Methodology for Coupling Computational Fluid Dynamics and Integral Transport Neutronics

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The CFD code STAR-CD was coupled to the integral transport code DeCART in order to provide high-fidelity, full physics reactor simulations. An interface program was developed to perform the tasks of mapping the STAR-CD mesh to the DeCART mesh, managing all communication between STAR-CD and DeCART, and monitoring the convergence of the coupled calculations. The interface software was validated by comparing coupled calculation results with those obtained using an independently developed interface program. An investigation into the convergence characteristics of coupled calculations was performed using several test models on a multiprocessor LINUX cluster. The results indicate that the optimal convergence of the coupled field calculation depends on several factors, to include the tolerance of the STAR-CD solution and the number of DeCART transport sweeps performed before exchanging data between codes. Results for a 3D, multi-assembly PWR problem on 12 PEs of the LINUX cluster indicate the best performance is achieved when the STAR-CD tolerance and number of DeCART transport sweeps are chosen such that the two fields converge at approximately the same rate.

KEYWORDS: code coupling, method of characteristics, integral transport, DeCART, computational fluid dynamics, CFD, STAR-CD

1. Introduction

As part of a US-ROK collaborative I-NERI project, a comprehensive high fidelity reactor core modeling capability is being developed for detailed analysis of current and advanced reactor designs. The work involves the coupling of advanced numerical models such as computational fluid dynamics (CFD) for thermal hydraulic calculations, whole core discrete integral transport for neutronics calculations, and thermo-mechanical techniques for structural calculations. Other papers have provided an overview of the project [1] and details on each of the computational tools employed. This paper focuses on the methodology for coupling the CFD code STAR-CD [4] to the integral transport neutronics code DeCART.

The coupling of DeCART and STAR-CD was achieved using an external interface program. Because the CFD and neutronics meshes are generally different, one of the first tasks required in the interface was to perform a geometric mapping operation. Typically, the CFD mesh is significantly finer than the neutronics mesh as can be seen in the example fuel pin meshes shown in Figure 1. The algorithm developed in the interface maps multiple CFD cells to a single DeCART zone based on the location of the CFD cell centroids. Partial mapping is not allowed for a CFD cell and therefore each CFD cell is associated with exactly one DeCART zone.

Fig.1 STAR-CD (left) and DeCART (right) Mesh for a Fuel Pin
(fuel:yellow, cladding:red, and moderator:blue)

The second major task performed by the interface is to manage the communication between the CFD and neutronics modules. The interface serves as the master process, with the CFD and neutronics modules as its clients. Each data exchange cycle, STAR-CD transfers the cell-wise temperature and moderator density distribution to the interface. The interface then volume-averages these distributions in order to map them to corresponding DeCART zone-wise distributions for the data transfer. DeCART then updates its cross sections with the new temperature/fluid data. Upon completion of the neutron transport calculation, DeCART sends the flux distribution to the interface. The interface then normalizes the flux distribution to the total core power and obtains the power density distribution. This distribution is then reverse-mapped to a CFD cell-wise distribution before being transferred to STAR-CD. These data exchange cycles continue throughout the calculation as depicted in the coupling scheme shown in Figure 2.

Fig.2 Schematic of the DeCART/STAR-CD Coupling Scheme.

The amount of data transferred each exchange can be significant for practical problems. For the ¼-assembly mini-core model described in another paper in this session [2], the CFD model has nearly 5 million cells. Each data exchange requires the transfer of three cell-wise distributions (temperature, coolant density, and power density). When double-precision numbers are used, this corresponds to a transfer of roughly 120 MB in each cycle. The communication task is further complicated by the fact that parallel processing is used for both STAR-CD and DeCART. The CFD and neutronics domains are decomposed onto each processor, such that each process only has knowledge of its part of the problem domain. This requires both STAR-CD and DeCART to have their own internal communication schemes which is based on the MPI message passing model. In order to avoid potential conflicts with

the message passing models of each code the data communication in the interface program is based on a set of socket-based communication subroutines developed specifically for this project. These socket subroutines were implemented into the interface, as well as into the corresponding DeCART and STAR-CD user subroutines.

The final task for the interface is to monitor and control the convergence of the coupled field solution. The interface monitors the CFD convergence by tracking the enthalpy residual which is calculated by STAR-CD after each iteration. The enthalpy residual is an indication of how well the temperature distribution has converged based on the most recent DeCART power distribution. Experience has shown that for reactor core problems, the enthalpy residual in the fuel is the last to converge in STAR-CD. DeCART also computes several residuals after each transport sweep. Typically these residuals are reduced very quickly, such that it is not necessary to monitor them closely except to ensure final convergence.

The interface computes changes in the zone-wise temperature and power distributions from consecutive data exchange cycles. For instance, the so-called interface power residual is defined for the kth data exchange as

$$\|q\| = \max_{izone}\left\{\frac{\left|q_{izone}^{k} - q_{izone}^{k-1}\right|}{q_{izone}^{k}}\right\},\qquad(1)$$

where q_{izone}^{k} is the most recently received power density in DeCART zone *izone*, and q_{izone}^{k-1} is the previously received power density in the same zone. The STAR-CD fuel enthalpy and interface power residuals are generally the important indicators of coupled calculation convergence.

Further details on execution of the coupled calculations and various modeling issues are provided in another paper in this session [2]. The focus of this paper is on the task of controlling the frequency of data exchanges between STAR-CD and DeCART. The data exchange criterion has an important effect on convergence and the overall execution time. On the neutronics side, data exchanges occur after a specified number of transport sweeps, *N,* which generally range from 1 to 5. On the CFD side, data exchanges occur when the fuel enthalpy residual has been reduced to a prescribed level. After each data exchange, the fuel enthalpy residual must be reduced by a factor α ($0<\alpha<1$). For instance, suppose that at the third data exchange, the fuel enthalpy residual was required to be less than 10. If $\alpha=0.1$, then STAR-CD will continue iterating until the residual is less than 1 before it updates the temperature and density distributions the fourth time. In general, if the criterion for the $(k-1)^{th}$ data exchange was that the fuel enthalpy residual must be less than ε_{k-1}, then the criterion for the kth data exchange is

$$\varepsilon_{k} = \alpha\varepsilon_{k-1} = \alpha^{k}\varepsilon_{0},\qquad(2)$$

where ε_0 is an initial tolerance. Cases tested so far have used values of α from 0.5 to 0.01. The selection of the values of N and α have an important effect on the rate of convergence of the coupled calculation.

The procedure for executing a coupled DeCART/STAR-CD calculation can be summarized as:

1. The interface computes the mapping of STAR-CD cells onto DeCART zones based on geometry input supplied by the user. The interface receives information about the STAR-CD

decomposition on the compute nodes, i.e. which cells are on which compute node.   It then transfers an initial power distribution to STAR-CD.

2. STAR-CD begins iterating using the power distribution supplied by the interface.   Once the fuel enthalpy residual is sufficiently small (i.e. Eqn. 2 is satisfied), the CFD cell-wise temperature and density distributions are transferred to the interface. STAR-CD waits until the power distribution is updated again. The interface volume-averages these distributions and transfers them to DeCART.

3. DeCART begins performing transport sweeps using the temperature and density distributions supplied by the interface.   Once the prescribed number of transport sweeps has been performed, the flux distribution is transferred to the interface.   DeCART waits until the temperature and density distributions are updated again.   The interface performs the reverse-mapping of the power distribution on to the CFD cells and transfers the data.

4. Steps 2 and 3 repeat until the interface determines that the coupled calculations have converged.

The completion of steps 2 and 3 comprise the completion of one data exchange cycle.   Typically between 5 and 20 data exchanges are required before the coupled calculations are converged for multi-assembly size problems.

2. Quality Assurance

The interface was verified by developing independently a second interface program that was different from the original interface in several ways.   Most notably the second interface was designed to use I/O files rather than sockets to communicate between the CFD and neutronics modules.

Two test models were developed for verifying the interfaces.   The first is a 3x3 array of PWR fuel pins: five UO_2 pins, three MOX pins, and a central guide tube.   The models were discretized such that DeCART had roughly 5,000 zones and STAR-CD has more than 1 million cells.   A detailed description of the 3x3 model is available in references [2] and [3].   The second test model was a multi-assembly PWR mini-core.   A checkerboard-style array of MOX and UO_2 fuel assemblies in a small PWR-type reactor was used to study the challenging coupled neutronics and thermo-fluid problem.   The CFD model is equivalent to ¼ of an assembly: one eighth of a UO_2 assembly adjacent to another one eight of a MOX assembly.   Because of symmetry limitations in the DeCART code, the neutronics model is equivalent to one full assembly, also half UO_2 and half MOX.   The model discretization is such that there are approximately 150,000 DeCART zones and 5 million STAR-CD cells.   When comparing execution times of STAR-CD and DeCART for this problem, it is important to note that the DeCART problem domain is four times larger than that of STAR-CD.   Nonetheless, the number of STAR-CD cells is 33 times larger than the number of DeCART zones.   A detailed description of the mini-core model is provided in another paper in this session [2].

In all cases tested, the results of the calculations performed with each interface matched within 1 pcm, providing confidence in the performance of the interface programs.   As an example of the agreement obtained, the percent difference in temperature for CFD cells is shown in Figure 3.   For this case, the maximum difference in temperature for any cell is less than 0.5%.

Fig. 3 Difference in Temperature Distribution Using Two Independently Developed Interface Programs.

3. Convergence Analysis

A convergence study was performed using the multi-assembly checkerboard model to investigate the effect of the values of N and α on convergence of the coupled field calculation. The problem was executed on 12 PEs of the ANL LCRC cluster *jazz*, a 350 node LINUX cluster. DeCART and STAR-CD shared the same 12 processors and the interface was executed on its own processor, thereby requiring a total of 13 PEs. For this model and parallelization scheme, the STAR-CD executable required 540 MB and the DeCART executable required 72 MB. Since each compute node has both processes, the memory requirement is 612 MB for each node, which fits well on *jazz* nodes which each have at least 1 GB of RAM.

For the application here, there was one important deviation from the standard coupling procedure outlined in the first section. Because of convergence difficulties encountered when using temperature-dependent thermophysical properties, the properties were held constant in the STAR-CD model. In order to provide a realistic moderator density distribution to DeCART, a density table was installed in the interface which was used the computed STAR-CD temperature distribution. Work is ongoing to resolve the convergence difficulties associated with temperature-dependent properties in STAR-CD.

Convergence analysis was performed using twelve cases with different combinations of N and α. A summary of the results is given in Tables 1 and 2. In Table 1, the resulting infinite medium eigenvalue is given along with a summary of the convergence characteristics: the total number of data exchange cycles, STAR-CD iterations, and DeCART transport sweeps performed before the calculations were converged. In the final column, the "bottleneck" for the convergence is listed. If the fuel enthalpy residual criterion was the last to be satisfied, then an "h" is displayed in this column. Conversely, if the interface power residual criterion is the last to be satisfied, then a "Q" is indicated. In the case with α=0.05 and N=3 (bold in the Table), both criteria were satisfied only at the last data exchange. A summary of the elapsed (wall-clock) time is given for each case in Table 2, which provides the time spent

in STAR-CD, DeCART, and communication, along with the total elapsed time and ratio of STAR-CD time to DeCART time.

Table 1 Summary of Convergence Data for Mini-Core Problem

Enthalpy Residual Reduction Factor (α)	DeCART Transport Sweeps/ Exchange (N)	k_∞	Total Number of Data Exchanges	Total STAR-CD Iterations	Total DeCART Transport Sweeps	Bottleneck Criterion
0.25	2	1.28230	15	416	31	h
0.10	2	1.28231	10	477	21	Q
0.05	2	1.28231	13	718	27	Q
0.01	2	1.28231	10	844	21	Q
0.25	3	1.28230	15	325	46	h
0.10	3	1.28231	9	366	28	h
0.05	**3**	**1.28231**	**7**	**358**	**22**	**-**
0.01	3	1.28231	8	573	25	Q
0.25	4	1.28230	15	304	61	h
0.10	4	1.28231	9	342	37	h
0.05	4	1.28231	7	345	29	h
0.01	4	1.28231	6	486	25	Q

Table 2 Summary of Execution Times for Mini-Core Problem

Enthalpy Residual Reduction Factor (α)	DeCART Transport Sweeps/ Exchange (N)	STAR-CD Time (min:sec)	DeCART Time (min:sec)	Comm. Time (min:sec)	Total Elapsed Time (min:sec)	STAR-CD time/ DeCART time
0.25	2	57:17	35:15	2:04	96:47	1.62
0.10	2	60:09	21:58	1:23	85:40	2.74
0.05	2	90:51	30:18	1:52	125:12	3.00
0.01	2	109:47	22:39	1:24	136:00	4.85
0.25	3	44:41	65:24	2:05	114:44	0.68
0.10	3	49:43	35:41	1:13	89:17	1.39
0.05	**3**	**46:22**	**26:17**	**1:06**	**76:01**	**1.76**
0.01	3	75:18	30:59	1:13	109:34	2.43
0.25	4	41:30	91:13	2:11	136:58	0.45
0.10	4	43:13	52:38	1:17	99:11	0.82
0.05	4	42:45	38:31	1:05	84:20	1.11
0.01	4	61:26	30:06	1:04	94:31	2.04

Several observations are immediately apparent from these tables.   As expected, the solution accuracy does not depend on the selection of α and *N*, as can be seen by the consistency of the eigenvalues calculated for all cases.   (Note: The CFD solution also is the same for each case.)   Next, it is worth

noting that the communication time is not a significant contribution to the total run time; it is usually less than 2% of the total time.   In terms of the total elapsed time, the best cases correspond to when the enthalpy and power distributions converge at the same rate.   The minimum execution time (α=0.05 and *N*=3) occurs when the two criteria are satisfied simultaneously.   The time spent in STAR-CD and DeCART are on the same order for the better cases, with the ratio of the two times being between 1 and 3 (Again, please note the DeCART physical problem is four times larger than the STAR-CD problem in this example).

Analysis of the results also provides insight about the impact of varying the tolerance on the convergence of the other field solution.   For example, consider the case when a value of *N* has been chosen and it is desired to search for the optimal value of α which will result in the smallest total elapsed time.   Larger values of α will cause STAR-CD to perform only a few iterations per exchange, and small values of α will cause STAR-CD to perform many iterations per data exchange.   By increasing α, the CFD solution will be better converged to the most recent DeCART power distribution.   The expectation is that this improved intermediate solution will result in faster convergence of DeCART and reduce the total number of data exchanges required.   This reduction in the total number of data exchanges will reduce the DeCART run time and therefore the total problem execution time.   The total elapsed time for each case is shown schematically in Figure 4.

Fig.4   Total Elapsed Time as a Function of α for Different values of *N*

Consider the cases where *N*=4.   As the value of α decreases, the number of data exchanges performed also decreases.   When α is varied from 0.25 to 0.05, the total run time decreases as well. For the α=0.01 case, however, the reduction in the number of data exchanges was not sufficient to offset the increase in the STAR-CD run time and the total problem time increased.   The cases with *N*=3 exhibit similar behavior, except for the α=0.01 case.   In this case, the number of data exchanges is greater than the α=0.05 case, which indicates that making the enthalpy residual tighter actually has a destabilizing effect on the convergence.   Consequently, the total run time for this case is substantially greater than that of the α=0.05 case.

For the case with three DeCART transport sweeps (N=3), the convergence behavior of the STAR-CD

fuel enthalpy residual is shown in Figure 5 for various enthalpy reduction factors.   As indicated each time STAR-CD receives an updated power density distribution, the fuel enthalpy residual increases sharply.   Typically these jumps in the residual are brought back down quickly.   As α decreases these jumps become larger and recovery becomes more difficult.   The α=0.25 case shows a reasonable CFD-side convergence with only modest jumps in the residual and a small number of total iterations. This comes at the expense of the neutronics-side convergence, however, as the increased number of data exchanges requires DeCART to perform additional transport sweeps.   At the other extreme, the α=0.01 case shows extraordinary jumps in the fuel enthalpy residual which are likely responsible for the poorer overall performance of this case.   The general relation between the number of data exchanges and the choice of α and N is the subject of ongoing investigation.

Fig. 5   Convergence Behavior of the Fuel Enthalpy Residual (N=3)

4.   Summary and Conclusions

A methodology has been demonstrated for coupling the CFD code STAR-CD to the integral transport code DeCART.   An interface program was developed to perform the tasks of mapping the STAR-CD mesh to the DeCART mesh, managing all communication between STAR-CD and DeCART, and monitoring the convergence of the coupled calculations.   The interface software was validated by comparing coupled calculation results with those obtained using an independently developed interface program.   An investigation into the convergence characteristics of coupled calculations was performed using several test models on a multiprocessor LINUX cluster.   The results indicate that the optimal convergence of the coupled field calculation depends on several factors, to include the tolerance of the STAR-CD solution and the number of DeCART transport sweeps performed before exchanging data between codes.   Results for a 3D, multi-assembly PWR problem on 12 PEs of the LINUX cluster indicate the best performance is achieved when the STAR-CD tolerance and number of DeCART transport sweeps are chosen such that the two fields converge at approximately the same rate.   Work is continuing on a more thorough

understanding of the convergence of the coupled fields, as well as testing of the interface for larger static and transient PWR applications.

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