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Short note

Notes on the PCICE method: Simplification, generalization, and compressibility properties

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Abstract

The pressure-based PCICE numerical method [R.C. Martineau, R.A. Berry, The pressure-corrected ICE finite element method (PCICE-FEM) for compressible flows on unstructured meshes, J. Comput. Phys. 198 (2004) 659] for computing transient fluid flows of all speeds from nearly incompressible to high supersonic with strong shocks is simplified and generalized. Its behavior is examined in the nearly incompressible limit and in the fully compressible limit. In the nearly incompressible limit the PCICE algorithm is found to reduce to a generalization of the incompressible MAC method, which includes the density gradient as a driving function in the pressure Poisson equation. In the fully compressible regime, it is found to reduce to an expression equivalent to density-based methods for high-speed flow.

Keywords: Compressible flow; Incompressible flow; All-speed flow; PCICE; ICE; Fractional-step method; Pressure-based method

1. Introduction

The pressure-corrected variant of the implicit continuous-fluid Eulerian (ICE) [2], or PCICE numerical method has been presented [1] as a finite element method, PCICE-FEM, for computing fluid flows of all speeds from low subsonic or nearly incompressible to high supersonic compressible. PCICE is a predictor–corrector method for approximating the solution of the conservative form of the Euler/Navier–Stokes equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{u} = 0, \tag{1}$$

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

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

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where ρ, $\vec{u}$, p, and T represent the fluid mass density, velocity, pressure, and temperature, respectively. In these equations, τ is the shear stress, $e_t = e + \frac{\vec{u}\cdot\vec{u}}{2}$ is the total energy density (where e is the internal energy density), $h_t = \frac{\rho e_t + p}{\rho}$ is the specific total enthalpy, and $i(T)$ is a temperature-dependent energy source term. Fourier's law for thermal conduction has been assumed with k denoting the thermal conductivity. These equations represent the balance of mass, momentum, and total energy, respectively. Because the PCICE method is not restricted to any specific equation of state, the general functional form

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

will be utilized throughout this development.

The objectives of this short note are twofold. First, it presents a simplified, yet generalized, description of the PCICE method, independent of specific spatial discretizations and equations of state. Second, the behavior of the PCICE method is examined in the nearly incompressible limit ($c\Delta t \gg l$, where c is the acoustic wave speed, Δt represents the time resolution of interest, and l represents the characteristic length of interest) as well as in the fully compressible limit ($c\Delta t \ll l$).

2. PCICE algorithm

The pressure-corrected implicit continuous-fluid Eulerian, or PCICE algorithm [1], is an ideal basis with which to construct a fully coupled unified physics computer analysis code. This scheme, developed for all-speed compressible and nearly incompressible flows, improves upon previous pressure-based methods in terms of accuracy and numerical efficiency and gives a wider range of applicability. Because of the need to simulate flows with shocks it is essential that both the governing equations and their discretized approximations be in conservative form [3,4]. Unlike other ICE variants that have been proposed in the past, most of which are entirely or partially in primitive form, the PCICE algorithm solves the conservative form of the governing equations.

Other researchers have coupled, to varying extent, energy effects into ICE-type algorithms [5–8], but most have utilized, entirely or partially, non-conservative forms which led to algorithms which are restricted to smooth transient solutions (no discontinuity waves) or to steady solutions with sonic- and lower speeds. Patnaik et al. [9] developed a "barely implicit" ICE-type algorithm in conservative form which primarily couples the momentum and energy equations, similar to that of Cassuli and Greenspan [5]. The PCICE algorithm efficiently incorporates an even higher degree of implicitness into a very general conservative framework which can be utilized with either finite difference, finite volume, or finite element spatial representations. In the PCICE algorithm, the total energy equation is sufficiently coupled to the pressure Poisson equation to avoid iteration between the pressure Poisson equation and the pressure–correction equations. Both the mass conservation and total energy equations are explicitly convected with the time-advanced explicit momentum. The pressure Poisson equation then has the time-advanced internal energy information it requires to yield an accurate implicit pressure. At the end of a time step, the conserved values of mass, momentum, and total energy are all pressure-corrected. As a result, the iterative process usually associated with pressure-based schemes is not required. This aspect has been found advantageous when computing transient compressible flows, including flows with significant energy deposition, chemical reactions, or phase change.

The pressure-based PCICE solution algorithm is composed of two fractional steps: an explicit predictor step and an implicit pressure correction step which includes an elliptic Poisson equation which is solved for new-time pressures and an explicit correction with the new pressures. The pressure, momentum, and density in the governing hydrodynamic equations are treated in an implicit fashion. The so-called mass–momentum coupling is obtained by substituting the momentum balance equations into the mass conservation equation to eliminate time-advanced momentum–density (or mass flux) as an unknown. The time rate of density change in the mass conservation equation is then expressed in terms of pressure and internal energy change by employing the equation of state. These substitutions result in a single second-order elliptic differential equation in terms of pressure (pressure Poisson equation). This semi-implicit treatment has two advantages over explicit schemes. First, the acoustic component from the explicit time step size stability criteria is removed, thus eliminating the time integration stiffness that results from slow flows. Second, the pressure obtained with this semi-implicit treatment corrects the momentum to satisfy mass conservation requirements. This allows nearly incompressible flows to be simulated with compressible flow equations, which can be used to simulate flows from very low speeds to supersonic, including mixed flows with all flow speeds present.

Though our original description of the PCICE algorithm was in the context of a finite element-based method, PCICE-FEM [1], with an ideal gas equation of state, it can be generally implemented within the context of other spatial discretization methods (finite difference, finite volume, grid-free, etc.). Therefore, the description of the PCICE algorithm given here will be kept free of specialized spatial discretizations and equations of state.

3. Temporal discretization

The PCICE algorithm is a predictor–corrector method for solving the following time discretization of balance equations (1)–(3) for mass, momentum, and energy, respectively:

$$\rho^{n+1} = \rho^n - \Delta t \nabla \cdot [\varphi(\rho\vec{u})^{n+1} + (1-\varphi)(\rho\vec{u})^n], \tag{5}$$

$$(\rho\vec{u})^{n+1} = (\rho\vec{u})^n - \Delta t \vec{\nabla} \cdot (\rho\vec{u} \otimes \vec{u})^{n+\varphi} - \Delta t \vec{\nabla}[\varphi p^{n+1} + (1-\varphi)p^n] + \Delta t \nabla \cdot \tau^n, \tag{6}$$

$$(\rho e_t)^{n+1} = (\rho e_t)^n - \Delta t \vec{\nabla} \cdot [\varphi(\rho\vec{u})^{n+1} h_t^{n+1} + (1-\varphi)(\rho\vec{u})^n h_t^n] + \Delta t \nabla \cdot (\tau^n \cdot \vec{u}^n) + \Delta t \nabla \cdot (k \nabla T^n) + \Delta t i^n. \tag{7}$$

These equations are approximated with the following fractional two-step process.

3.1. Fractional Step 1

The predictor step first solves a portion of Eqs. (5)–(7), *in order*:

Momentum:

$$(\rho\vec{u})^* = (\rho\vec{u})^n - \Delta t \vec{\nabla} \cdot (\rho\vec{u} \otimes \vec{u})^{n+\varphi} + \Delta t \nabla \cdot \tau^n, \tag{8}$$

where the divergence term is at a partially time-advanced level obtained by utilizing an explicit two-step or predictor–corrector technique such as Lax-Wendroff, etc. (in the PCICE-FEM method [1], an efficient Taylor–Galerkin method was used).

Mass:

$$\rho^* = \rho^n - \Delta t \nabla \cdot [\varphi(\rho\vec{u})^* + (1-\varphi)(\rho\vec{u})^n] = \rho^n - \Delta t \nabla \cdot \{\varphi[(\rho\vec{u})^* - (\rho\vec{u})^n] + (\rho\vec{u})^n\}. \tag{9}$$

Total energy:

$$\begin{aligned}(\rho e_t)^* &= (\rho e_t)^n - \Delta t \vec{\nabla} \cdot [\varphi(\rho\vec{u})^* + (1-\varphi)(\rho\vec{u})^n] h_t^n + \Delta t \nabla \cdot (\tau^n \cdot \vec{u}^n) + \Delta t \nabla \cdot (k \nabla T^n) + \Delta t i^n \\ &= (\rho e_t)^n - \Delta t \nabla \cdot \{\varphi[(\rho\vec{u})^* - (\rho\vec{u})^n] + (\rho\vec{u})^n\} h_t^n + \Delta t \nabla \cdot (\tau^n \cdot \vec{u}^n) + \Delta t \nabla \cdot (k \nabla T^n) + \Delta t i^n.\end{aligned} \tag{10}$$

It is important that the quantities ρ^*, $(\rho\vec{u})^*$, and $(\rho e_t)^*$ be advanced with high-order monotonic algorithms such as FCT, TVD, ENO, etc. or that they be smoothed with another appropriate smoother such as the variable diffusion method of Swanson and Turkel [10] used in the finite element version PCICE-FEM [1]. Using the same notation $(\cdot)^*$ for smoothed variables, the other variables are then obtained from

$$\vec{u}^* = \frac{(\rho\vec{u})^*}{\rho^*}, \quad e_t^* = \frac{(\rho e_t)^*}{\rho^*}, \quad e^* = e_t^* - \frac{\vec{u}^* \cdot \vec{u}^*}{2}, \quad T^* = \frac{e^*}{c_v}, \quad p^* = f(\rho^*, e^*). \tag{11}$$

The pressure gradient term is not included in the partial momentum balance equation (8) because it will be included implicitly in the next fractional step. Therefore the time step stability restriction for this fractional step is the satisfaction of the material Courant condition, or the Courant condition based on flow speed. Because the shear stress term in Eq. (8) and the heat conduction and energy source terms in Eq. (10) are treated explicitly, a stable time step based on these terms may still be too restrictive. To obtain additional stability with larger time steps, these terms can be treated implicitly, either here in this fractional step, or in an additional (subsequent or previous) fractional step (for which case these terms would not even appear in this fractional step).

3.2. Fractional Step 2

This step seeks to solve the following portion of the original discretized equations (5)–(7) to obtain new time pressure.

Momentum:

$$(\rho\vec{u})^{n+1} = (\rho\vec{u})^* - \Delta t\nabla[\varphi p^{n+1} + (1-\varphi)p^n] = (\rho\vec{u})^* - \varphi\Delta t\nabla(p^{n+1} - p^n) - \Delta t\nabla p^n. \tag{12}$$

Mass:

$$\rho^{n+1} = \rho^* - \varphi\Delta t\nabla\cdot\left[(\rho\vec{u})^{n+1} - (\rho\vec{u})^*\right]. \tag{13}$$

Total energy:

$$(\rho e_t)^{n+1} = (\rho e_t)^* - \varphi\Delta t\nabla\cdot\left[(\rho\vec{u})^{n+1}h_t^{n+1} - (\rho\vec{u})^* h_t^n\right]. \tag{14}$$

This is accomplished in a couple of steps, first by constructing a pressure Poisson equation which is solved to obtain pressures at the new-time level, then correcting the dependent variables with these new-time pressures to obtain Eqs. (12)–(14).

The pressure Poisson equation is constructed as follows. Substituting (12) into (13) gives

$$\rho^{n+1} = \rho^* + \varphi^2\Delta t^2\nabla\cdot\nabla(p^{n+1} - p^n) + \varphi\Delta t^2\nabla\cdot\nabla p^n$$

or

$$\begin{aligned}\rho^{n+1} - \rho^n &= \rho^* - \rho^n + \varphi^2\Delta t^2\nabla\cdot\nabla(p^{n+1} - p^n) + \varphi\Delta t^2\nabla\cdot\nabla p^n \\ &= \delta\rho + \varphi^2\Delta t^2\nabla\cdot\nabla(p^{n+1} - p^n) + \varphi\Delta t^2\nabla\cdot\nabla p^n,\end{aligned} \tag{15}$$

where $\delta\rho = \rho* - \rho^n$. Note that $\delta\rho$ is a smoothed quantity because $\rho*$ has been smoothed.

Alternatively, using Eq. (9)

$$\delta\rho = -\Delta t\nabla\cdot\{\varphi[(\rho\vec{u})^* - (\rho\vec{u})^n] + (\rho\vec{u})^n\},$$

where, again, a smoothed $\delta\rho$ is obtained by using the smoothed value $(\rho\vec{u})^*$. Adopting this approach, Eq. (15) can be written as

$$\rho^{n+1} - \rho^n = -\Delta t\nabla\cdot\{\varphi[(\rho\vec{u})^* - (\rho\vec{u})^n] + (\rho\vec{u})^n\} + \varphi^2\Delta t^2\nabla\cdot\nabla(p^{n+1} - p^n) + \varphi\Delta t^2\nabla\cdot\nabla p^n. \tag{16}$$

From the equation of state (EOS)

$$p = f(\rho, e)$$

one can obtain

$$\delta\rho = \frac{1}{\frac{\partial f}{\partial\rho}}\delta p - \frac{\frac{\partial f}{\partial e}}{\frac{\partial f}{\partial\rho}}\delta e,$$

where δ just indicates a perturbation or change in a quantity (not to be confused, at this point, with the δ of Eq. (15)). This leads to the simple approximation

$$\rho^{n+1} - \rho^n \approx \frac{1}{\left(\frac{\partial f}{\partial\rho}\right)^*}(p^{n+1} - p^n) - \frac{\left(\frac{\partial f}{\partial e}\right)^*}{\left(\frac{\partial f}{\partial\rho}\right)^*}(e^* - e^n). \tag{17}$$

The pressure Poisson equation, in terms of $\delta p = p^{n+1} - p^n$, is finally obtained by substituting (17) into (16) giving

$$\begin{aligned}&\frac{1}{\left(\frac{\partial f}{\partial\rho}\right)^*}(p^{n+1} - p^n) - \frac{\left(\frac{\partial f}{\partial e}\right)^*}{\left(\frac{\partial f}{\partial\rho}\right)^*}(e^* - e^n) \\ &\quad = \varphi^2\Delta t^2\nabla\cdot\nabla(p^{n+1} - p^n) - \Delta t\nabla\cdot\{\varphi[(\rho\vec{u})^* - (\rho\vec{u})^n] + (\rho\vec{u})^n\} + \varphi\Delta t^2\nabla\cdot\nabla p^n\end{aligned}$$

or

$$\frac{1}{\left(\frac{\partial f}{\partial \rho}\right)^*}(p^{n+1}-p^n) - \varphi^2 \Delta t^2 \nabla \cdot \nabla (p^{n+1}-p^n)$$
$$= \frac{\left(\frac{\partial f}{\partial e}\right)^*}{\left(\frac{\partial f}{\partial \rho}\right)^*}(e^* - e^n) - \Delta t \nabla \cdot \{\varphi[(\rho\vec{u})^* - (\rho\vec{u})^n] + (\rho\vec{u})^n\} + \varphi \Delta t^2 \nabla \cdot \nabla p^n. \quad (18)$$

Numerical solution of this equation by an efficient, elliptic partial differential equation solver yields the new pressure distribution, p^{n+1}.

The other dependent variables are then updated, or corrected, with the new-time pressures as follows, *in order*:

Momentum:

$$(\rho\vec{u})^{n+1} = (\rho\vec{u})^* - \Delta t \nabla[\varphi p^{n+1} + (1-\varphi)p^n]. \quad (19)$$

Mass:

$$\rho^{n+1} = \rho^* - \varphi \Delta t \nabla \cdot [(\rho\vec{u})^{n+1} - (\rho\vec{u})^*]. \quad (20)$$

Total energy:

$$h_t^{n+1} = \frac{(\rho e_t)^* + p^{n+1}}{\rho^{n+1}}, \quad (21)$$

$$(\rho e_t)^{n+1} = (\rho e_t)^* - \varphi \Delta t \nabla \cdot \left[(\rho\vec{u})^{n+1} h_t^{n+1} - (\rho\vec{u})^* h_t^n\right]. \quad (22)$$

4. Compressible and incompressible limits

The objective here is to examine the compressible and incompressible limiting forms of the PCICE algorithm. For simplicity, the particular form resulting from choosing $\varphi = 1.0$ will be examined. For this case, the pressure Poisson equation (18) becomes

$$\frac{1}{\left(\frac{\partial f}{\partial \rho}\right)^*}(p^{n+1}-p^n) = \Delta t^2 \nabla^2 p^{n+1} + \frac{\left(\frac{\partial f}{\partial e}\right)^*}{\left(\frac{\partial f}{\partial \rho}\right)^*}(e^* - e^n) - \Delta t \nabla \cdot (\rho\vec{u})^*. \quad (23)$$

Dividing by Δt, noting that the isentropic sound speed c^* is given by

$$(c^*)^2 = \frac{p^*}{(\rho^*)^2}\left(\frac{\partial f}{\partial e}\right)^* + \left(\frac{\partial f}{\partial \rho}\right)^*,$$

and introducing

$$\frac{1}{\left(\frac{\partial f}{\partial \rho}\right)^*} = \frac{A^*}{(c^*)^2}, \quad \text{where } A^* = \left[1 + \frac{p^*\left(\frac{\partial f}{\partial e}\right)^*}{(\rho^*)^2\left(\frac{\partial f}{\partial \rho}\right)^*}\right],$$

gives

$$\frac{A^*}{(c^*)^2}\frac{p^{n+1}-p^n}{\Delta t} = \Delta t \nabla^2 p^{n+1} + \frac{A^*\left(\frac{\partial f}{\partial e}\right)^*}{(c^*)^2}\frac{e^*-e^n}{\Delta t} - \nabla \cdot (\rho\vec{u})^*. \quad (24)$$

If Eq. (24) is multiplied by a characteristic length, l, and a characteristic time, $\tau_c = \frac{l}{c^*}$, is introduced, the pressure Poisson equation becomes

$$\tau_c \frac{p^{n+1}-p^n}{\Delta t} = \frac{lc^* \Delta t}{A^*}\nabla^2 p^{n+1} + \tau_c \left(\frac{\partial f}{\partial e}\right)^* \frac{e^*-e^n}{\Delta t} - \frac{lc^*}{A^*}\nabla \cdot (\rho\vec{u})^*. \quad (25)$$

The characteristic time τ_c approximates the time it takes an acoustic wave (traveling with velocity c^*) to propagate the distance (l) characterizing the portion of our solution domain of interest and effecting the solution change. While incompressible fluids do not physically exist, such a mathematical model can be conceived by supposing the time resolution of interest corresponds to Δt. Thus, if the case is desired in which $\tau_c \ll \Delta t$, then necessarily the resolution of the physical acoustic waves which produce the solution change is not of interest. Furthermore, a characteristic time $\tau_u = \frac{l}{|\vec{u}|}$ can be identified which approximates the time it takes to advect the solution a distance l. In the incompressible limit $\tau_c \ll \Delta t < \tau_u$, or in other words $c^*\Delta t \gg l$, which implies that $\frac{\tau_c}{\Delta t} \to 0$ and the pressure Poisson equation (25) effectively reduces to

$$\nabla^2 p^{n+1} = \frac{\nabla \cdot (\rho\vec{u})^*}{\Delta t}. \tag{26}$$

Obviously the incompressible limit also implies that $\frac{|\vec{u}|}{c^*} \ll \frac{|\vec{u}|\Delta t}{l} < 1$, or the *Mach Number* $\ll 1$. The corresponding, traditional MAC-type pressure Poisson equation [11], without convective terms, is

$$\nabla^2 p^{n+1} = \frac{\rho^n \nabla \cdot \vec{u}^*}{\Delta t}. \tag{27}$$

In this equation, the computed pressure field will be consistent with the requirement for incompressible flow fields that the velocity field be divergence-free. However, Eq. (26) additionally allows for potentially important spatial gradients in the density field to drive the pressure Poisson equation, and thus to be coupled with the pressure and velocity fields.

On the other hand, for fully compressible flows $\tau_u > \tau_c \gg \Delta t$, or $c^*\Delta t \ll l$, and the pressure Poisson equation (25) can be rewritten as

$$\frac{1}{\left(\frac{\partial f}{\partial \rho}\right)^*} \frac{p^{n+1} - p^n}{\Delta t} - \frac{\left(\frac{\partial f}{\partial e}\right)^*}{\left(\frac{\partial f}{\partial \rho}\right)^*} \frac{e^* - e^n}{\Delta t} = -\nabla \cdot (\rho\vec{u})^* \tag{28}$$

(as seen from Eq. (17)) which is effectively a density-based compressible flow algorithm since it is easily recognized that the left side of this equation is an approximation for the term $\frac{\partial \rho}{\partial t}$. In fact, the combination of fractional step 1 above with pressure equation (28) and the correction equations (19)–(22), to which the PCICE methods reduces in this limit, constitutes an explicit, predictor–corrector algorithm for fully compressible flows.

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