1. Business
   a. Teams
   b. Schedule
   c. Don't be afraid to explore → gridding

2. Review (Where are we?)
   - Equilibrium
   - Detailed Chemistry
   - Turbulent Reacting Gaseous Flow (Fluent)

3. Now add a condensed phase!
   - Droplet combustion ⇒ engines for transportation
   - Particle combustion
     ⇒ pulverized coal ⇒ electricity
     ⇒ biomass
     ⇒ propellants

4. Class Outline (Typed sheet)
**Eulerian**

- Solve on a grid
- Transport properties between cells based on \( \rho, T, P \)
- Finite volume approach
- Use void fraction
  \[ \theta = \frac{V_{gas}}{V_{gas} + V_{solid}} \]
  dispersed when \( \theta \approx 1 \)

**Advantages**

- Easy

**Disadvantages**

- Hard to get Eulerian transport properties for particles (no energy for particles)
- Particle history effects not modeled
- Turbulence affects particles differently than gas

**Lagrangian**

- Solve along particle trajectories
  - Continuity, momentum, energy
  - \( \frac{dx}{dt} \)
  - \( \frac{dy}{dt} \)
  - \( \frac{dz}{dt} \)
  (i.e., solve time-dependent particle eqns.)
- Save source terms for gas phase eqns.
- Use gas properties from Eulerian approach
  - Gas phase
  - Solid particle phase

**Advantages**

- Easy to get physical parameters to solve conservative equations
- History effect modeled
- Particle properties dependent on path (to the cell)
- Can use small time steps when needed

**Disadvantages**

- Need lots of particles to represent system
- Interface with gas phase is sometimes hard
Table 1. Summary of Conservation Equations for Gas–Particle Mixtures

### Continuity equation

<table>
<thead>
<tr>
<th>Phase</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas phase</td>
<td>$\frac{\partial \rho_g}{\partial t} + \nabla \cdot (\rho_g \mathbf{v}_g) = r_p$</td>
</tr>
<tr>
<td>Particle phase</td>
<td>$\frac{\partial \rho_p}{\partial t} + \nabla \cdot (\rho_p \mathbf{v}_p) = -r_p$</td>
</tr>
<tr>
<td>Mixture</td>
<td>$(\frac{\partial}{\partial t})(\rho_p + \rho_g) + \nabla \cdot (\rho_g \mathbf{v}_g + \rho_p \mathbf{v}_p) = 0$</td>
</tr>
</tbody>
</table>

### Momentum equation

<table>
<thead>
<tr>
<th>Phase</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas phase</td>
<td>$(\frac{\partial}{\partial t})(\rho_g \mathbf{v}_g) + \nabla \cdot (\rho_g \mathbf{v}_g \mathbf{v}_g) = -\nabla p + \nabla \cdot [\theta \tau + (1 - \theta)\tau_a] - \mathbf{f}_p + \rho_g \mathbf{g} + \mathbf{v}_p \mathbf{r}_p$</td>
</tr>
<tr>
<td>Particle phase</td>
<td>$(\frac{\partial}{\partial t})(\rho_p \mathbf{v}_p) + \nabla \cdot (\rho_p \mathbf{v}_p \mathbf{v}_p) = \mathbf{f}_p + \rho_p \mathbf{g} - \mathbf{v}_p \mathbf{r}_p$</td>
</tr>
<tr>
<td>Mixture</td>
<td>$(\frac{\partial}{\partial t})(\rho_g \mathbf{v}_g + \rho_p \mathbf{v}_p) + \nabla \cdot (\rho_g \mathbf{v}_g \mathbf{v}_g + \rho_p \mathbf{v}_p \mathbf{v}_p) = -\nabla p + \nabla \cdot [\theta \tau + (1 - \theta)\tau_a] + (\rho_g + \rho_p) \mathbf{g}$</td>
</tr>
</tbody>
</table>

### Energy equation (total)

<table>
<thead>
<tr>
<th>Phase</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas phase</td>
<td>$(\frac{\partial}{\partial t})[\rho_g (i_g + v_g^2/2)] + \nabla \cdot [\rho_g \mathbf{v}_g (h_g + v_g^2/2)]$</td>
</tr>
<tr>
<td></td>
<td>$= -\nabla \cdot [\theta q + (1 - \theta)q_{s,s}] - q_{cp} + q_{rg} + r_p (\bar{h}_s + v_p^2/2 + w_s^2/2) - \nabla \cdot [(1 - \theta)p \mathbf{v}_p]$</td>
</tr>
<tr>
<td></td>
<td>$+ \nabla \cdot [\theta \tau \cdot \mathbf{v}_g + (1 - \theta)\tau_a \cdot \mathbf{v}_p] - \mathbf{v}_p \cdot \mathbf{f}_p + \rho_g \mathbf{g} \cdot \mathbf{v}_g + \bar{s}_s \mathbf{v}_v$</td>
</tr>
<tr>
<td>Particle phase</td>
<td>$(\frac{\partial}{\partial t})[\rho_p (i_p + v_p^2/2)] + \nabla \cdot [\rho_p \mathbf{v}_p (i_p + v_p^2/2)]$</td>
</tr>
<tr>
<td></td>
<td>$= -r_p (\bar{h}_s + v_p^2/2 + w_s^2/2) + \mathbf{v}_p \cdot \mathbf{f}<em>p + \rho_p \mathbf{g} \cdot \mathbf{v}<em>p + q</em>{cp} + q</em>{rg} - \bar{s}_s \mathbf{v}_v$</td>
</tr>
<tr>
<td>Mixture</td>
<td>$(\frac{\partial}{\partial t})[\rho_g (i_g + v_g^2/2) + \rho_p (i_p + v_p^2/2)] + \nabla \cdot [\rho_g \mathbf{v}_g (h_g + v_g^2/2) + \rho_p \mathbf{v}_p (i_p + p/\rho_p + v_p^2/2)]$</td>
</tr>
<tr>
<td></td>
<td>$= -\nabla \cdot [\theta q + (1 - \theta)q_{s,s}] + \theta q_{rg} + q_{rg} + \nabla \cdot [\theta \tau \cdot \mathbf{v}_g + (1 - \theta)\tau_a \cdot \mathbf{v}_p]$</td>
</tr>
<tr>
<td></td>
<td>$+ \mathbf{g} \cdot (\rho_p \mathbf{v}_p + \rho_g \mathbf{v}_g)$</td>
</tr>
</tbody>
</table>

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PSI-Cell Technique

Idea: What is the source term to gas phase from particles

A. Mass

\[ \nabla \cdot \vec{\rho} \vec{v} = S_p^m \]

\[ S_p^m = \frac{\Delta m_p}{V_{cell}} \]

\[ \Delta m_p = n_p \left[ \rho_{in} - \rho_{out} \right] \]

\# of particles represented by this trajectory
time

Procedure:
- Compute \( \Delta m_p \) whenever particle crosses cell boundaries
- Interpolate to get gas properties based on neighboring cells

B. Momentum

Axial

\[ \dot{\rho} \vec{v} = \frac{1}{V} n_p \left[ (u_p \vec{x}_p)_{in} - (u_p \vec{x}_p)_{out} \right] \]

Same for \( \vec{w} \) velocities \( \dot{\rho} \vec{w} \)
c. Energy (neglecting radiation for now)

\[ S_p^h = \frac{1}{\nu_p} [ (h_p \alpha_p)_\text{in} - (h_p \alpha_p)_\text{out} ] \]

⇒ more complicated when radiation is involved
⇒ includes chemical reaction and convective heat transfer effects

In practice, many different particles are used
\( i = \) index for particle size
\( j = \) index for starting location, etc.

\[ S_{\text{cell}}^m = \frac{1}{\nu} \left( \sum \Delta m_{pj} \right) \]

(sum contributions from all particles)

If we wanted to do species continuity

\[ S_{pjk}^m = \text{species or element contribution} \]

d. To start trajectories, need

- Size distribution
- Starting location
- Composition
Turbulence Effects on Particle Motion

A. Ignore Turbulence $\frac{d\bar{e}}{dt} = f(\text{mean gas properties})$

B. $\bar{u}_p = \bar{u}_p^m(y - y_g) + \bar{u}_p^t$

1. Empirical way to get $\bar{u}_p^t$ based on gradient analogies (Smith & Smol, 1985)

\[
\bar{u}_p^t = -\frac{1}{\rho_p} \nabla \bar{n}_p
\]

\[
\bar{n}_p = \text{particle number density (volume)}
\]

\[
\bar{\rho}^t = \frac{\bar{\rho}_p - \bar{\rho}_n}{\bar{\rho}_p} \rightarrow \text{turbulent eddy viscosity}
\]

\[
\bar{\nu}_p^t \rightarrow \text{turbulent Schmidt number (empirical)}
\]

Problems: 1. Have to use Eulerian eqn. to get $\bar{n}_p$

2. Physics not right (not gradient-dependent, since it is not a continuum)

2. Stochastic methods (Shah et al., AIAA J., 23:3, 376-404, 1985)

$\bar{u}_p = \bar{u}_p^m(y - y_g) + \bar{u}_p^t$

\[
\bar{u}_p^t = \text{random element based on } k, \varepsilon
\]

\[
\bar{u}_p^t \rightarrow \text{randomly select from Gaussian PDF with isotropic standard deviations } \frac{\bar{K}}{4},
\]

$\bar{U} = \bar{V} = \bar{W} = 0$

Keep this "extra" velocity for eddy lifetime or distance

\[
\tau_e = \frac{L_e}{(\bar{K}/4)}
\]

$\tau_e = \frac{C_{14}^4}{\rho} K^{3/2} / \varepsilon$

+ Lots of PARTICLES ($\times 5000$)
3. Cloud method

- Compute "mean" particle trajectory
- Compute distribution as a function of time assuming a distribution function

\[ R = -\int_0^t T_g(t') \, dt' \]
\[ T_g = \frac{c^{2/3} \xi^{3/2}}{E (2k_0)^{1/2}} \]

- Get contribution to cell from different clouds, weight appropriately
- Distribution function sacrifices physics
- "Easy" to use (not so many particles)
- Gas properties computed only at mean position
- Wall boundaries are complicated


Bottom Line: No perfect method

Fluent \Rightarrow \text{Stochastic}
PCGE-3 \Rightarrow \text{Empirical} \, \overline{N_p} \text{ (want to change)} \, \text{gradient method}
Jasper \Rightarrow \text{Cloud
Figure 4. Lagrangian view of dispersion in a one-dimensional flow. Each circle is a measure of the spatial extent of a pdf for particle position at successive times during the flow. The position of a typical Eulerian computational cell is also illustrated. Particles of many different residence times contribute to the overall population of particles in the cell.