CFD simulations of AM processes using JAX

Shuheng Liao*

November 2022

1 Equations

The governing equations we considered here are the incompressible N-S equation and energy conservation:

$$\nabla \cdot \boldsymbol{u} = 0 \tag{1}$$

$$\frac{\partial(\rho \boldsymbol{u})}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = \nabla \cdot (\mu \nabla \boldsymbol{u}) - \nabla p + f \tag{2}$$

$$\rho c_{\mathrm{p}} \frac{\partial T}{\partial t} + \rho c_{\mathrm{p}} \nabla \cdot (\boldsymbol{u} T) + \rho L \frac{\partial f_{\mathrm{L}}}{\partial t} + \rho L \boldsymbol{u} \cdot \nabla f_{\mathrm{L}} = \nabla \cdot (k \nabla T) + Q \tag{3}$$

To solve the above transient equations, the convection terms are treated explicitly while the diffusion terms are treated implicitly. E.g., for the engergy conservation, i.e., Equation (3):

$$\rho \bar{c}^{n-1} \frac{T^n - T^{n-1}}{\Delta t} + \rho \bar{c}^{n-1} \nabla \cdot (\boldsymbol{u}^{n-1} T^{n-1}) = \nabla \cdot (k^n \nabla T^n) + Q^n \tag{4}$$

Finite volume method is used for spatial discretization. Central difference scheme is used for the diffusion term while the QUICK scheme is used for the convection term. Note that $\bar{c}$ is the apparent heat capacity:

$$\bar{c} = c_{\mathrm{p}} + L \frac{\partial f_{\mathrm{L}}}{\partial T} \tag{5}$$

Because of the temperature dependence of the thermal conductivity k, Equation (4) leads to a set of nonlinear equations and Newton's method is used to iterative solve the equations. The gradients are calculated using automatic differentiation.

To solve the N-S equation, the fractional step method is used. At each time step, we first estimated the velocity using the pressure gradient at the last step:

$$\rho \frac{\boldsymbol{u}^* - \boldsymbol{u}^{n-1}}{\Delta t} + \rho \cdot \nabla(\boldsymbol{u}^{n-1} \boldsymbol{u}^{n-1}) = \nabla \cdot (\mu \nabla \boldsymbol{u}^*) - \nabla p^{n-1} + f^n \tag{6}$$

Then, a Poisson equation is solved for correcting the pressure:

$$p^n = p^{n-1} + p' \tag{7a}$$

$$\nabla^2 p' = \frac{\rho}{\Delta t} \nabla \cdot \boldsymbol{u}^* \tag{7b}$$

The velocity can be then updated by

$$\boldsymbol{u}^n = \boldsymbol{u}^* - \frac{\Delta t}{\rho} \nabla p' \tag{8}$$

Note that the equations we need to solve are: Equations (4), (6) and (7), and all of them are Poisson-type equations.

*github link