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A ONE AND TWO DIMENSIONAL PCICE-BASED MULTIPHYSICS ALGORITHM FOR USE IN REACTOR CORE SIMULATIONS

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ABSTRACT

The current research in the field of reactor design investigates numerical tools which are spatially and temporally accurate with number of physical phenomena. The objective is, therefore, to simulate the thermal behavior of next generation reactors with a high level of detail. The simultaneous simulation of neutron transport, solid heat conduction and hydrodynamics can be obtained by applying the unifying principle of energy conservation. Following this principle, a one and two dimensions multiphysics algorithm is explored by expanding the PCICE solution algorithm for fluid flow. In one dimension, a variable area finite element method is developed and coupled to a quasi-one dimensional solid-state conduction and neutron transport solvers. In two dimensions, a finite volume formulation of the PCICE scheme is outlined. Moreover, the foundations for incorporating solid state heat transfer into the finite volume formulation are defined. Additionally, the coupling with the radiation transport code EVENT is also highlighted. Such methods will allow to model different physics of the same problem in a unified way with high accuracy.

Key Words: PCICE, Compressible Flow, Pressure-based Method, Multiphysics coupling, Radiation Transport, Solid-state Heat Conduction

1 INTRODUCTION

One of the driving forces for the development of multiphysics algorithms is the demand for high fidelity reactor simulations. Within these simulations, it is desirable to numerically couple the various physical phenomena taking place within the reactor. Physically, these phenomena are linked to one another by internal energy. To numerically couple the phenomena, the PCICE solution algorithm for fluid flow is expanded to include the effects of solid state heat conduction and a temperature dependent heat generation provided by the solution to the neutron transport equation. This expansion was performed in one and two dimensions. The purpose of the quasi-one dimensional formulation was to test the temporal coupling between the multiple physical processes. With the temporal behavior characterized, the formulation is extended to two dimensions using a finite volume formulation. In this paper, the PCICE algorithm will first be outlined. Next, the quasi-one dimensional finite element formulation will be explained and the coupling between the codes modeling the solid state heat transfer and neutron transport will be detailed. Finally, an overview of the finite volume formulation of the PCICE method will be given with a special emphasis on the incorporation of solid phase conduction into the algorithm.

2 The PCICE Method

In this section, a brief outline of the PCICE method will be presented. For a full explanation of the method, the reader should refer to [4].

The PCICE method is a pressure corrected, semi-implicit method used to solve the Eulerian/Navier Stokes equations in conservative form:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{u} = S \tag{1}$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) = -\nabla p + \nabla \cdot \tau + \vec{B} \tag{2}$$

$$\frac{\partial \rho e_t}{\partial t} + \nabla \cdot (\rho \vec{u} h_t) = \nabla \cdot (\tau \cdot \vec{u}) + \nabla \cdot k \nabla T + i(T) \tag{3}$$

$$p = f(\rho, e) \tag{4}$$

where $\rho, \vec{u}, p$, and T are the fluid density, velocity, pressure and temperature, respectively. The variables e_t and h_t are the total specific energy and enthalpy, $\underline{\tau}$ is the viscous stress tensor and S, $\vec{B}$ and $i(T)$ are source terms for the mass, momentum and energy equations respectively. Additionally, Fourier's Law was assumed for the conduction within the fluid, where k is the thermal conductivity. Here, the energy source term is written as a function of temperature to emphasize the nonlinear aspect of the term. The PCICE method is advantageous due to its semi-implicit nature and the strong coupling between the energy and pressure Poisson equations. This strong coupling eliminates the need for iterations between the energy and pressure-correction equation, in contrast to traditional pressure based methods. The semi-implicit nature of the method allows for the elimination of the acoustic component of the Courant stability limit.
Additionally, the PCICE method is valid over the entire range of compressibility, from fully compressible to nearly incompressible [[3]]. This applicability to all speed flows and the improved numerical efficiency makes the method ideal for multiphysics solvers, where computational efficiency and flexibility are required. The target discretization for the PCICE scheme used in the following formulations is given below.

$$\rho^{n+1} = \rho^n + \Delta t S^n - \frac{\Delta t}{2} \nabla \cdot (\rho \vec{u}^{n+1} + \rho \vec{u}^n) \tag{5}$$

$$\rho \vec{u}^{n+1} = \rho \vec{u}^n - \frac{\Delta t}{2} \nabla \cdot (\rho \vec{u} \otimes \vec{u}^p + \rho \vec{u} \otimes \vec{u}^n) - \frac{\Delta t}{2} \nabla (P^{n+1} + P^n) + \Delta t \nabla \cdot (\underline{\tau}^n) + \Delta t B^n \tag{6}$$

$$\rho e_t^{n+1} = \rho e_t^n - \frac{\Delta t}{2} \nabla \cdot (\rho \vec{u} h_t^{n+1} + \rho \vec{u} h_t^n) + \Delta t \nabla \cdot (\underline{\tau} \cdot \vec{u}^n) + \Delta t \nabla \cdot (k \nabla T)^n + \Delta t i(T)^n \tag{7}$$

$$\tag{8}$$

To obtain this discretization, four steps are performed. First, the solution variables are advected using a two step predictor-corrector formulation. Next, the variables are further updated with the viscosity, conduction and source terms. This update step is treated in a fully explicit manner for the purposes of this work. After the solution variables are updated with the viscous and thermal terms, the pressure at $n + 1$ is estimated by solving a pressure Poisson equation which tightly couples the mass and momentum equations. Finally, in step four of the scheme, the solution variables are corrected using the estimated pressure calculated in step three.
In step one of the scheme, the variables are explicitly advected using a two-step, predictor-corrector method. This two step advancement is shown in compact form below.

$$\vec{U}^p = \vec{U}^n - \Delta t \nabla \cdot (\vec{F}_c^{\,n}) \quad (9)$$

$$\vec{U}^c = \vec{U}^n - \frac{\Delta t}{2} \nabla \cdot (\vec{F}_c^{\,n} + \vec{F}_c^{\,p}) \quad (10)$$

$$where: \quad (11)$$

$$\vec{U} = \left\{ \begin{array}{c} \rho \\ \rho\vec{u} \\ \rho e_t \end{array} \right\} \quad (12)$$

$$and: \quad (13)$$

$$\vec{F}_c = \left\{ \begin{array}{c} \rho\vec{u} \\ \rho\vec{u} \otimes \vec{u} \\ \rho\vec{u}h_t \end{array} \right\} \quad (14)$$

In these equations, the solution variables are updated using only the convective flux vectors. Notice that at the predictor time level, partially updated primitive variables such as temperature, velocity and pressure are calculated. These partially updated primitive variables are used to calculate the flux at the predictor and corrector time levels.
With the variables explicitly advected, the solution vectors are updated using the diffusive/viscous flux vectors. For this work, this step is carried out using a one step, fully explicit time integration and is shown below.

$$\vec{U}^d = \vec{U}^c + \Delta t \nabla \cdot \vec{F}_v^{\,n} + \Delta t \vec{Q}^n \quad (15)$$

$$where: \quad (16)$$

$$\vec{F}_v = \left\{ \begin{array}{c} 0 \\ \tau \\ \tau \cdot \vec{u} + k\nabla T \end{array} \right\} \quad (17)$$

$$and: \quad (18)$$

$$\vec{Q} = \left\{ \begin{array}{c} S \\ \vec{B} \\ i(T) \end{array} \right\} \quad (19)$$

To predict the pressure in an implicit manner, a Poisson equation for the pressure is constructed. To construct this equation, the discretized formulas for density and momentum are combined and the equation of state is used to relate pressure to density. Beginning with the target discretization, the density and momentum equations are:

$$\rho^{n+1} = \rho^n - \frac{\Delta t}{2} \nabla \cdot (\rho\vec{u}^{n+1} + \rho\vec{u}^n) \quad (20)$$

$$\rho\vec{u}^{n+1} = \rho\vec{u}^n - \frac{\Delta t}{2} \nabla \cdot (\rho\vec{u} \otimes \vec{u}^p + \rho\vec{u} \otimes \vec{u}^n) - \frac{\Delta t}{2} \nabla (P^{n+1} + P^n) + \Delta t \nabla \cdot (\underline{\tau}^n) + \Delta t B^n \quad (21)$$

$$(22)$$

In the above equation, the mass source term was taken to be zero. In Equation 21 above, all of the terms on the right hand side of the equation, aside from the pressure term can be replaced by the partially updated momentum after the diffusion step (step 2) of the scheme. Additionally, the momentum at time step n can be added to both sides of the equation. With this manipulation, the Equation 21 becomes:

$$\rho\vec{u}^{n+1} + \rho\vec{u}^{n} = \rho\vec{u}^{d} + \rho\vec{u}^{n} - \frac{\Delta t}{2}\nabla(P^{n+1} + P^{n}) \tag{23}$$

By substituting Equation 23 into Equation 20, the momentum and mass equations become tightly coupled. The result of this substitution is below.

$$\rho^{n+1} - \rho^{n} = -\frac{\Delta t}{2}(\rho\vec{u}^{d} + \rho\vec{u}^{n}) + \frac{\Delta t^2}{4}\nabla\cdot\nabla(P^{n+1} + P^{n}) \tag{24}$$

Finally, the equation of state is used to relate the change in density to the change in pressure for that time step. This relationship is found by taking the derivative of the equation of state and approximating it using a simple backward differencing.

$$\hat{P}^{n+1} - P^{n} = \left(\frac{\partial f}{\partial \rho}\right)^{d}(\rho^{n+1} - \rho^{n}) + \left(\frac{\partial f}{\partial \rho}\right)^{d}(e^{d} - e^{n}) \tag{25}$$

In this equation, $\hat{P}^{n+1}$ is the estimated value of the pressure at the new time step. It is this estimated pressure for which the pressure Poisson equation solves. By substituting the above relationship into Equation 24, the final form of the pressure Poisson equation is obtained.

$$\frac{\hat{P}^{n+1} - P^{n}}{\left(\frac{\partial f}{\partial \rho}\right)^{d}} - \frac{\Delta t^2}{4}\nabla\cdot\nabla(P^{n+1} - P^{n}) = \frac{\left(\frac{\partial f}{\partial e}\right)^{d}}{\left(\frac{\partial f}{\partial \rho}\right)^{d}}(e^{d} - e^{n}) - \frac{\Delta t}{2}(\rho\vec{u}^{d} + \rho\vec{u}^{n}) + \frac{\Delta t^2}{2}\nabla\cdot\nabla(P^{n}) \tag{26}$$

Once the above equation is solved for the estimated pressure at time $n+1$, the solution variables can be corrected using the pressure information. First, the momentum is updated using the following formula.

$$\rho\vec{u}^{n+1} = \rho\vec{u}^{d} - \frac{\Delta t}{2}\nabla(P^{n+1} + P^{n}) \tag{27}$$

Using the momentum at new time step, the other variables are corrected according to the following equations.

$$\rho^{n+1} = \rho^d - \frac{\Delta t}{2}\nabla \cdot (\rho\vec{u}^{n+1} - \rho\vec{u}^d) \tag{28}$$

$$\rho e_t^{n+1} = \rho e_t^d - \frac{\Delta t}{2}\nabla \cdot (\rho\vec{u}h_t^{n+1} - \rho\vec{u}h_t^d) \tag{29}$$

$$where: \tag{30}$$

$$h_t^{n+1} = \frac{\rho e_t^d + \hat{P}^{n+1}}{\rho^{n+1}} \tag{31}$$

With the solution variables found at the new time step, the primitive variables are recalculated, including the pressure at new time step.

3 Quasi-one Dimensional PCICE Scheme

3.1 General Formulation in quasi-one dimensional

The original PCICE algorithm [4] has been simplified to a quasi-one dimensional formulation in order to focus on the temporal aspect of the multiphysics coupling.
In a one-dimensional calculation, the flow is treated as constant-area flow. In quasi-one dimensional flows, the previous constrain is relaxed and the cross sectional area is allowed to change with direction x. Therefore, for steady and unsteady flow, the variables will be $A = A(x)$, $p = p(x)$, $\rho = \rho(x)$, $\rho u = \rho u(x)$, $\rho e_t = \rho e_t(x)$ and $A = A(x,t)$, $p = p(x,t)$, $\rho = \rho(x,t)$, $\rho u = \rho u(x,t)$, $\rho e_t = \rho e_t(x,t)$ respectively. The derivation of the Navier-Stokes equations in quasi-one dimensional form can be obtained from [2] and will not be developed here. Below is the compact writing form of the quasi-one dimension Navier-Stokes equations:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = \frac{\partial F_v}{\partial x} + Q \tag{32}$$

where the column vector of the conservative variables is given by:

$$U = \left\{ \begin{array}{c} A\rho \\ A\rho u \\ A\rho e_t \end{array} \right\} \tag{33}$$

The advective flux vector is defined by:

$$F = \left\{ \begin{array}{c} A\rho u \\ A\rho u^2 + AP \\ A\rho u H \end{array} \right\} \tag{34}$$

In one-dimensional analysis, friction is treated as a source term instead of considering a viscous stress tensor. Therefore, the only contributing term in the flux vector $\vec{f_v}$ is the heat flux vector:

$$F_v = \left\{ \begin{array}{c} 0 \\ 0 \\ -Aq_x \end{array} \right\} \tag{35}$$

The source term is:

$$Q = \left\{ \begin{array}{c} AS \\ -\tau_w P_w + AB \\ Ai(T) \end{array} \right\} \tag{36}$$

where S, B and $i(T)$ are the sources introduced in equation (16), τ_w is the frictional shear stress and P_w is the wetted perimeter. The shear stress can be expressed in terms of a friction coefficient f, defined as $\tau_w = \frac{1}{2}\rho u^2 f$.
The Navier-Stokes formulation displayed previously (section) is discretized in space using the Finite Element Method and time, and the PCICE-FEM scheme is utilized to solve them.

The first fractional step is the explicit predictor which advects the solution field neglecting pressure and source terms followed by a step taking friction, thermal diffusion and source terms into consideration. The third and fourth steps include an elliptic Poisson equation which is solved for new-time pressures and an explicit correction with the new pressures.

3.2 MultiPhysics Coupling

In order to have an accurate representation of the temperature distribution within a nuclear core, the equations for neutron diffusion, solid heat transfer and fluid dynamics have to be coupled together. The basis for this coupling is the unifying principle of energy conservation.

In the present work, two phases are considered for the reactor core: a solid phase which represents the core itself and a fluid phase which represents the coolant. Conduction and fission are the only phenomena considered within the core, while conduction and convection are the predominant mechanisms in the fluid. A numerical resolution of a coupled thermal problem follows the following procedure. During the first time step, only the hydrodynamic equations are solved with the PCICE-FEM scheme. At the second iteration and until convergence, the coupling will be taken into account. The first step of the PCICE-FEM adverts the variables. During the second step, the heat equation is solved for the solid phase with the fluid temperature distribution as an input. From the temperature distribution obtained, a neutron balance is performed within the core in order to obtain a power distribution. The power distribution is fed into the solid heat transfer equation which produces a source term processed by the diffusion step of the PCICE-FEM. The Poisson equation and the pressure correction steps are kept identical to the previous PCICE formulation.

3.2.1 Neutronics/Energy Coupling

For the purpose of the thermal analysis of the reactor core, the neutron flux has to be determined. The neutron flux distribution will lead to the power distribution in the core which will be used as an internal heat generation source. Two formulations have been explored: the finite element diffusion equation and the disconitnous discrete ordinates method. Only the finite element diffusion formulation will be outlined in this paper. The time-dependent diffusion equation in quasi one-dimension is given here

$$\frac{1}{v_{th}}A_s(x)\frac{\partial\phi(x)}{\partial t} - \frac{\partial}{\partial x}\left(D(x,T)A_s(x)\frac{\partial}{\partial x}\phi(x)\right) + A_s(x)\Sigma_a(x,T)\phi = A_s(x)\nu\Sigma_f(x,T)\phi(x) \quad (37)$$

where v_{th} is the thermal neutron velocity, A_s is the cross sectional area of the solid phase, D is the diffusion coefficient, Σ_a is the absorption cross section and Σ_f is the fission cross section. Equation (37) is discretized in time and space (using the Finite Element Method) and solved with the Thomas algorithm.

The coupling between the neutronics and the solid heat conduction takes place via the temperature and heat generation. Therefore, after solving the diffusion equation, the internal heat generation source $i(T)$ is extracted for each cell

$$\int_V dV\, Ai(T) = Q\int_V dV\, A\nu\Sigma_f(T)\phi(x) \quad (38)$$

In this equation, Q represents the amount of energy released per fission reaction and the integral term represents the total number of fission reactions within the volume V_i.

The challenge of this procedure is to generate temperature dependent cross sections. The temperature distribution has to be provided by the solid heat transfer calculation. From this point, cross sections at determined temperatures will have to be provided by external codes and the values of the cross sections will be interpolated.

3.2.2 Solid-Fluid Coupling

The same formulation can be applied to the solid phase. However, some conditions have to be enforced. In fact, the velocity within the solid is zero and the system of equations (1) becomes

$$\frac{\partial A\rho}{\partial t} = 0 \quad (39)$$

$$\frac{\partial A\rho\vec{u}}{\partial t} = 0 \quad (40)$$

$$\frac{\partial A\rho e_t}{\partial t} = \frac{\partial}{\partial x}Ak\frac{\partial}{\partial x}T + Ai(T) \quad (41)$$

The energy equation can be reduced to the well known solid heat equation, which results, after discretization in time

$$A\rho C_v(T^{n+1} - T^n) = \Delta t\frac{\partial}{\partial x}\left(Ak\frac{\partial}{\partial x}T\right) + \Delta t Ai^{n+1} \quad (42)$$

where T_s is the temperature of the solid phase and T_f is the temperature of the fluid.

The solid heat equation is a crucial part of the coupling. In fact, it relates directly the hydrodynamics to the neutronics of the problem. The source term $i(T)$ presented in the previous section has to be modified to take the fluid contribution into account. This term takes the form of a convective term between the fluid and the solid. Therefore, the solid heat equation, combining the fission heat source and the convective term, becomes:

$$A\rho C_v(T^{n+1} - T^n) = \Delta t \frac{\partial}{\partial x}\left(Ak\frac{\partial}{\partial x}T\right) + \Delta t A\left[Q\int_V dV\, A\nu\Sigma_f(T)\phi(x) + h\left(T_f - T_s\right)\right] \tag{43}$$

In a same way, the energy equation for the fluid becomes:

$$A\rho(e_t^{n+1} - e_t^n) = \frac{\Delta t}{2}\frac{\partial}{\partial x}\left(A\rho\vec{u}^{n+1}h_t^{n+1} - A\rho\vec{u}^n h_t^n\right)\Delta t\frac{\partial}{\partial x}\left(Ak\frac{\partial}{\partial x}T\right)h\left(T_s - T_f\right) \tag{44}$$

3.3 Benchmark

The quality of the results produced by the scheme have been verified with a series of benchmark problems for which the solution is known. The purpose of these tests is to verify the capabilities of the PCICE-FEM scheme in a wide range of flow regimes. The first simulation demonstrated here is of transient flow to verify the accuracy of the PCICE scheme to propagate wave forms. The problem utilized for this purpose is the Riemann problem for which an analytical solution exists. Next, three steady-state simulations are presented. The first steady-state simulation consists of a flow passing through a converging-divergent nozzle at different flow regimes. The second and third test cases are a pipe flow with the addition of wall friction in a first approach and, secondly a pipe flow with heat addition .

3.3.1 The Shock Tube Problem

The shock tube is a classic test for the validation of compressible flow schemes and codes. The problem can be characterized by the sudden rupture of a diaphragm in a long one-dimensional tube separating two initial gas states at different pressures and densities. After rupture of the diaphragm, three major compressible flow phenomena appear: a shock wave propagating downstream followed by a contact discontinuity traveling with the fluid, and a rarefaction wave traveling upstream. The figure 1 represents the pressure field for a pipe of 100 meters long with an initial pressure discontinuity at $x = 40$m with $P_1 = 1013250.0$Pa and $P_2 = 101325.0$Pa. The mesh utilized contains 100 nodes.

3.3.2 Steady State simulations

The first problem of the following steady-state test cases is the converging-diverging nozzle. This problem is an extend of a one-dimensional, inviscid, non-heat conducting flow problem. Here, the streamtube area is allowed to vary with distance x. The last two problems of the benchmark are constant area flows that are modified either by the presence of friction, or the addition of heat.

Convergent-Divergent Nozzle

The converging-diverging nozzle is a verification case for an inviscid non-heat conduction air through a variable area duct. This problem is largely described in [2] and allows to verify the validity of the scheme

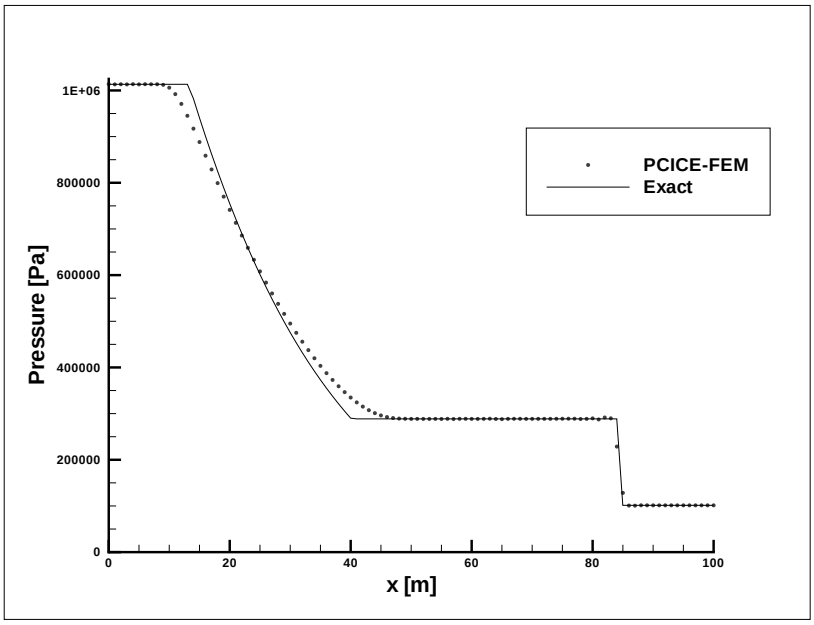

Figure 1. PCICE FEM shock tube solution for pressure at time t=0.08 s.

Table I. Table 1: Flow Conditions

Plenum Total Pressure (psi)	1.0
Plenum Total Temperature (R)	100.0
Exit Static Pressures (psi)	0.89 0.75 0.16

for different flow regimes: subsonic isentropic flow, supersonic with a normal shock in the diffusing section and supersonic, isentropic flow. The three regimes correspond to a pressure drop of $p_{exit}/P_t = 0.89$, $p_{exit}/P_t = 0.75$ and $p_{exit}/P_t = 0.16$ respectively. The following data from the benchmark problem is obtained from the NASA library of CFD validation problems.

The pressure profile given by the PCICE-FEM is compared to the analytical solution in Fig. 3.

Again, the numerical solution accuracy when compared to the analytical solution is excellent. The next step in the benchmark of the code is the validation of the second step of the PCICE-FEm by the analysis of a one-dimensional flow with friction and with addition of heat.

Pipe Flow with Heat Addition

Another source of change in a one dimensional flow is heat addition. If heat is extracted or added within a certain region, the properties of the flow will change within that particular region. The analysis of the heat addition within a fluid is very delicate even in one-dimensional flow and a numerical solution is generally required. However, for a calorically perfect gas, closed -form analytical expressions exist. The solution to a

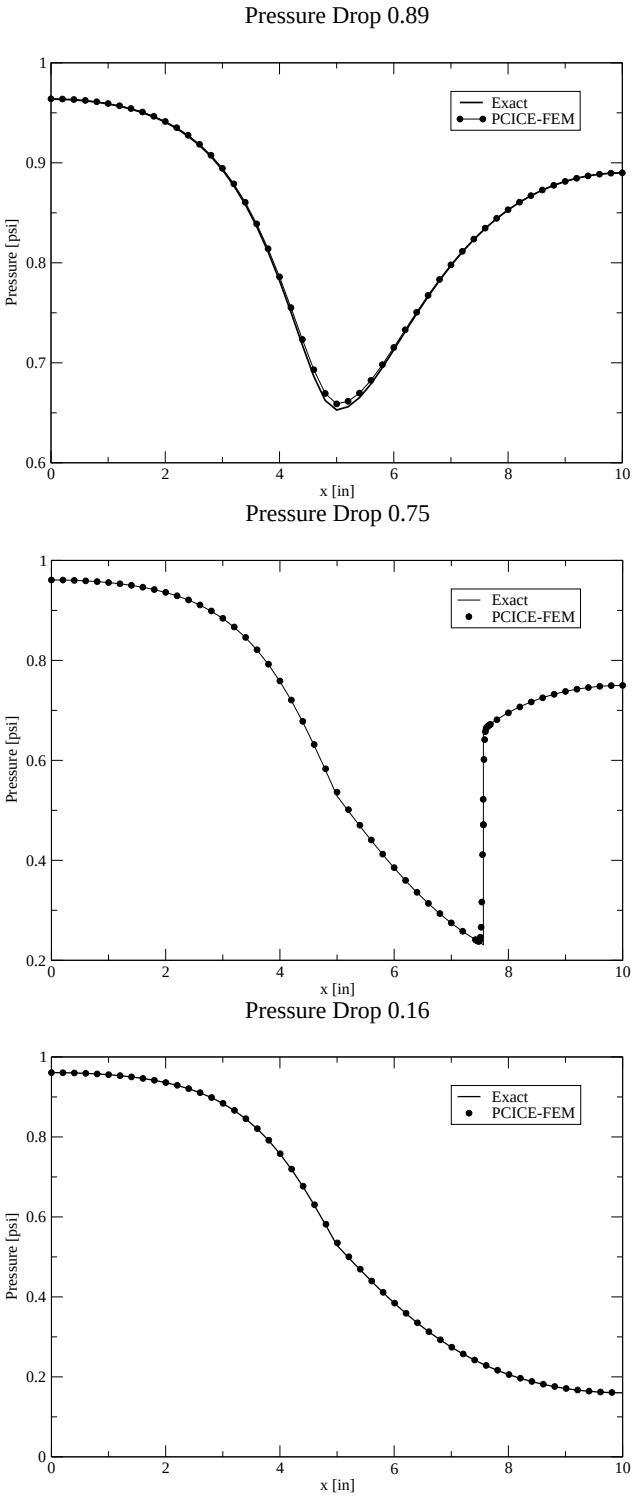

Figure 2. Different Flow Regimes for the Converging Diverging Nozzle

pipe flow problem with heat addition is shown below.

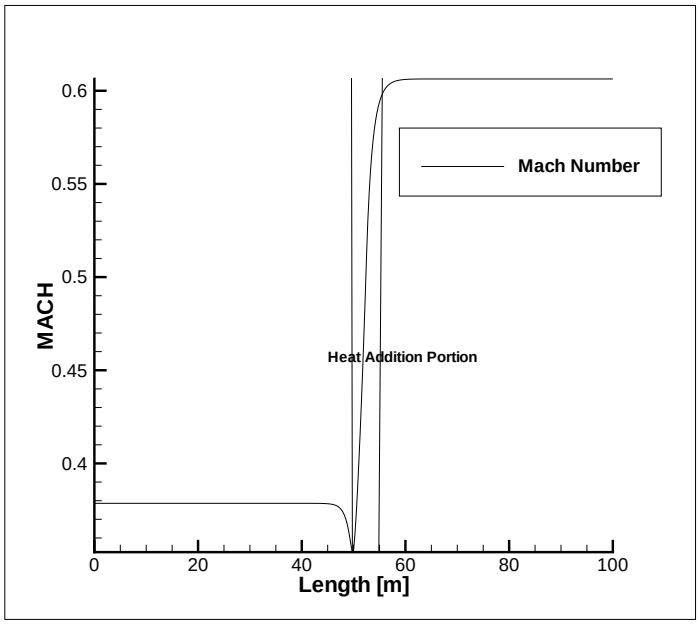

Figure 3. Pipe Flow with Heat Addition

4 Finite Volume based PCICE Scheme

4.1 General Finite Volume Formulation

In this section, the general finite volume formulation used for this work will be outlined. This outline will include the interpolation scheme used for the convective and diffusive fluxes. First, the full Navier Stokes equations are reduced to two dimension Cartesian space. The compact form of the equations in this frame is given below.

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{f}}{\partial x} + \frac{\partial \vec{g}}{\partial y} = \frac{\partial \vec{f_v}}{\partial x} + \frac{\partial \vec{g_v}}{\partial y} + \vec{Q} \tag{45}$$

$$where: \tag{46}$$

$$\vec{U} = \left\{ \begin{array}{c} \rho \\ \rho u \\ \rho v \\ \rho e_t \end{array} \right\} \tag{47}$$

$$and: \tag{48}$$

$$\vec{f} = \left\{ \begin{array}{c} \rho u \\ \rho u^2 + P \\ \rho uv \\ \rho u h_t \end{array} \right\} \tag{49}$$

$$\vec{g} = \left\{ \begin{array}{c} \rho v \\ \rho uv \\ \rho v^2 + P \\ \rho v h_t \end{array} \right\} \tag{50}$$

$$and: \tag{51}$$

$$\vec{f_v} = \left\{ \begin{array}{c} 0 \\ \tau_{xx} \\ \tau_{yx} \\ \tau_{xx} u + \tau_{yx} v - q_x \end{array} \right\} \tag{52}$$

$$\vec{g_v} = \left\{ \begin{array}{c} 0 \\ \tau_{xy} \\ \tau_{yy} \\ \tau_{xy} u + \tau_{yy} v - q_y \end{array} \right\} \tag{53}$$

$$and: \tag{54}$$

$$\vec{Q} = \left\{ \begin{array}{c} S \\ B_x \\ B_y \\ i(T) \end{array} \right\} \tag{55}$$

$$\tag{56}$$

For this work, the shear stress tensor was assumed to correspond to one of a newtonian fluid. Additionally, it was assumed that the heat conduction was characterized by Fourier's law. These assumptions give the following expressions for the shear stress tensor and heat flux vector.

$$\underline{\tau} = \left(\begin{array}{cc} \frac{2}{3}\mu(2\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}) & \mu(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}) \\ \mu(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}) & \frac{2}{3}\mu(2\frac{\partial v}{\partial y} - \frac{\partial u}{\partial x}) \end{array} \right) \tag{57}$$

$$\vec{q} = \left(\begin{array}{c} k_x \frac{\partial T}{\partial x} \\ \\ k_y \frac{\partial T}{\partial y} \end{array} \right) \tag{58}$$

To establish the discretized equations for each cell, the above set of equations is integrated over a volume corresponding to a single grid cell. Additionally, by utilizing the divergence theorem, the derivative terms can be transformed into integrals over the surface area of the cell. Using this process, the integral equation for a cell is given by:

$$\frac{\partial}{\partial t}\int_{V_i}\vec{U}dV + \int_{A_i}(\vec{f}\hat{i} + \vec{g}\hat{j})\cdot d\vec{A} = \int_{A_i}(\vec{f}_v\hat{i} + \vec{g}_v\hat{j})\cdot d\vec{A} + \int_{V_i}\vec{Q} \tag{59}$$

To simplify the above equation, the integral over volume is replaced by the average value of the solution in that cell (the solution at the cell center) multiplied by the volume of the cell. Additionally, the integral over the surface is replaced by a sum over the faces of the cell and the flux along that face takes on an average value. Finally, the differential area vector is approximated using the following:

$$d\vec{A} = \left\{ \begin{array}{c} dy \\ -dx \end{array} \right\} \tag{60}$$

where dy and dx refer to the displacement in the X and Y directions of the two nodes of the face relative to one another. With these simplifications, the equation for each cell is given by:

$$V_i\frac{\partial\vec{U}_i}{\partial t} + \sum_k(\vec{f}_k dy_k - \vec{g}_k dx_k) = \sum_k(\vec{f}_{v,k}dy_k - \vec{g}_{v,k}dx_k) + V_i\vec{Q}_i \tag{61}$$

where $\vec{U}_i$ is the solution value at the cell center, $\vec{Q}_i$ is the source term evaluated using the cell centered solution value, $\vec{f}_k$ and $\vec{g}_k$ are the average advective flux vectors at the k^{th} face and likewise for the viscous/diffusive flux vectors.

Finally, to complete the spatial discretization, the flux vectors at each face must be approximated in some manner. For the convective flux vectors, linear interpolation was used. For this interpolation, the flux at the k^{th} face is taken to be a weighted average of the flux evaluated at the centers of the cells adjacent to the face, known as cells i and j for the remainder of this paper. The weighting for this interpolation is simply based on the distance of the cell centers from face.

$$f_k = \frac{|\vec{r}_k - \vec{r}_i|}{|\vec{r}_j - \vec{r}_i|}f_i + \frac{|\vec{r}_k - \vec{r}_j|}{|\vec{r}_j - \vec{r}_i|}f_j \tag{62}$$

On a structured grid, this interpolation reduces to central differencing and is second order accurate. For second order accuracy, the midpoint of the face must lie on the line connecting the centers of the cells sharing that face. As this requirement becomes less valid, the spatial accuracy of the scheme will be reduced [1].

To evaluate the diffusive flux vectors and implement the PCICE scheme, the gradient of various quantities at the cell face must be approximated. To approximate the gradient normal to a face, it was assumed again

that the face center is located on the line between the centers of the cells adjacent to the face. Additionally, it was assumed that the normal to the face was parallel to the line connecting the cell centers. For this normal gradient, the approximation is:

$$(\nabla\Phi \cdot d\vec{A})_k = |dA_k| \frac{\Phi_j - \Phi_i}{\vec{r_j} - \vec{r_i}} \tag{63}$$

For the derivatives in the viscous stress tensor, a similar approach could have been employed; however, on a non-Cartesian grid, a local coordinate system for the momentum and velocity would need to be defined. To avoid this step, the derivative of each velocity component with respect to x and y were calculated directly. The cell centered derivative with respect to X can be defined in the following manner.

$$\int_{V_i} dV \frac{\partial\Phi}{\partial x} = \int_{V_i} dxdy \frac{\partial\Phi}{\partial x} \tag{64}$$

$$\int_{V_i} dxdy \frac{\partial\Phi}{\partial x} = \int_A dy\Phi \tag{65}$$

$$\int_A dy\Phi = \sum_k \Phi_k dy_k \tag{66}$$

$$\frac{\partial\Phi}{\partial x}_i = \frac{1}{V_i} \sum_k \Phi_k dy_k \tag{67}$$

In a similar manner, the cell centered derivative with respect to y can be defined. Finally, to approximate this derivative at the cell face, linear interpolation was again used.

The formulation outlined above is meant to give a basic idea of the discretization utilized in the finite volume formulation of the PCICE algorithm. A detailed development of the finite volume PCICE scheme is beyond the realm of this work and will be presented in a separate publication.

4.2 Multiphysics Coupling within PCICE finite volume formulation

For this work, it was necessary to couple the equations of solid state heat transfer and neutron transport to the fluid dynamics formulation. This coupling was carried out using the energy equation. For this work, a tight coupling was possible between the solid state conduction and the fluids equations. The neutron transport aspect of the problem was linked to the fluids by use of the volumetric heat generation term.

4.2.1 Solid-Fluid Linking

In order to link the solid phase to the fluid phase, no changes were required to the actual formulation. The changes merely came in implementing the code numerically. When the velocity is forced to zero, the Navier Stokes equations reduce to the following set of equations.

$$\frac{\partial \rho}{\partial t} = 0 \tag{68}$$

$$\frac{\partial \rho \vec{u}}{\partial t} = 0 \tag{69}$$

$$\frac{\partial \rho e}{\partial t} = \nabla \cdot (k \nabla T) + Q(T) \tag{70}$$

where the mass and momentum source terms have been taken to equal zero. Notice that the first two equations simply show that the density and momentum are constant. Therefore, provided the initial conditions in the solid are physical, i.e. Density set to proper value and Velocity set to zero, these variables will remain unchanged as they should for a solid. In the energy equation, by setting the velocity to zero, this equation has reduced to the standard heat equation for a solid. This equation takes on its familiar form when the specific internal energy is replaced by the temperature and specific heat.

$$\rho c_v \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q(T) \tag{71}$$

Because the solid state and fluid energy equations are equivalent for zero velocity, the formulation outlined required little modification in order to simulation solid heat conduction.

In order to tightly couple the two phases, it is desired to model the entire domain using the same formulation and simply making modifications to cell properties in order to accurately model the physics. Therefore, the boundary between the Solid and Fluid is not treated though the use of boundary conditions and the information is propagated between the two phases at each time step. By eliminating the boundary condition between the two phases, both the temperature and heat flux at the phase boundary can be matched.

At the fluid/solid interface, there is a large discontinuity in thermal conductivities between the two cells with faces adjacent to the boundary. Due to the presence of this discontinuity, the traditional form of the thermal diffusion operator in a finite volume formulation must be modified. Typically on a uniform grid, the heat across a face would be given by the following:

$$\int_{A_k} \vec{q} d\vec{A}_k = |dA| \frac{(k_j + k_i)}{2} \frac{T_j - T_i}{|r_j - r_i|} \tag{72}$$

This approximation assumes that the variation of the thermal conductivity is linear and that the gradient in temperature is continuous across the face. For a fluid/solid interface, both of these approximations are invalid. To solve this problem, the two physical constraints present at the face were enforced. First, the heat flux leaving one cell must be equal to the heat flux entering the adjacent cell. Second, the temperature at the boundary must be continuous. To approximate the heat flux, a one sided difference was used to approximate the temperature gradient on each side of the interface. These one sided differences were then set equal to one another and the temperture at the cell face was set equal between the two approximations. The result of this process is found below.

$$(\int_{A_k} \vec{q_k} d\vec{A}_k)_i = -(\int_{A_k} \vec{q_k} d\vec{A}_k)_j \tag{73}$$

$$q_i |dA_k| = -q_j |dA_k| \tag{74}$$

$$k_i \frac{T_b - T_i}{|r_b - r_i|} = -k_j \frac{T_b - T_j}{|r_b - r_j|} \tag{75}$$

where T_b is the temperature at the face, T_i is the temperature at the center of the i^{th}, T_j is the temperature at the center of the j^{th} cell and k_i and k_j are the thermal conductivities of the respective cells. To find the heat flux leaving the cell, the above equation is solved for T_b. This value of T_b is then put into the expression for the heat flux.

$$T_b = \frac{\frac{k_j T_j}{|r_b - r_j|} + \frac{k_i T_i}{|r_b - r_i|}}{\frac{k_j}{|r_b - r_j|} + \frac{k_i}{|r_b - r_i|}} \tag{76}$$

$$q_{i,k} = -k_i \frac{T_b - T_i}{|r_b - r_i|} \tag{77}$$

By approximating the heat flux in the above manner, large changes in thermal conductivity and consequently, temperature gradient can be taken into account between cells. The above approximation assumes that the thermal conductivity within a cell is constant. For this work, this limitation is acceptable due to the approximations ability to handle large changes in thermal conductivity at cell interfaces.

In terms of the PCICE algorithm, little change is required to simulate systems containing fluids and solids. For the explicit predictor-corrector step, none of the variables within the solid change provided that the variables within the solid region have been initialized to physical conditions (velocity of zero). In the diffusion step, the density and momentum equations remain unchanged due to the zero velocity. For the energy equation, the diffusion step is equivalent to a one step, fully explicit time integration of the heat equation. This energy diffusion step becomes

$$(\rho e)^d = (\rho e)^c - \frac{\Delta t}{V_i} \sum_k q_k^n |dA_k| \tag{78}$$

where q^n is calculated as outlined above using the temperature at time level n.

The pressure Poisson equation within the solid is irrelevant to the calculations as the thermodynamic pressure within the solid has no meaning. Because this is the case, the pressure change within the solid was set equal to zero and initialize to be a uniform pressure. This lack of pressure gradients within the solid ensures that the momentum variables remain unchanged during the pressure correction step. A consequence of this assumption is that the pressure at the solid/fluid interface is no longer continuous and without special treatment, would cause mass conservation to be violated. To avoid this problem, the solid and fluid domains were decoupled while solving the pressure Poisson equation. Therefore, at the fluid/solid interface, the pressure at the boundary was extrapolated from the interior of the fluid domain and the fluid cell receives no pressure information from the solid.

4.2.2 Neutronics/Energy Coupling

For the purposes of this work, the neutron flux through out the domain will be somewhat of a given. To find this neutron flux, the code EVENT will be used. EVENT solves the even-parity transport equation and produces a detailed, energy dependent flux distribution throughout the domain. By using the same mesh for EVENT and the Fluid/solid solver, information can easily be exchanged between the two domains. The Coupling between the two codes will take place via the temperature and heat generation. EVENT provides the fluid/solid solver with an internal heat generation source for each cell, $i(T)$. This heat generation source, ignoring gamma heating, is given in general by the following equation.

$$V_i i(T) = \int_{V_i} dV \int_0^\infty dE \int_{4\pi} d\vec{\Omega} Q(E) \Sigma_f(E,T) \Psi(\vec{r}, \vec{\Omega}, E) \tag{79}$$

In this equation, Q represents the amount of energy released per fission reaction and the integral term represents the total number of fission reactions within the volume V_i. Obviously, the above generalization depends on knowing the exact solution of the energy dependent angular flux and fission cross-section. EVENT uses a multigroup treatment of the energy and a finite element discretization for the spatial dependence of the flux. Given these approximations, the heat generation source per cell is given by:

$$V_i i(T) = \sum_{g=1}^{G} Q^j < \Sigma_f^g >_e \phi_e^g V_i \tag{80}$$

In the above equation, ϕ_e^g is the elemental value of the scalar flux in energy group g, and Σ_f^g is the homogenized fission cross section for energy group g and element e.

In terms of the neutronics calculations, the temperature of distribution of the medium is needed. This information will be provided to EVENT by the fluid/solid solver. Using the internal heat generation, the fluid/solid solver will solve the energy equation throughout the entire domain. Since the same mesh is used between Event and the fluid/solid solver, the temperature information is easily transfered to EVENT with no need for interpolation or restriction of the domain. The calculation of cross-sections based on these temperatures is then handled internally by EVENT. The treatment of these cross-section is not addressed as part of this work.

5 Conclusion

The PCICE scheme is a prime candidate for use within a multiphysics algorithm due to its applicability to all flow regimes and its improved stability properties. Additionally, the operator splitting procedure of the PCICE facilitate the incorporation of other physics, for instance, radiative heat transfer, chemical reactions and neutronics. The quasi-one dimensional algorithm developed here demonstrates the value of PCICE as a multiphysics solver and provides a basis for such an algorithm in higher dimensions. In order to apply such a scheme to higher dimensions, a finite volume PCICE formulation was developed and a practical implementation of conjugate heat transfer into the formulation was introduced. To increase the applicability of the scheme presented, the solver must be expanded to include various working fluids, such

as water and Sodium. This addition would allow for the simulation of a broader spectrum of reactors types. These improvements are areas of active work.

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