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LLNL contributions to ANL Report ANL/NE-16/6 "Sharp User Manual"

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Disclaimer

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Using Diablo in the SHARP framework

Diablo is a Multiphysics implicit finite element code with an emphasis on coupled structural/thermal analysis. In the SHARP framework, it is used as the structural solver, and may also be used as the mesh smoother.

In the current SHARP implementation, Diablo receives temperatures from Nek5000, which are calculated in a coupled fashion with the PROTEUS neutronics code. The change in temperatures induces thermal stresses in the structural model. Diablo then performs one or more Newton (or Quasi-Newton) iterations until the structural solve is converged (meaning the structure is once more in equilibrium), and then returns the deformed configuration to the rest of SHARP.

Diablo may also be used as the mesh smoother for SHARP (currently this is the only method tested). Diablo accomplishes this task by solving a solid mechanics problem for a domain that includes the entire domain, including the fluid domain. The two tools by which this is accomplished are "pseudo-materials" and "duplication"

Pseudo-materials are simply choices of material parameters for regions which are not structural, e.g. the fluid regions and other regions for which a structural calculation is not desired. Typically one would choose an elastic material (e.g. material model 1, 15, or 27) with small values of elastic constants, e.g. $1/100^{th}$ or $1/1000^{th}$ of the typical values of the structural materials. The smaller the value the more accurate the structural solution, but the more difficult the conditioning of the resulting linear system is, which may result in a less efficient solution. Choosing a direct linear solver such as WSMP or MUMPS is generally preferable because they are less sensitive to the condition number of the matrix. Typically it is advantageous to provide pseudo-materials with a realistic value of the coefficient of thermal expansion

Duplication allows an element set to be "duplicated", including all the associated nodes and elements. This allows the mesh smoother to operate independently, in some sense, from the solid mechanics solution.

An example of duplication is the provided by the following diagram:

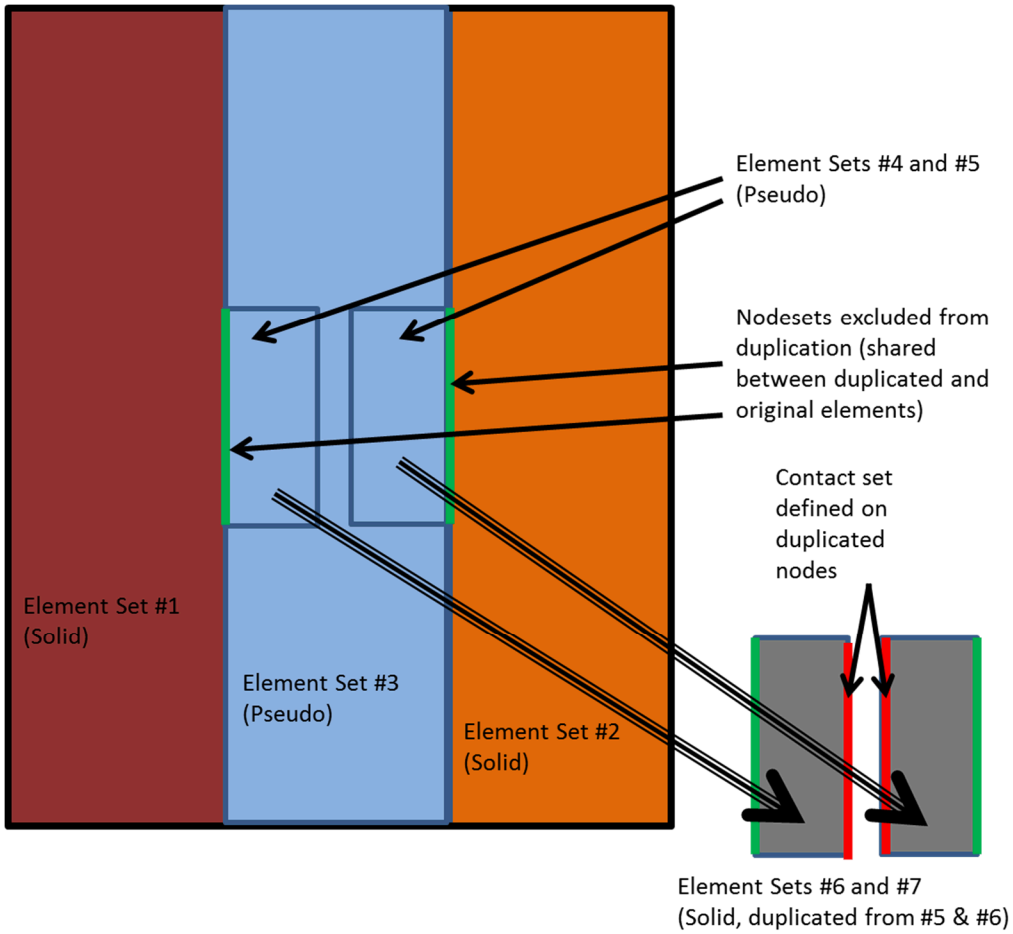

Figure 1 - SHARP/Diablo usage

In the figure, element sets #1 and #2 represent structural material that is shared between the rest of SHARP (e.g. PROTEUS and NEK) and Diablo. Element Set #3 represents fluid material that is modeled as pseudo-material in Diablo. Element sets #5 and #6 represent material that is structural, but represented as fluid in Nek and PROTEUS (e.g. pads). In order to represent the structural response, the element sets are duplicated as element sets #6 and #7. A contact set between the two duplicated element sets(e.g. 6 and 7) is defined on the duplicated nodes (in red). The green node set (or, equivalently, sideset) represents nodes that are shared by both the duplicated and the unduplicated elements (in order that the duplicated elements may be coupled structurally to the rest of the mesh). By means of selective use of duplicated element sets, and duplicated and excluded node sets, the structural response of a reactor may be modeled, as per Figure 2.

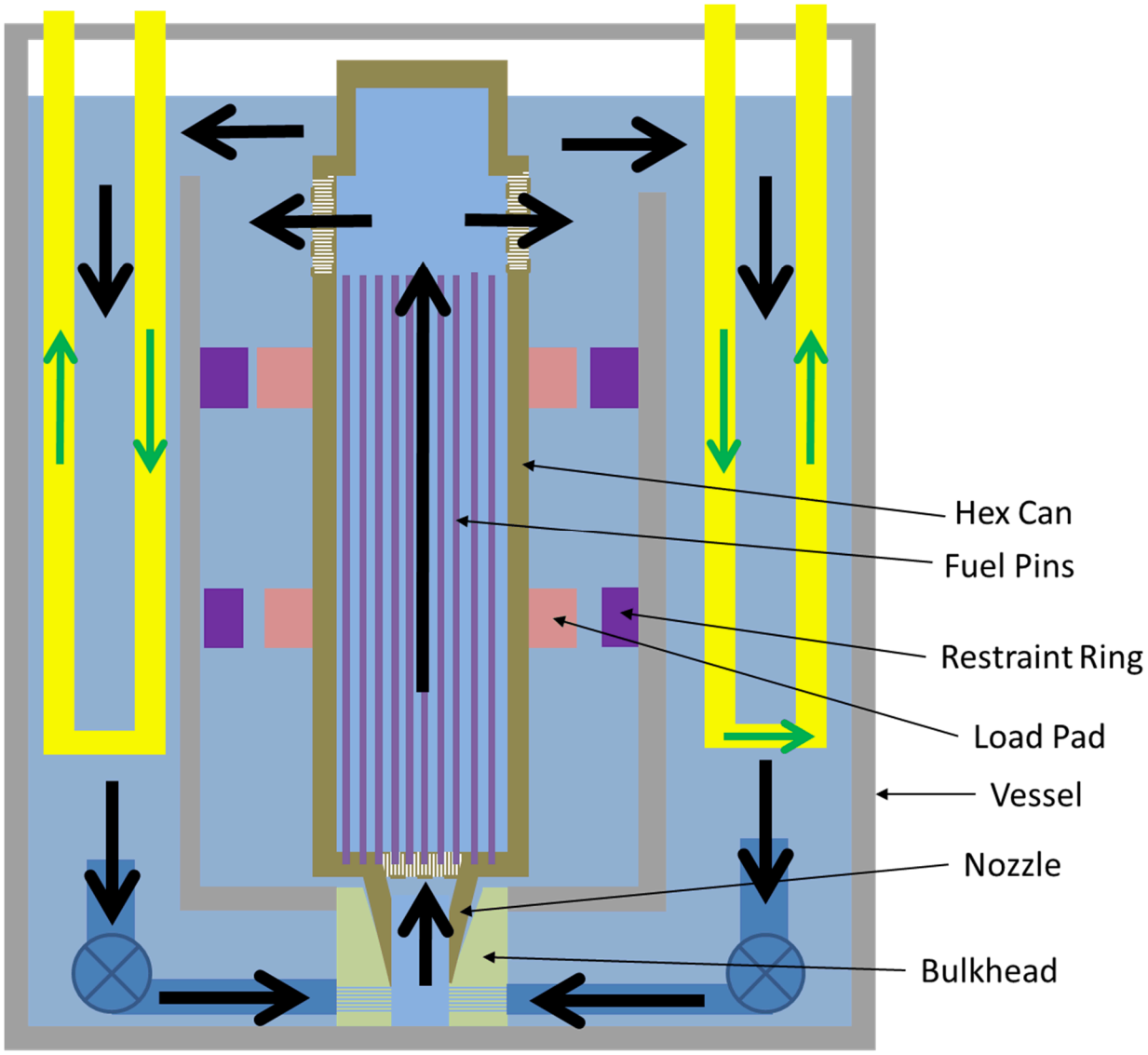

Figure 2 - Notional reactor model

All valid Diablo syntax is valid within the SHARP framework, with the exception that time stepping (e.g. choice of time step) is controlled via SHARP, and all temperature information is also provided by SHARP. Duplication and the associated other features are provided only within the context of the exodus reader. The Diablo manual consistent with the current release of SHARP is in the modules/Diablo/documents directory.

To create a duplicate element set, use the following command or variations thereof in the subassembly file within an element set definition

```
#start_element_topo_exodus
   #exodus_block_id 5
  #duplicate_nodes_flag .TRUE.
  #exclude_duplicates_sideset 5
 #exclude_duplicates_nodeset 6
#end_element_topo_exodus
```

In a Neumann, Dirichlet, or Contact Set definition, the duplicated nodes can be selected (instead of the original nodes) via the #map_nodes_flag

```
#start_bc_topo_exodus
    #exodus_sideset_id 5
    #map_nodes_flag .TRUE.
#end_bc_topo_exodus
```