### Introduction

In scientific computing, code verification ensures the reliability and numerical accuracy of a model simulation by comparing the simulation results to experimental data or known analytical solutions. The model is typically defined by a set of partial differential equations with initial and boundary conditions, and verification ensures that the software is used to model high-consequence systems which cannot be physically tested in a fully operational environment.

Verifying the simulation to experimental data or known analytical solutions. The model is typically defined by a set of partial differential equations with initial and boundary conditions, and verification ensures that the software is used to model high-consequence systems which cannot be physically tested in a fully operational environment. The exercise of verification and validation should follow the guidelines of Oberkampf and Trucano (2007), which describes four essential elements in high-quality verification benchmark construction: (1) conceptual description, (2) mathematical description, (3) accuracy assessment, and (4) additional documentation and user information.

- **Validation:**
  - “Are we building the right software?”
- **Verification:**
  - “Are we building the software right?”

### QA Test Suite Work Flow

We implement several tests using a structured hierarchical approach which results in widespread test coverage. Test execution is automated through controlled Bash scripting.

A script executes the test suite:

```
#!/bin/bash
```

Start with a physical model component (energy, flow, transport, etc.)

For each physical model component, set up a steady and transient problem

For each steady and transient test, set up a problem for each dimension

For each dimension, set up all possible boundary and initial condition types

For every boundary/initial condition type, run the test in each simulation mode

Each test results in simulation output that is stored for later comparison

A python script compares the PFLTRAN solution to the analytical solution

Analytical solutions for each test problem are obtained from literature

The relative error is calculated to decide passing/failing grade

- **PASS** error < 2%
- **FAIL** error > 2%

### 1D Steady Heat Conduction

### Problem

\[
\frac{\partial}{\partial t} \left( \frac{\partial p^2}{\partial x^2} \right) = 0
\]

The domain is a 100x10x10 meter cube made up of 10x10x10 cubic grid cells with dimensions 0.05x0.05x0.05 meters. The cube is composed of two materials with the following properties:

- Thermal conductivity: \(k_1 = 300 \text{ W/mK}\), \(k_2 = 30 \text{ W/mK}\)
- Specific heat: \(c_p = 1 \text{ kJ/kgK}\)
- Density: \(\rho = 1 \text{ kg/m}^3\)

### Initial and Boundary Conditions

The initial temperature is 1.0°C. At the left \((x = 0)\) and right \((x = 1)\) boundaries, a Dirichlet boundary condition is applied: \(T(x = 0) = 3.0°C\), \(T(x = 1) = 1.0°C\) at the right

The simulation is run until a steady-state solution develops.

### Solution

\[
\begin{align*}
T(x) &= T_g + x - 0.5 \quad \text{for} \quad 0 < x < 0.5 \\
T(x) &= T_g + (1 - x) - 0.5 \quad \text{for} \quad 0.5 < x < 1
\end{align*}
\]

### 2D Transient Liquid Flow

### Problem

\[
\frac{\partial}{\partial t} \left( \frac{\partial p^2}{\partial x^2} \right) = 0
\]

The domain is a 10x10x10 meter plate made up of 10x10x10 hexahedral grid cells with dimensions 0.2x0.2x0.2 meters. The column is composed of a single material with the following properties:

- Permeability: \(k = 1 \times 10^{-14} \text{ m}^2\)
- Porosity: \(\phi = 0.20\)
- Fluid viscosity: \(\mu = 1 \times 10^{-3} \text{ Pa s}\)
- Fluid density: \(\rho = 1 \times 10^{-3} \text{ kg/m}^3\)
- Fluid saturation: \(S_w = 0.50\)

### Initial and Boundary Conditions

The initial pressure is described by \(p(0,y,t) = 0\ \text{ Pa}\) at the north and south boundaries, a no-flow boundary condition is applied: \(\nabla \cdot q = 0\) at the west and east boundaries. A Dirichlet boundary condition is applied: \(p(x,0,t) = 0\ \text{ Pa}\)

### Solution

\[
\begin{align*}
p(x,y,t) &= 0.5 \cos \frac{\pi x}{L} \cos \frac{\pi y}{L} \sin \omega t \\
p(x,y,t) &= 0.5 \cos \frac{\pi x}{L} \cos \frac{\pi y}{L} \sin \omega t \\
p(x,y,t) &= 0.5 \cos \frac{\pi x}{L} \cos \frac{\pi y}{L} \sin \omega t
\end{align*}
\]

### 3D Steady Gas Flow

### Problem

\[
\frac{\partial}{\partial t} \left( \frac{\partial p^2}{\partial x^2} \right) = 0
\]

The domain is a 1x1x1 meter cube made up of 2x2x2 cubic grid cells with dimensions 0.5x0.5x0.5 meters. The cube is composed of a single material with the following properties:

- Gas viscosity: \(\mu = 1 \times 10^{-5} \text{ Pa s}\)
- Gas density: \(\rho = 1 \times 10^{-2} \text{ kg/m}^3\)
- Specific heat: \(c_p = 1 \text{ kJ/kgK}\)

### Initial and Boundary Conditions

The initial pressure is \(p(0,y,z) = 0\ \text{ Pa}\) at each face of the cube. A specific gas flow is applied:

\[
\begin{align*}
q(x,y,z) &= 1 \times 10^{-2} \text{ m}^3\text{s}^{-1} \\
q(x,y,z) &= 1 \times 10^{-2} \text{ m}^3\text{s}^{-1}
\end{align*}
\]

### Solution

\[
\begin{align*}
p(x,y,z) &= 0.5 \cos \frac{\pi x}{L} \cos \frac{\pi y}{L} \cos \frac{\pi z}{L} \\
p(x,y,z) &= 0.5 \cos \frac{\pi x}{L} \cos \frac{\pi y}{L} \cos \frac{\pi z}{L}
\end{align*}
\]