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ISCES: A SPECTRAL ELEMENT CODE WITH DYNAMIC REZONING AND VARIABLE DIFFUSIVITY

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ABSTRACT

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1. MODEL

1.1. *Pseudo-Incompressible Equations*

We start from the fully compressible equations of hydrodynamics in an irrotational system without magnetic fields (e.g. Braginsky & Roberts (2006)),

$$\rho \frac{D}{Dt}\mathbf{u} = -\nabla p - \rho\nabla\Phi + \nabla\cdot\mathbf{\Pi}, \tag{1a}$$

$$\frac{D}{Dt}\rho = -\rho\nabla\cdot\mathbf{u}, \tag{1b}$$

$$\rho T\frac{D}{Dt}s = \nabla\mathbf{u} : \mathbf{\Pi} + \sum_i \mu_i\nabla\cdot\mathbf{C}_i - \nabla\cdot\mathbf{H}, \tag{1c}$$

$$\rho\frac{D}{Dt}\xi_i = -\nabla\cdot\mathbf{C}_i, \tag{1d}$$

where ρ is the mass density, $\mathbf{u}$ is the velocity, Φ is the gravitational potential energy, s is the entropy, and ξ_i is the fractional abundance of the ith compositional component of the fluid.

Given an equation of state of the form $e(\rho, s, \xi_1, \xi_2, \dots)$, we can formally define

$$p \equiv \rho^2\frac{\partial e}{\partial \rho}, \tag{2a}$$

$$T \equiv \frac{\partial e}{\partial s}, \tag{2b}$$

$$\mu_i \equiv \frac{\partial e}{\partial \xi_i}, \tag{2c}$$

which are the pressure, temperature, and chemical potentials, respectively. The remaining quantities, **Pi**, **H**, and $\mathbf{C_i}$ are the stress tensor, heat flux vector, and compositional flux vectors, respectively.

These equations as they are conserve momentum through Equation 1a, mass through Equation 1b, and energy as follows:

$$\rho\frac{D}{Dt}\left(\mathbf{u}^2/2 + e + \Phi\right) + \nabla\cdot\mathbf{u} = \nabla\cdot\left(\Pi\cdot\mathbf{u} - \mathbf{H}\right), \tag{3}$$

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which can be derived trivially using Equations 1a through 1d and the first law of thermodynamics:

$$de = Tds + \frac{p}{\rho^2}d\rho + \sum_i \mu_i d\xi_i. \tag{4}$$

Vasil et al. (2013) show that in the absence of any nonconservative effects, such as diffusion, and under the approximation that the fluid is constrained to be in pressure balance, the pseudo-incompressible equations take the following form:

$$\rho\frac{D}{Dt}\mathbf{u} = -\nabla p_0 - p_0^{\frac{c_p}{c_V}}\nabla\left(\frac{p_1}{p_0^{\frac{c_p}{c_V}}}\right) - \rho\nabla\Phi, \tag{5a}$$

$$\frac{D}{Dt}\rho = -\rho\nabla\cdot\mathbf{u}, \tag{5b}$$

$$\nabla\cdot p_0^{\frac{c_p}{c_V}}\mathbf{u} = 0, \tag{5c}$$

where p_0 is a nonuniform but static reference pressure, p_1 is a small pressure perturbation, and c_V and c_p are the specific heat capacities at constant volume and pressure, respectively. As an additional assumption to arrive at this expression, it must be assumed that $\frac{c_p}{c_V} = \frac{\rho}{p}\left.\frac{\partial p}{\partial \rho}\right|_s$ is constant, which is the case for an ideal gas. It should be noted that these equations do not take the same form as those from the original ones in Durran (1989), rather they are derived to conserve mass and energy.

Wood (private communication) has used these results to derive a set of equations with varying composition and allowing for diffusion while still conserving energy and mass:

$$p_0\left(\mathbf{x}\right) = p\left(\rho, s, \xi_1, \xi_2, \dots\right), \tag{6a}$$

$$\rho \frac{D}{Dt}\mathbf{u} = -\nabla\left(p_0 + p_1\right) + \frac{p_1}{\rho}\left(\frac{\partial p}{\partial \rho}\right)^{-1}\nabla p_0 - \rho\nabla\Phi + \nabla\cdot\mathbf{\Pi}, \tag{6b}$$

$$\frac{D}{Dt}\rho = -\rho\nabla\cdot\mathbf{u}, \tag{6c}$$

$$\rho T\frac{D}{Dt}s = \left(\nabla\mathbf{u} : \mathbf{\Pi} - \nabla\cdot\mathbf{H}\right)\left(1+Q\right) + \sum_i \mu_i \nabla\cdot\mathbf{C}_i, \tag{6d}$$

$$\rho\frac{D}{Dt}\xi_i = -\nabla\cdot\mathbf{C}_i, \tag{6e}$$

where Q is a source term that will enforce energy conservation.

This necessitates the use of an equation of state.

1.2. *Equation of State*

To close these equations, we need an equation of state, for which we'll simply use an ideal gas, ie. $p = \rho kT/\overline{m}$. The full expression is $e = \frac{k}{(\gamma-1)\overline{m}}\left(\frac{\rho\Phi}{\overline{m}}e^{\frac{s}{\overline{m}}k}\right)^{\gamma-1}$. With this, we can express the velocity equation as

$$\rho\frac{D}{Dt}\mathbf{u} = -\nabla\left(p_0 + p_1\right) + \frac{p_1}{p\gamma}\nabla p_0 - \rho\nabla\Phi + \nabla\cdot\mathbf{\Pi}. \tag{7}$$

From the equation of state, we can derive a temperature of $T = e\overline{m}\left(\gamma-1\right)/k$. We can then derive a temperature equation by taking

$$\frac{dT}{T} = \gamma\frac{d\rho}{\rho} + \left(\gamma-1\right)\frac{\overline{m}}{k}dS \tag{8}$$

1.3. *Velocity Constraint*

We can use these to derive a velocity constraint. Expanding the pressure constraint into its differential components, we find

$$\frac{D}{Dt}p_0 = \frac{\partial p}{\partial\rho}\frac{D}{Dt}\rho + \frac{\partial p}{\partial s}\frac{D}{Dt}s + \frac{\partial p}{\partial\xi_i}\frac{D}{Dt}\xi_i. \tag{9}$$

Since $p = \rho\left(\gamma-1\right)e$, we derive the following, substituting in the full equations where convenient:

$$\mathbf{u}\cdot\nabla p_0 = -\gamma p_0\nabla\cdot\mathbf{u} + \left(\gamma-1\right)\left(\nabla\mathbf{u} : \mathbf{\Pi} - \nabla\cdot\mathbf{H}\right)\left(1+Q\right), \tag{10}$$

which can be reorganized as

$$\nabla\cdot p_0^{\frac{1}{\gamma}} = \frac{\gamma-1}{\gamma}p_0^{\frac{1}{\gamma}-1}\left(\nabla\mathbf{u} : \mathbf{\Pi} - \nabla\cdot\mathbf{H}\right)\left(1+Q\right). \tag{11}$$

1.4. *Energy Conservation*

To conserve energy, we add up all possible stores of energy:

$$\rho\frac{D}{Dt}\left(\frac{\mathbf{u^2}}{2} + \Phi\right) + \mathbf{u}\cdot\nabla\left(p_0+p_1\right) = \frac{p_1}{\gamma p_0}\mathbf{u}\cdot\nabla p_0 + \mathbf{u}\cdot\nabla\cdot\mathbf{\Pi}, \tag{12}$$

$$\rho T\frac{D}{Dt}s = \left(\nabla\mathbf{u} : \mathbf{\Pi} - \nabla\cdot\mathbf{H}\right)\left(1+Q\right) + \sum_i \mu_i\nabla\cdot\mathbf{C}_i, \tag{13}$$

$$\rho\frac{D}{Dt}\xi_i = -\nabla\cdot\mathbf{C}_i. \tag{14}$$

Using the first law of thermodynamics ($de = Tds + \mu_i d\xi_i + p_0 d\rho/\rho^2$, we can combine these:

$$\rho\frac{D}{Dt}\left(\frac{\mathbf{u^2}}{2} + \Phi + e\right) + \nabla\cdot\mathbf{u}\left(p_0+p_1\right) - p_1\nabla\cdot\mathbf{u} = \frac{p_1}{\gamma p_0}\mathbf{u}\cdot\nabla p_0 + \mathbf{u}\cdot\nabla\cdot\mathbf{\Pi} + \rho \tag{15}$$

Applying our velocity constraint and substituting our governing equations, we get

$$\rho\frac{D}{Dt}\left(\frac{\mathbf{u^2}}{2} + \Phi + e\right) + \nabla\cdot\mathbf{u}\left(p_0+p_1\right) \tag{16}$$

$$= \left(\frac{p_1}{p_0}\frac{\gamma-1}{\gamma} + 1\right)\left(\nabla\mathbf{u} : \mathbf{\Pi} - \nabla\cdot\mathbf{H}\right)\left(1+Q\right) + \mathbf{u}\cdot\nabla\cdot\mathbf{\Pi}. \tag{17}$$

To ensure energy conservation, the right hand side must be

$$\nabla\mathbf{u} : \mathbf{\Pi} - \nabla\cdot\mathbf{H} + \mathbf{u}\cdot\nabla\cdot\mathbf{\Pi}, \tag{18}$$

which is true only when $Q = -p_1\left(\gamma-1\right)/\left(p_0\gamma + p_1\left(\gamma-1\right)\right)$. Unfortunately, this proves to be somewhat analytically untractable. We can approximate $Q \approx -p_1\left(\gamma-1\right)/p_0\gamma$, which undermines our attempt for perfect energy conservation

1.5. *Temperature Equation*

Using the equation of state and the new entropy equation, we can derive an equation for temperature. Recall that for an ideal gas, $T = \overline{m}\left(\gamma-1\right)e/k$, so

$$\frac{D}{Dt}T = \frac{\partial T}{\partial\rho}\frac{D}{Dt}\rho + \frac{\partial T}{\partial s}\frac{D}{Dt}s + \frac{\partial T}{\partial\xi_i}\frac{D}{Dt}\xi_i. \tag{19}$$

Substituting in our governing equations, we find

$$\rho\frac{D}{Dt}T = -\left(\gamma-1\right)\rho T\nabla\cdot u + \left(\gamma-1\right)\frac{\overline{m}}{k}\left(\nabla\mathbf{u} : \mathbf{\Pi} - \nabla\cdot\mathbf{H}\right)\left(1+Q\right). \tag{20}$$

1.6. *Non-dimensionalization*

We can non-dimensionalize the equations as follows:

$$p_0 = \frac{\rho T}{\overline{m}} \tag{21}$$

$$\frac{D}{Dt}\rho\mathbf{u} = -\nabla\left(p_0 + p_1\right) + \frac{p_1}{\gamma p_0}\nabla p_0 - \rho\hat{y} + \nabla\cdot\mathbf{\Pi} \tag{22}$$

$$\frac{D}{Dt}\overline{m} = \nabla\cdot\rho\tau\nabla\frac{\overline{m}}{\rho} \tag{23}$$

$$\frac{1}{\gamma-1}\frac{D}{Dt}\rho T = -\rho T\nabla\cdot\mathbf{u} + \overline{m}\left(\nabla\mathbf{u}:\mathbf{\Pi} + \nabla\cdot\frac{\rho}{\overline{m}}\nabla T\right)(1+Q) \tag{24}$$

$$\nabla\cdot p_0^{\frac{1}{\gamma}} = \frac{\gamma-1}{\gamma}p_0^{\frac{1}{\gamma}-1}\left(\nabla\mathbf{u}:\mathbf{\Pi} - \nabla\cdot\frac{\rho}{\overline{m}}\nabla T\right)(1+Q) \tag{25}$$

$$\Pi_{ij} = \rho\mathrm{Pr}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\nabla\cdot\mathbf{u}\right) \tag{26}$$

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