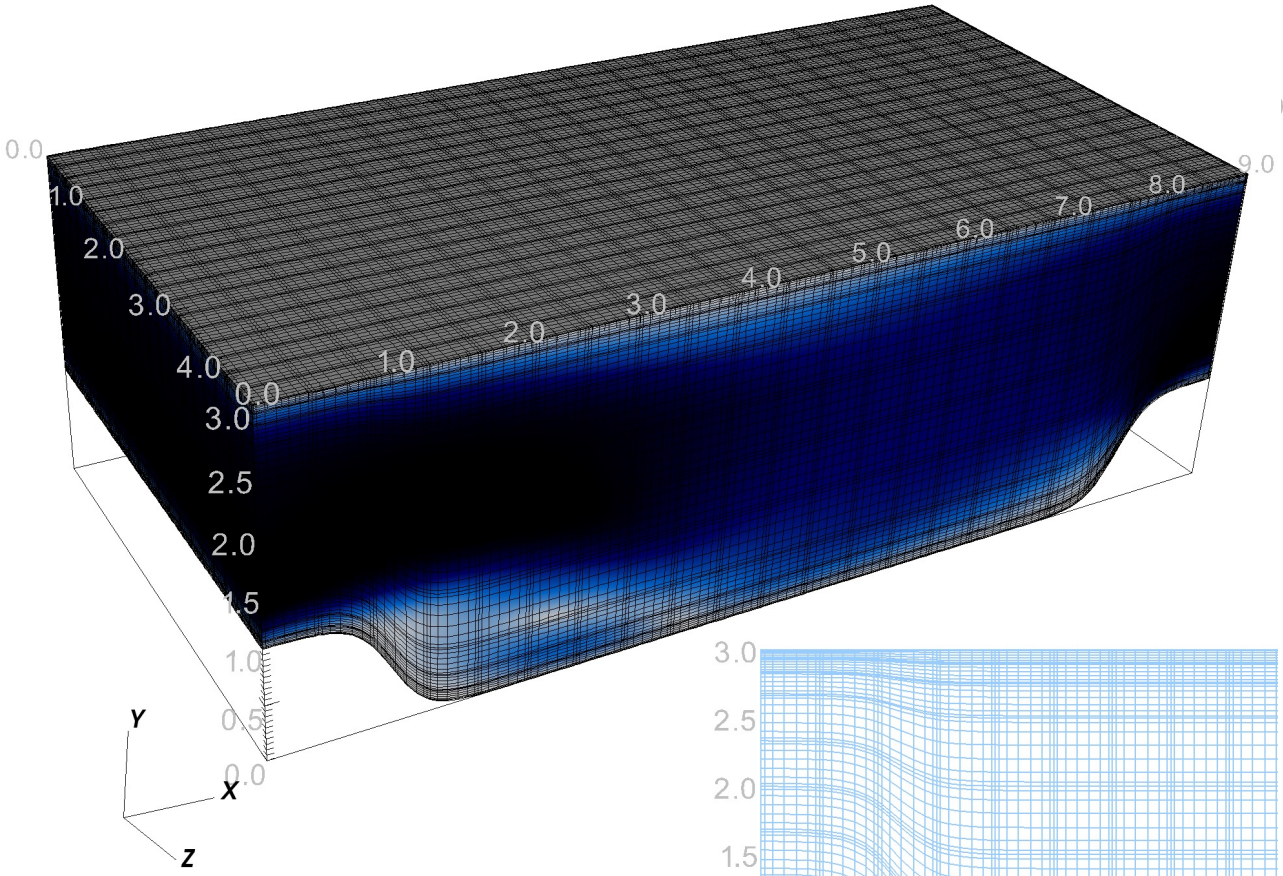
[2] MITTAL, K., DUTTA, S., & FISCHER, P. (2021). Multirate timestepping for the incompressible Navier-Stokes equations in overlapping grids. *Journal of Computational Physics*, *437*, 110335.

[3] MITTAL, K. (2019). Highly scalable solution of incompressible Navier-Stokes equations using the spectral element method with overlapping grids. *University of Illinois at Urbana-Champaign.*

Today I will focus only on how to use NEKNEK.

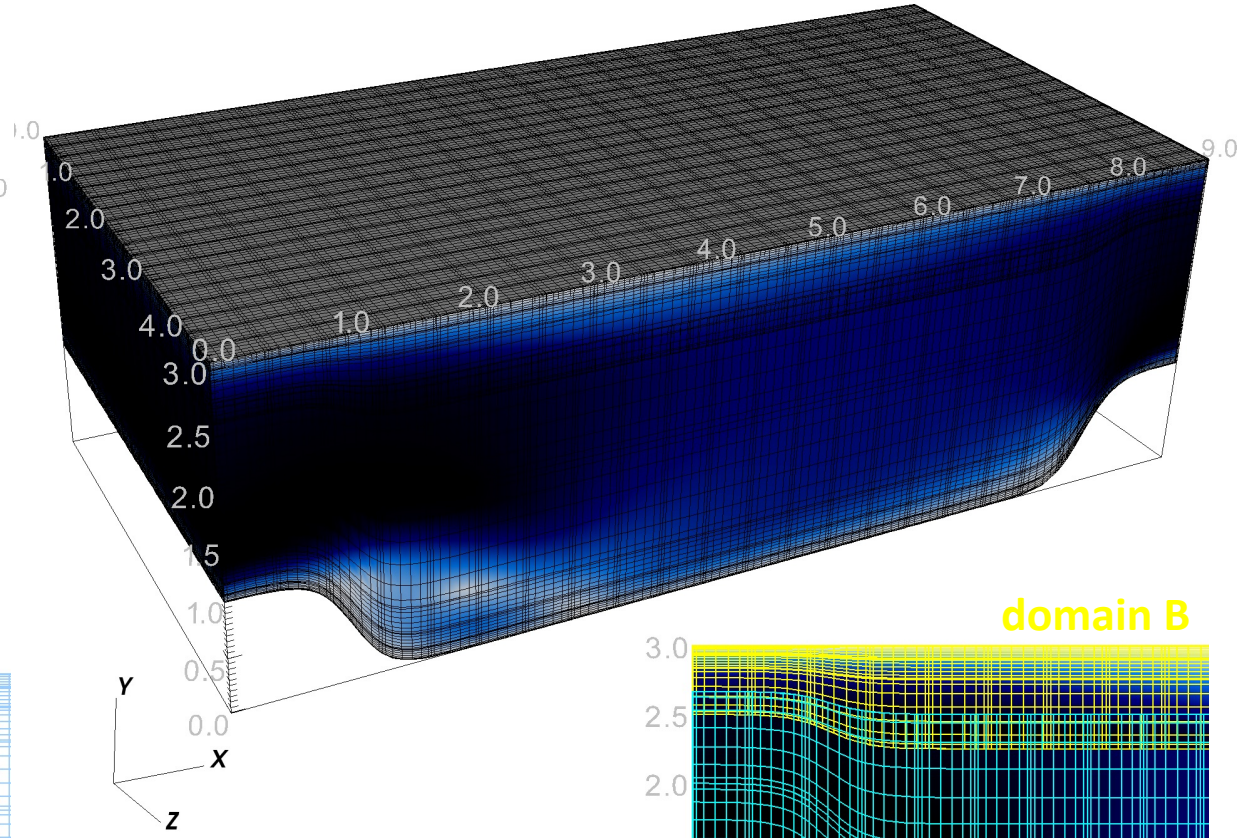
Periodic hill example

NEK5000 – mono-domain simulation

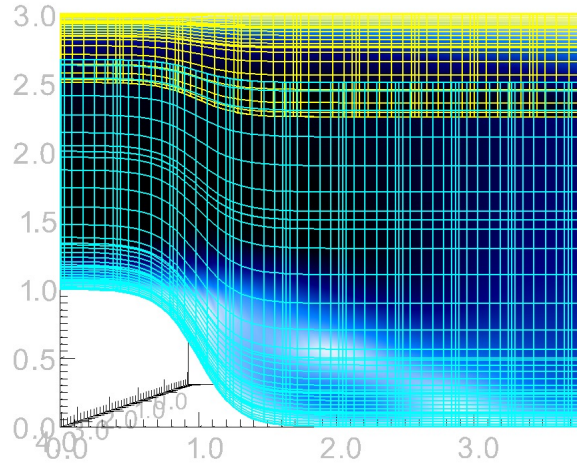


mono-domain

NEK5000 - multiple domain simulation (NEKNEK)



domain B



domain A

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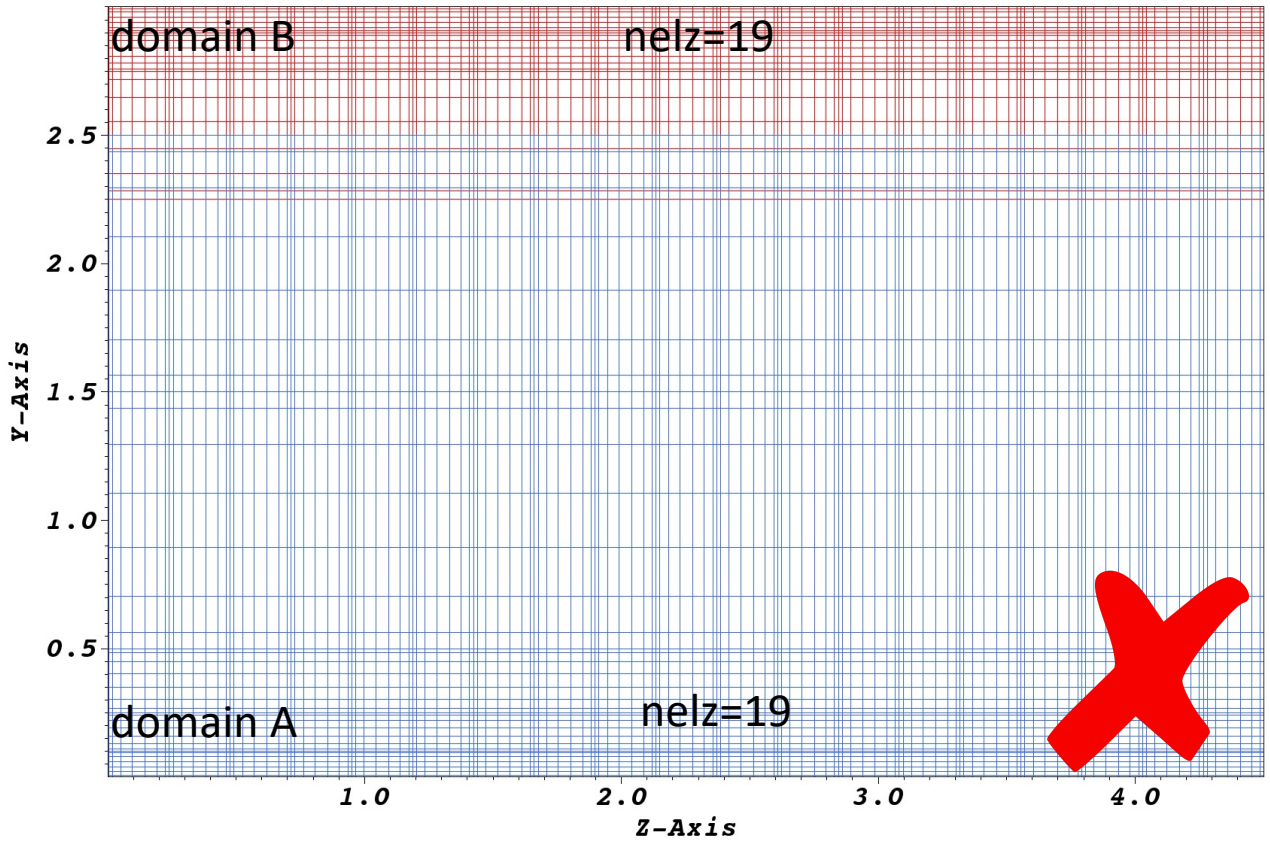
DOs and DON'Ts

- Currently, applying a **constant mass flux** with param(54) and param(55) is **not supported** with overlapping overset grids.
  (this is why we drive the flow using a constant acceleration term in userf)

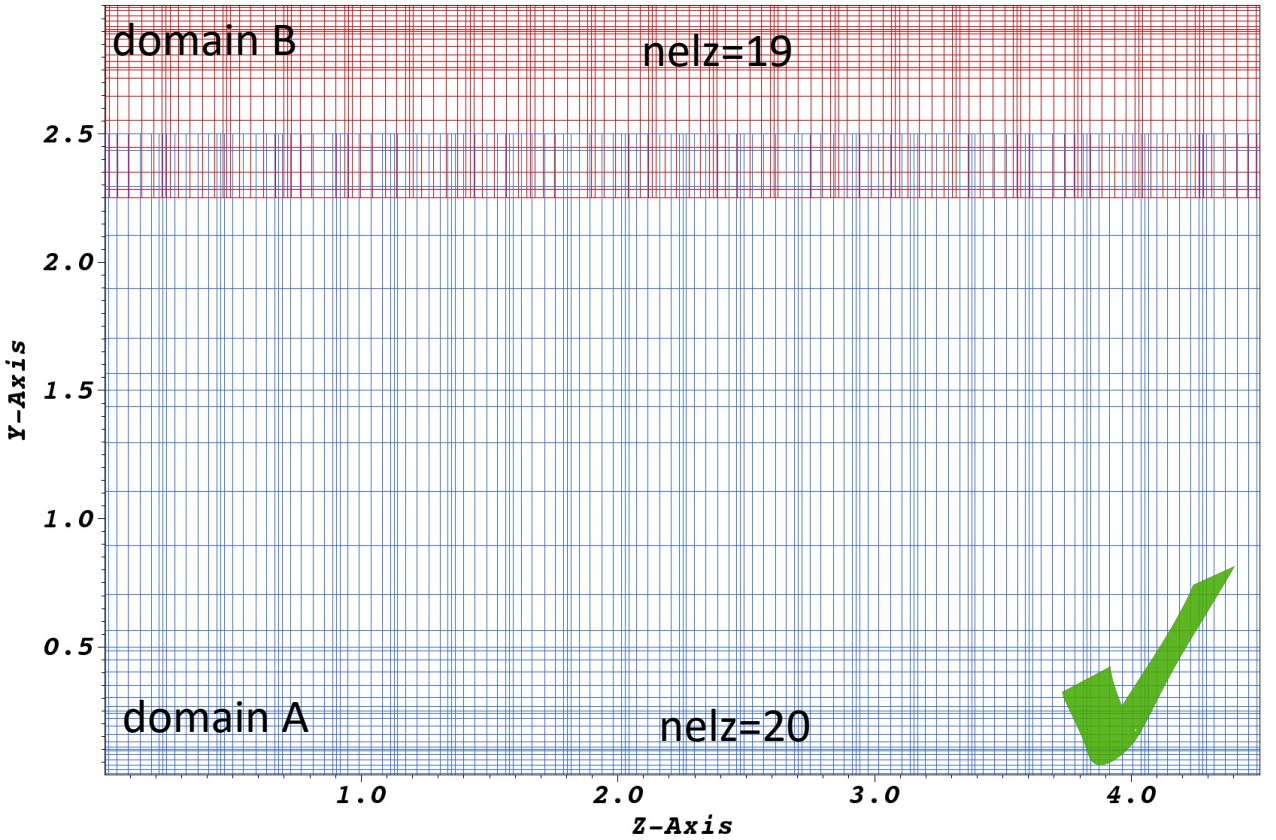
- multiple scalars
- RANS models
- moving geometries
- …

DOs and DON'Ts

avoid aligned/exactly overlapped 1-1 GLL points
at the int interface



prefer not aligned GLL points
at the int interface



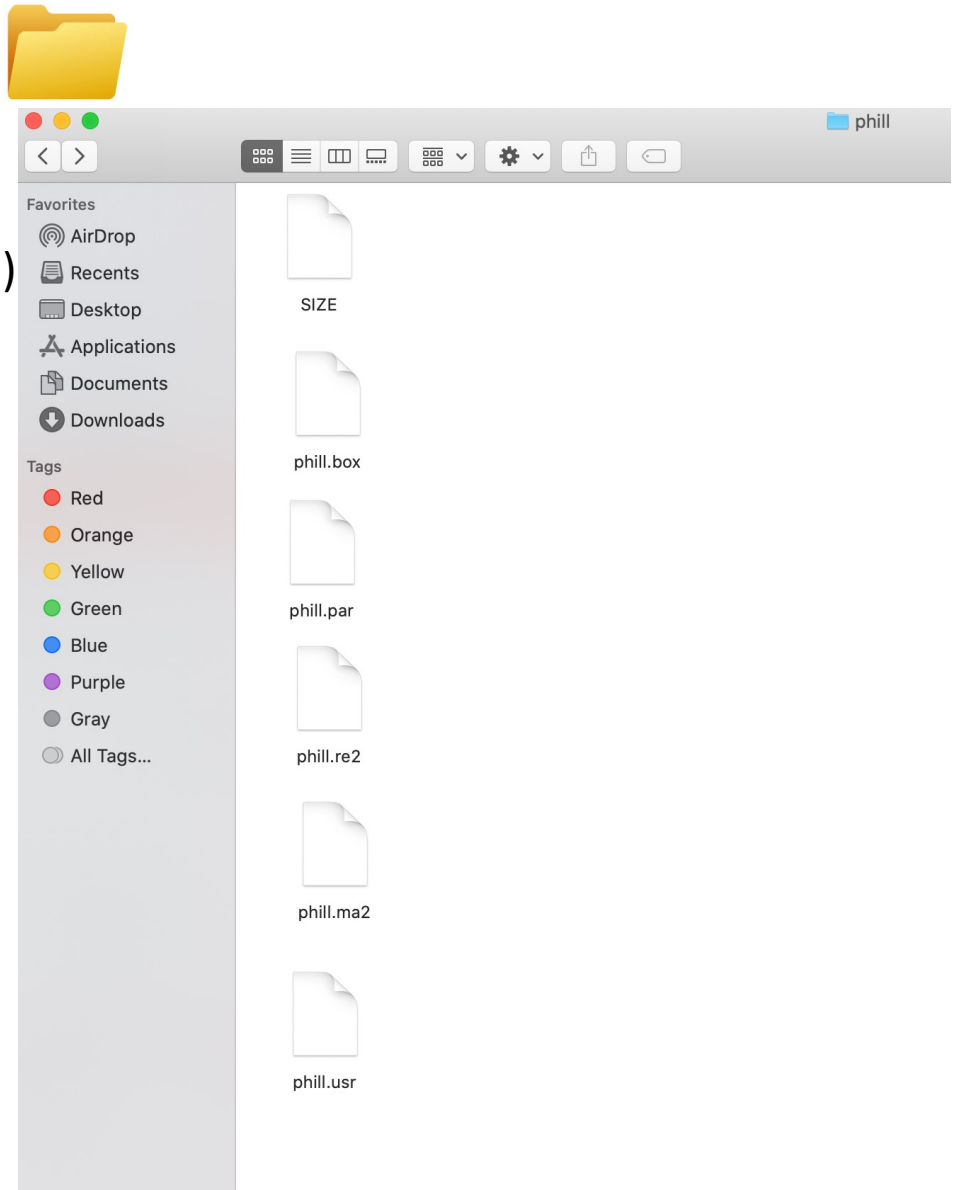
Workflow & files needed for a mono-domain/ single session NEK5000 simulation

files:

- 1 SIZE file
- 1 *box file (optional. used in case genbox is used for the grid generation)
- 1 *.rea (or *.par) file
- 1 *.map (or *.ma2) file
- 1 *.re2 (optional for large problems) file
- 1 *.usr file

steps:

- generate rea or re2 using genbox
  >genbox
  (…)
- generate map files using genmap
  >genmap
  (…)
- compile the code
  >makenek case_name(*.usr)
- run the code
  >nekmpi case_name np



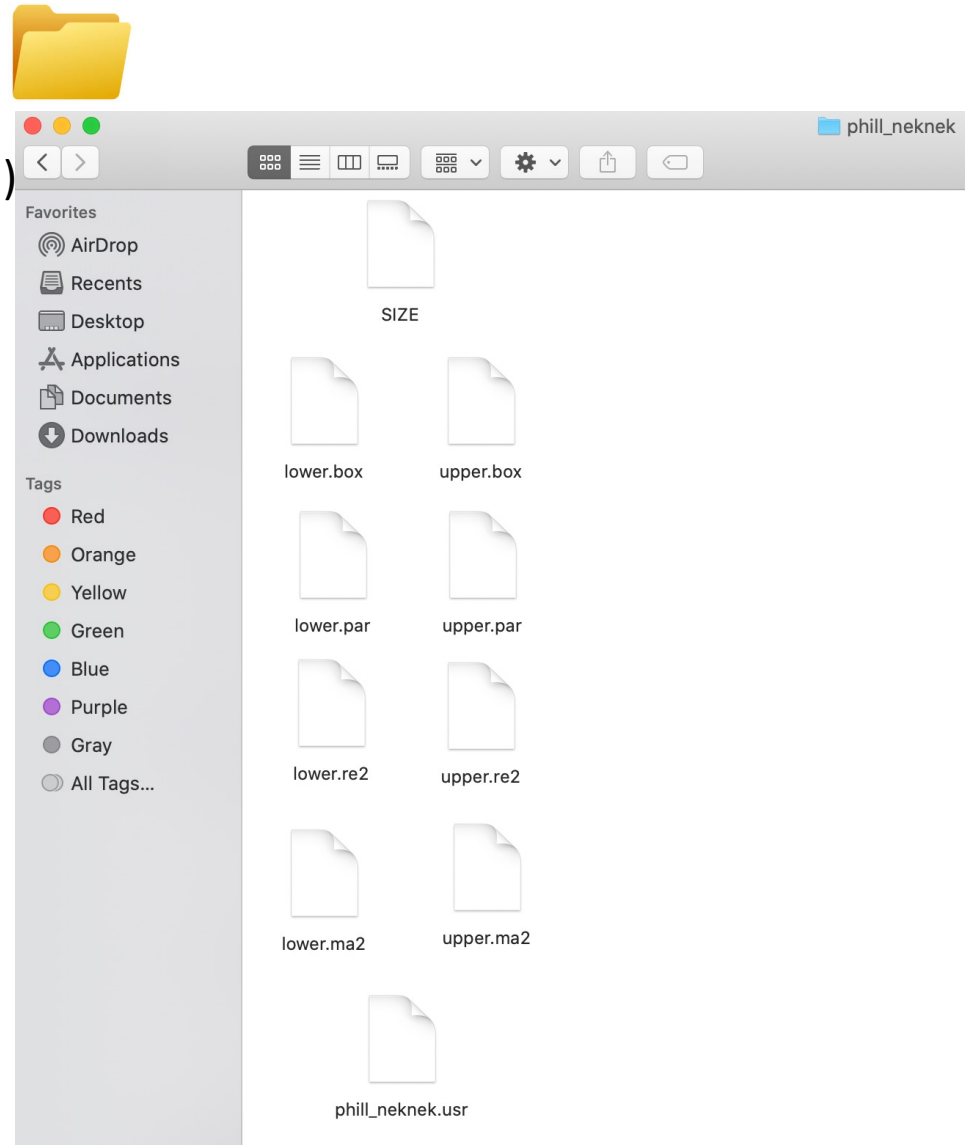
Workflow & files needed for a 2-domain/ 2-session NEKNEK simulation

files:

- 1 SIZE file
- 2 *box files (optional. used in case genbox is used for the grid generation)
- 2 *.rea (or *.par) file
- 2 *.map (or *.ma2) file
- 2 *.re2 (optional for large problems) file
- 1 *.usr file

steps:

- generate rea or re2 using genbox
  >genbox
  (…) 1st domainA
  >genbox
  (…) 2nd domainB
- generate map files using genmap
  >genmap
  (…) 1st domainA
  >genmap
  (…) 2nd domainB
- compile the code
  >makenek case_name(*.usr)
- run the code
  >neknek domainA domainB np np



From a NEK5000 case to NEKNEK

The three key steps to running a case with NekNek are:

1. setting up the mesh with appropriate boundary conditions for the overlapping interface.
   using **int** at the interfaces between the overlapping grids.

lower domain A:

```
#=======================================================================
#
Box
-22 5  -20                              nelx,nely for Box
0.0 9.0 1.0                             x0,xn,gain
0.0 0.1 0.25 0.5 1.5 2.5                y0 y1 ratio
0.0 4.5 1.0                             z0,zn,gain
P  ,P  ,W  ,int,P  ,P
```

upper domain B:

```
#=======================================================================
#
Box
-21 3  -19                              nelx,nely for Box
0.0 9.0 1.0                             x0,xn,gain
2.25 2.75 2.9 3.0                       y0 y1 ratio
0.0 4.5 1.0                             z0,zn,gain
P  ,P  ,int,W  ,P  ,P
```

2. specifying parameters to control stability and accuracy for the overlapping-Schwarz iterations.
   defining the # of sub-iterations at each time-step **ngeom** and **ninter** in usrdat().

```
subroutine usrdat()   ! This routine to modify element vertices

c      implicit none

       include 'SIZE'
       include 'TOTAL'
       include 'NEKNEK' ! DKF: needed for neknek

       ngeom = 5  !DKF: 4 sub-iterations ($ngeom=5$) at each time-step
       ninter = 2 !DKF: the temporal extrapolation order ($ninter$) is 2.


       return
       end
```

3. modifying userbc to read Dirichlet boundary data for the overlapping interfaces.
   typically using **valint(ix,iy,iz,ie,1), valint(ix,iy,iz,ie,2) etc** in userbc()

```
subroutine userbc(ix,iy,iz,iside,eg) ! set up boundary conditions
c
  ...

 if (imask(ix,iy,iz,ie).eq.0) then
  ux=0.0
  uy=0.0
  uz=0.0
  temp=0.0
 else
  ux = valint(ix,iy,iz,ie,1)
  uy = valint(ix,iy,iz,ie,2)
  uz = valint(ix,iy,iz,ie,3)
 if (nfld_neknek.gt.3) temp = valint(ix,iy,iz,ie,ldim+2)
 end if
```

From a NEK5000 case to NEKNEK

SIZE files:

mono-domain case:

```
c
c     Include file to dimension static arrays
c     and to set some hardwired run-time parameters
c
      integer ldim,lx1,lxd,lx2,lx1m,lelg,lelt,lpmin,ldimt
      integer lpelt,lbelt,toteq,lcvelt
      integer lelx,lely,lelz,mxprev,lgmres,lorder,lhis
      integer maxobj,lpert,nsessmax,lxo
      integer lfdm,ldimt_proj,lelr

      ! BASIC
      parameter (ldim=3)               ! domain dimension (2 or 3)
      parameter (lx1=8)                ! GLL points per element along each direction
      parameter (lxd=12)               ! GL  points for over-integration (dealiasing)
      parameter (lx2=lx1-2)            ! GLL points for pressure (lx1 or lx1-2)

      parameter (lelg=13000)            ! max number of global elements
      parameter (lpmin=32)             ! min number of MPI ranks
      parameter (lelt=lelg/lpmin + 3)  ! max number of local elements per MPI rank
      parameter (ldimt=1)              ! max auxiliary fields (temperature + scalars)

      ! OPTIONAL
      parameter (ldimt_proj=1)         ! max auxiliary fields residual projection
      parameter (lelr=lelt)            ! max number of local elements per restart file
      parameter (lhis=1)               ! max history/monitoring points
      parameter (maxobj=2)             ! max number of objects
      parameter (lpert=1)              ! max number of perturbations
      parameter (toteq=1)              ! max number of conserved scalars in CMT
      parameter (nsessmax=1)           ! max sessions to NEKNEK
      parameter (lxo=lx1)              ! max GLL points on output (lxo>=lx1)
      parameter (mxprev=20,lgmres=30)  ! max dim of projection & Krylov space
      parameter (lorder=3)             ! max order in time
      parameter (lx1m=1)               ! GLL points mesh solver
      parameter (lfdm=0)               ! unused
      parameter (lelx=1,lely=1,lelz=1) ! global tensor mesh dimensions

      parameter (lbelt=1)              ! lelt for mhd
      parameter (lpelt=1)              ! lelt for linear stability
      parameter (lcvelt=1)             ! lelt for cvode

      ! INTERNALS
      include 'SIZE.inc'
```

2-domain case:

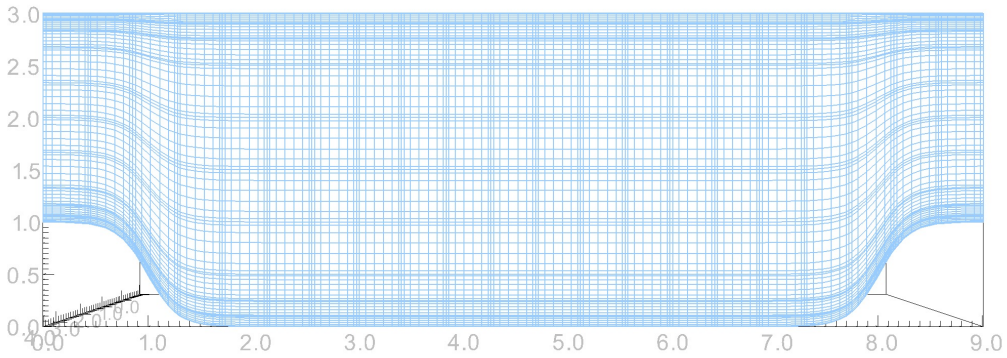
```
c
c     Include file to dimension static arrays
c     and to set some hardwired run-time parameters
c
      integer ldim,lx1,lxd,lx2,lx1m,lelg,lelt,lpmin,ldimt
      integer lpelt,lbelt,toteq,lcvelt
      integer lelx,lely,lelz,mxprev,lgmres,lorder,lhis
      integer maxobj,lpert,nsessmax,lxo
      integer lfdm,ldimt_proj,lelr

      ! BASIC
      parameter (ldim=3)               ! domain dimension (2 or 3)
      parameter (lx1=8)                ! GLL points per element along each direction
      parameter (lxd=12)               ! GL  points for over-integration (dealiasing)
      parameter (lx2=lx1-2)            ! GLL points for pressure (lx1 or lx1-2)

      parameter (lelg=13000)            ! max number of global elements
      parameter (lpmin=32)             ! min number of MPI ranks
      parameter (lelt=lelg/lpmin + 3)  ! max number of local elements per MPI rank
      parameter (ldimt=1)              ! max auxiliary fields (temperature + scalars)

      ! OPTIONAL
      parameter (ldimt_proj=1)         ! max auxiliary fields residual projection
      parameter (lelr=lelt)            ! max number of local elements per restart file
      parameter (lhis=1)               ! max history/monitoring points
      parameter (maxobj=2)             ! max number of objects
      parameter (lpert=1)              ! max number of perturbations
      parameter (toteq=1)              ! max number of conserved scalars in CMT
      parameter (nsessmax=2)           ! max sessions to NEKNEK                    !DKF: 1 --> 2 for two domains
      parameter (lxo=lx1)              ! max GLL points on output (lxo>=lx1)
      parameter (mxprev=20,lgmres=30)  ! max dim of projection & Krylov space
      parameter (lorder=3)             ! max order in time
      parameter (lx1m=1)               ! GLL points mesh solver
      parameter (lfdm=0)               ! unused
      parameter (lelx=1,lely=1,lelz=1) ! global tensor mesh dimensions

      parameter (lbelt=1)              ! lelt for mhd
      parameter (lpelt=1)              ! lelt for linear stability
      parameter (lcvelt=1)             ! lelt for cvode

      ! INTERNALS
      include 'SIZE.inc'
```

From a NEK5000 case to NEKNEK

*.box files:

mono-domain case:

```
-3                      spatial dimension
1                       number of fields (U)
#=======================================================================
#
#   .box file for channel flow
#
#    If nelx (y or z) < 0, then genbox automatically generates the
#                          grid spacing in the x (y or z) direction
#                          with a geometric ratio given by "ratio".
#                          ( ratio=1 implies uniform spacing )
#
#    Note that the character bcs _must_ have 3 spaces.
#
#=======================================================================
#
Box
-21 10 -19                              nelx,nely for Box
0.0 9.0 1.0                             x0,xn,gain
0.0 0.1 0.25 0.5 1.0
1.5 2.0 2.5 2.75  2.9 3.0               y0 y1 ratio
0.0 4.5 1.0                             z0,zn,gain
P  ,P  ,W  ,W  ,P  ,P
```



mono-domain

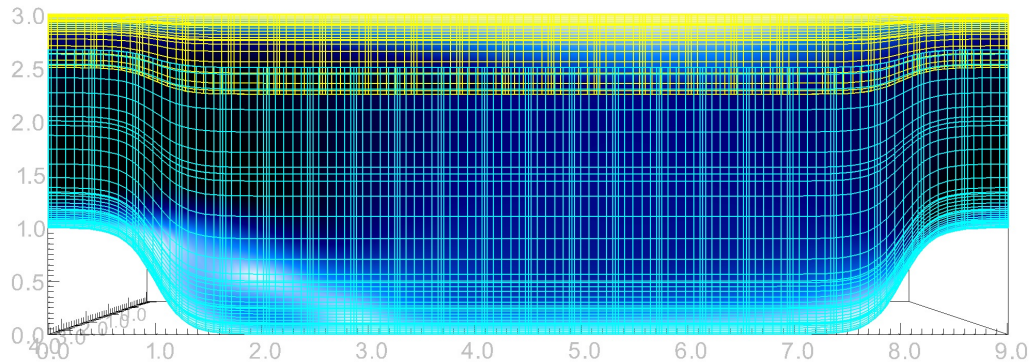
2-domain case:

domain A

```
-3                      spatial dimension
1                       number of fields (U)
#=======================================================
#
#   .box file for channel flow
#
#    If nelx (y or z) < 0, then genbox automaticall
#                          grid spacing in the x (y
#                          with a geometric ratio g
#                          ( ratio=1 implies unifor
#
#    Note that the character bcs _must_ have 3 spac
#
#=======================================================
#
Box
-22 5  -20                      nelx,nely for Box
0.0 9.0 1.0                     x0,xn,gain
0.0 0.1 0.25 0.5 1.5 2.5        y0 y1 ratio
0.0 4.5 1.0                     z0,zn,gain
P  ,P  ,W  ,int,P  ,P
```

domain B

```
-3                      spatial dimension
1                       number of fields (U)
#=======================================================
#
#   .box file for channel flow
#
#    If nelx (y or z) < 0, then genbox automatical
#                          grid spacing in the x (
#                          with a geometric ratio
#                          ( ratio=1 implies unifo
#
#    Note that the character bcs _must_ have 3 spa
#
#=======================================================
#
Box
-21 3  -19                      nelx,nely for Box
0.0 9.0 1.0                     x0,xn,gain
2.25 2.75 2.9 3.0               y0 y1 ratio
0.0 4.5 1.0                     z0,zn,gain
P  ,P  ,int,W  ,P  ,P
```



domain B

domain A

From a NEK5000 case to NEKNEK

*.par files:

mono-domain case:

```
#
# nek parameter file
#
[GENERAL]
#startFrom =
stopAt = endTime #endTime numSteps
endTime = 200.0
numSteps =500

dt = 5e-03
timeStepper = bdf3 #char #steady
variableDt = yes
targetCFL = 0.4

writeControl = runTime #runTime timeStep
writeInterval = 0.1

dealiasing = yes
filtering = hpfrt #hpfrt, none, explicit
filterWeight = 10.0
filterCutoffRatio = 0.9

[PROBLEMTYPE]
equation = incompNS
stressFormulation = no
variableProperties = no

[PRESSURE]
preconditioner = semg_xxt
residualTol = 1e-5
residualProj = yes

[VELOCITY]
residualTol = 1e-8
residualProj = yes
density = 1.0
viscosity = -100
advection = yes
```

2-domain case:

domain A

```
#
# nek parameter file
#
[GENERAL]
#startFrom =
stopAt = endTime #endTime numSteps
endTime = 200.0
numSteps =500

dt = 5e-03
timeStepper = bdf3 #char #steady
variableDt = yes
targetCFL = 0.4

writeControl = runTime #runTime timeStep
writeInterval = 0.1

dealiasing = yes
filtering = hpfrt #hpfrt, none, explicit
filterWeight = 10.0
filterCutoffRatio = 0.9

[PROBLEMTYPE]
equation = incompNS
stressFormulation = no
variableProperties = no

[PRESSURE]
preconditioner = semg_xxt
residualTol = 1e-5
residualProj = yes

[VELOCITY]
residualTol = 1e-8
residualProj = yes
density = 1.0
viscosity = -100
advection = yes
```

domain B

```
#
# nek parameter file
#
[GENERAL]
#startFrom =
stopAt = endTime #endTime numSteps
endTime = 200.0
numSteps =500

dt = 5e-03
timeStepper = bdf3 #char #steady
variableDt = yes
targetCFL = 0.4

writeControl = runTime #runTime timeStep
writeInterval = 0.1

dealiasing = yes
filtering = hpfrt #hpfrt, none, explicit
filterWeight = 10.0
filterCutoffRatio = 0.9

[PROBLEMTYPE]
equation = incompNS
stressFormulation = no
variableProperties = no

[PRESSURE]
preconditioner = semg_xxt
residualTol = 1e-5
residualProj = yes

[VELOCITY]
residualTol = 1e-8
residualProj = yes
density = 1.0
viscosity = -100
advection = yes
```

From a NEK5000 case to NEKNEK

*.usr files (1/3, usrdat & usrdat2):

mono-domain case:

```
c-----------------------------------------------------------------------
      subroutine usrdat()   ! This routine to modify element vertices

c      implicit none

      include 'SIZE'
      include 'TOTAL'


      return
      end
c-----------------------------------------------------------------------
      subroutine usrdat2()  ! This routine to modify mesh coordinates

c      implicit none

      include 'SIZE'
      include 'TOTAL'


      integer ntot
      real sa,sb,sc,xx,argx,A1

      ntot = nx1*ny1*nz1*nelt

      sa   = 4.5
      sb   = 3.5
      sc   = 1./6

      do i=1,ntot
        xx   = xm1(i,1,1,1)
        argx = sb*(abs(xx-sa)-sb)
        A1   = sc + sc*tanh(argx)
        ym1(i,1,1,1) = ym1(i,1,1,1) + (3-ym1(i,1,1,1))*A1
      enddo

      return
      end
c-----------------------------------------------------------------------
```

2-domain case:

```
c-----------------------------------------------------------------------
      subroutine usrdat()   ! This routine to modify element vertices

c      implicit none

      include 'SIZE'
      include 'TOTAL'
      include 'NEKNEK' ! DKF: needed for neknek

      ngeom = 5    !DKF: 4 sub-iterations ($ngeom=5$) at each time-step.
      ninter = 2   !DKF: the temporal extrapolation order ($ninter$) is 2.


      return
      end
c-----------------------------------------------------------------------
      subroutine usrdat2()  ! This routine to modify mesh coordinates

c      implicit none

      include 'SIZE'
      include 'TOTAL'


      integer ntot
      real sa,sb,sc,xx,argx,A1

      ntot = nx1*ny1*nz1*nelt

      sa   = 4.5
      sb   = 3.5
      sc   = 1./6

      do i=1,ntot
        xx   = xm1(i,1,1,1)
        argx = sb*(abs(xx-sa)-sb)
        A1   = sc + sc*tanh(argx)
        ym1(i,1,1,1) = ym1(i,1,1,1) + (3-ym1(i,1,1,1))*A1
      enddo

      return
      end
c-----------------------------------------------------------------------
```

From a NEK5000 case to NEKNEK

domain A
domain B

*.usr files (2/3, userf):

mono-domain case:

```
c-----------------------------------------------------------------------
      subroutine userf(ix,iy,iz,eg) ! set acceleration term
c
c     Note: this is an acceleration term, NOT a force!
c     Thus, ffx will subsequently be multiplied by rho(x,t).
c
c      implicit none
      integer ix,iy,iz,eg

      include 'SIZE'
      include 'TOTAL'
      include 'NEKUSE'

      integer e
!     e = gllel(eg)

      ffx = 0.052
      ffy = 0.0
      ffz = 0.0
      return
      end
c-----------------------------------------------------------------------
```

2-domain case:

```
c-----------------------------------------------------------------------
      subroutine userf(ix,iy,iz,eg) ! set acceleration term
c
c     Note: this is an acceleration term, NOT a force!
c     Thus, ffx will subsequently be multiplied by rho(x,t).
c
c      implicit none
      integer ix,iy,iz,eg

      include 'SIZE'
      include 'TOTAL'
      include 'NEKUSE'

      integer e
!     e = gllel(eg)

      ffx = 0.052
      ffy = 0.0
      ffz = 0.0
      return
      end
c-----------------------------------------------------------------------
```

no changes needed

From a NEK5000 case to NEKNEK

domain A
domain B

*.usr files (3/3, userbc & useric):

mono-domain case:

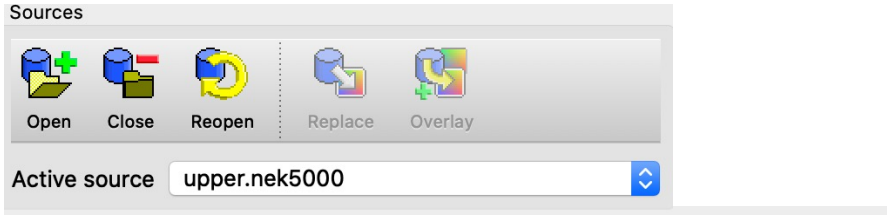
```
c-----------------------------------------------------------------------
      subroutine userbc(ix,iy,iz,iside,eg) ! set up boundary conditions
c
c     NOTE ::: This subroutine MAY NOT be called by every process
c
c      implicit none

      integer ix,iy,iz,iside,eg

      include 'SIZE'
      include 'TOTAL'
      include 'NEKUSE'

      ie = gllel(eg) ! global element number to processor-local element #
       ux=0.0
       uy=0.0
       uz=0.0
       temp=0.0

      return
      end
c-----------------------------------------------------------------------
      subroutine useric(ix,iy,iz,eg) ! set up initial conditions

c      implicit none

      integer ix,iy,iz,eg

      include 'SIZE'
      include 'TOTAL'
      include 'NEKUSE'

      ux   = 1.0
      uy   = 0.0
      uz   = 0.0
      temp = 0.0

      return
      end
c-----------------------------------------------------------------------
```

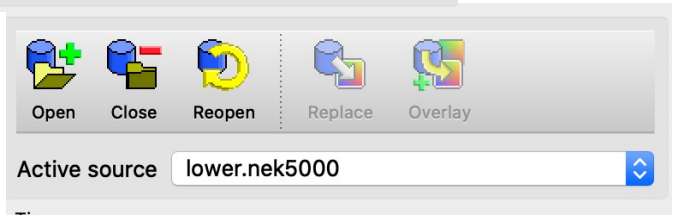
2-domain case:

```
c-----------------------------------------------------------------------
      subroutine userbc(ix,iy,iz,iside,eg) ! set up boundary conditions
c
c     NOTE ::: This subroutine MAY NOT be called by every process
c
c      implicit none

      integer ix,iy,iz,iside,eg

      include 'SIZE'
      include 'TOTAL'
      include 'NEKUSE'
      include 'NEKNEK' !DKF: needed for neknek

      ie = gllel(eg) ! global element number to processor-local element #

      !DKF: imask.eq.0 at points with

      if (imask(ix,iy,iz,ie).eq.0) then
       ux=0.0
       uy=0.0
       uz=0.0
       temp=0.0
      else
       ux = valint(ix,iy,iz,ie,1)
       uy = valint(ix,iy,iz,ie,2)
       uz = valint(ix,iy,iz,ie,3)
      if (nfld_neknek.gt.3) temp = valint(ix,iy,iz,ie,ldim+2)
      end if

      return
      end
c-----------------------------------------------------------------------
      subroutine useric(ix,iy,iz,eg) ! set up initial conditions

c      implicit none

      integer ix,iy,iz,eg

      include 'SIZE'
      include 'TOTAL'
      include 'NEKUSE'

      ux   = 1.0
      uy   = 0.0
      uz   = 0.0
      temp = 0.0

      return
      end
c-----------------------------------------------------------------------
```

Visualization using visit

- Load each domain's*.nek5000 file individually





- Create an "index database correlation"