**DISCRETIZATION EXAMPLE: CHEMICAL SPECIES TRANSPORT IN A FLOW FIELD**

Consider the transport equation for a chemical species in a flow field:

$$\frac{\partial}{\partial x_i} (u_i c) = \frac{\partial}{\partial x_i} \left( D \frac{\partial c}{\partial x_i} \right) + S$$

- $c$ : species concentration
- $D$ : diffusion coefficient
- $S$ : source term

Alternate form:

$$\nabla \cdot (c \mathbf{V}) = \nabla \cdot (D \nabla c) + S$$

This equation is to be solved over the following computational domain:

**STEP 1: INTEGRAL FORM OF THE GOVERNING EQUATION**

The governing equation is integrated over a CV:

The divergence theorem is used to convert integrals over CV into integrals over CS.

Divergence theorem: $\int_{CV} \nabla \cdot \mathbf{f} \ dV = \oint_{CS} \mathbf{f} \cdot d\mathbf{A}$

Convective term:

Diffusive term:
**STEP 2: EQUATION LINEARIZATION**
Each surface integral is expressed in terms of a sum over all cell faces.

Convective term:

Diffusive term:

Face values for $c$ and $u$ are not known a priori (values are stored at computational nodes). They are obtained using different interpolation techniques:
- Upwind discretization scheme (UDS)
- Central differencing scheme (CDS)
- Power law scheme
- Quadratic upwind scheme (QUICK – quadratic interpolation for convective kinematics)