COMPUTER & COMPUTATIONAL SCIENCES

Subgrid Scale Mixture Models for Hybrid Miscible/Immiscible Multifluid/Multimaterial Simulations

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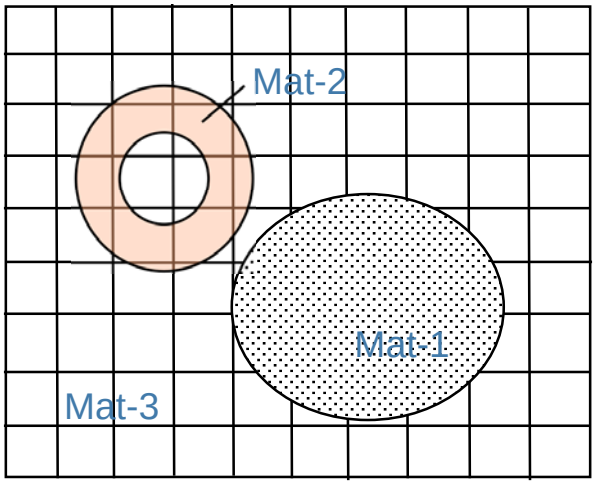
Overview

- Flow Regimes
- Formulation Issues – mean strain rate with void compression
  - Basic Equations
  - Mixture Model
  - Void Compression
- Multimaterial Formulation – pressure equilibration extensions
  - Pressure Relaxation
  - Strain Partitioning (*omitted*)
- Multispecies Formulation
  - General EOS closure
  - Gamma-law gas EOS closure
- Hybrid models
- Summary

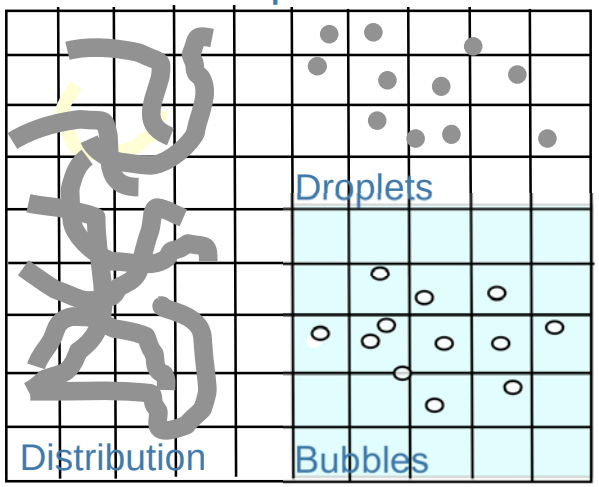
Multifluid, multimaterial and hybrid problems span a spectrum of flow regimes

Multimaterial/Multifluid



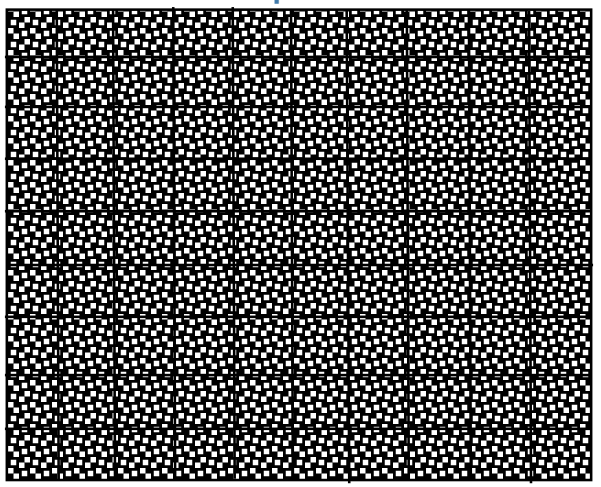
- Materials are immiscible
- Modest number of sharp interfaces are represented numerically
- Typically relies on the “mean-strain” approximation -- Each material has a unique stress and energy
- Incorporates treatment of void
- Sub-cell pressure equilibrium can be enforced, but it can be expensive to do so exactly
- Can also be extended to partition deviatoric strain

Multiphase



- Large number of small material domains that are not resolved by a single element
- Too many interfaces to treat individually
- Relies on spatially-averaged mixture approximations, i.e., homogenized equations
- Multiphase fluid formulations may be used in the multimaterial limit, but still a research area with few production-level codes

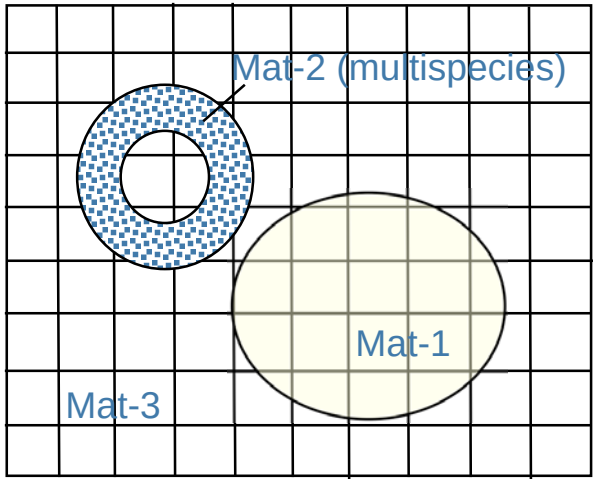
Multispecies



- Components are completely miscible from a continuum view
- Typically applied to gases or materials at high temperatures, i.e., plasmas
- Use pressure-temperature equilibrium, i.e., Amagat model for gases
- Extensible to a carrier material with stress deviator and advective transport of multiple species
- Can include reaction chemistry

The hybrid approach permits multiple mixture models to coexist

- Multimaterial and Multispecies
  - Individual materials can be designated as multispecies in the formulation
  - Requires material model definitions with multispecies EOS and species concentrations as state variables
  - Species cannot advect (or diffuse) between a multispecies material and “conventional” material

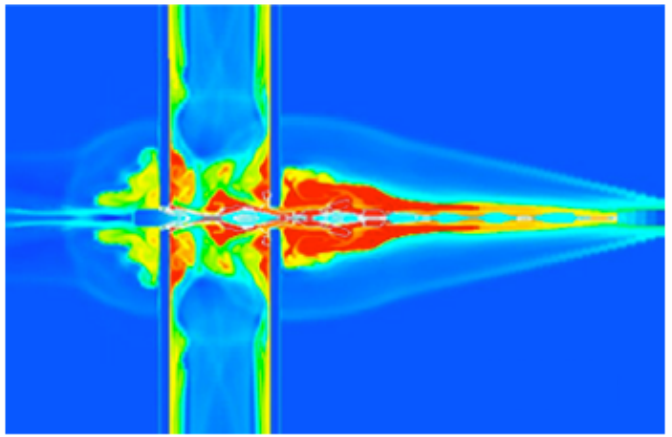


- Multimaterial and Multiphase
  - Multiphase materials, represented via homogenization, may be used in the multimaterial formulation, e.g., embedded rebar
  - State variables for multiphase (homogenized) materials can not mix with single phase materials or multispecies materials
- Materials can not be redefined as a problem evolves

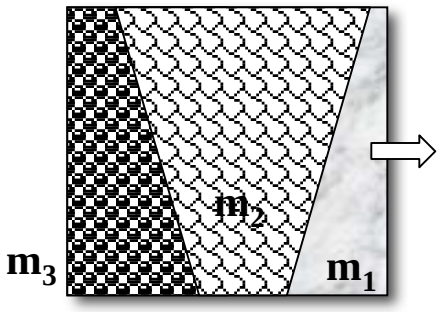
The development of multifluid/multimaterial methods have evolved with volume-tracking

- KRAKEN, de Bar (1974)
- SLIC, Noh & Woodward (1976)
- Youngs (1982, 1987)
  Parker and Youngs (1992)
- MESA, Mandell, et al. (1989)
- CTH, McGlaun, et al. (1990),
  Bell & Hertel (1992)
- ALEGRA, Peery & Carrol (2000) } started ~ 1990
- ALE3D, Sharp (2004)
- LS-DYNA, Hallquist, et al. (~2005)

  … and too many others to mention here



- Virtually all these multimaterial codes rely on:
  - A Lagrangian phase and a volume-tracking/remap phase
  - Some form of Young's reconstruction algorithm
  - Onion-skin approach to reconstructing multiple material interfaces, i.e., order-dependent material advection

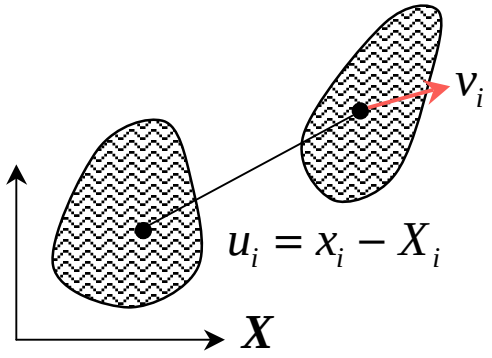


Lagrangian equations are based on the "mean-strain" assumption with a single velocity mixture model

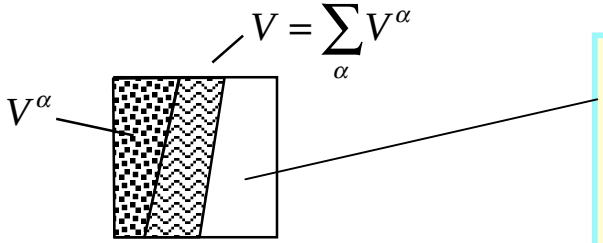
$$\bar{\rho} J = \bar{\rho}_0 \;\; where \;\; J = \det\left[\frac{\partial x_i}{\partial X_j}\right]$$

$$\bar{\rho}\dot{v}_i = \bar{\sigma}_{ij,j} + \bar{\rho} f_i$$

$$\bar{\rho}\dot{\bar{e}} = D_{ij}\bar{\sigma}_{ij} + \bar{Q}, \quad \text{where} \quad \bar{Q} = \sum_{\alpha} Q^{\alpha}$$



- Conservation of angular momentum requires: $\bar{\sigma}_{ij} = \bar{\sigma}_{ji}$



$$\mathcal{F}^{\alpha} = \frac{V^{\alpha}}{V} \qquad \alpha \in \{0, \ldots, Nmat\}$$

$$\mathcal{F}^{0} = \mathcal{F}^{\text{void}}$$

$$\sum_{\alpha} \mathcal{F}^{\alpha} = 1 \;\text{ and }\; \mathcal{F}^{\alpha} \geq 0 \;\; \forall \alpha$$

Void Material

$$\rho^0 = \rho^{\text{void}} = 0$$

$$p^0 = p^{\text{void}} = 0$$

$$\sigma_{ij}^0 = \sigma_{ij}^{\text{void}} = 0$$

$$c_d^0 = c_d^{\text{void}} = 0$$

Mixture Relations

$$\bar{\rho} = \sum_{\alpha} \mathcal{F}^{\alpha}\rho^{\alpha}$$

$$\bar{e} = \frac{\sum_{\alpha} e^{\alpha}\rho^{\alpha}V^{\alpha}}{\sum_{\alpha} \rho^{\alpha}V^{\alpha}} = \frac{\sum_{\alpha} \mathcal{F}^{\alpha} e^{\alpha}\rho^{\alpha}}{\sum_{\alpha} \mathcal{F}^{\alpha}\rho^{\alpha}}$$

$$\bar{T} = \frac{\sum_{\alpha} \mathcal{F}^{\alpha}\rho^{\alpha}C_v^{\alpha}T^{\alpha}}{\sum_{\alpha} \mathcal{F}^{\alpha}\rho^{\alpha}C_v^{\alpha}}$$

$$\bar{p} = \sum_{\alpha} \mathcal{F}^{\alpha} p^{\alpha}, \qquad \bar{\sigma}_{ij} = \sum_{\alpha} \mathcal{F}^{\alpha}\sigma_{ij}^{\alpha}$$

$$\bar{c}_d = \sum_{\alpha} \mathcal{F}^{\alpha} c_d^{\alpha} \quad OR \quad \bar{c}_d = \sqrt{\frac{\sum_{\alpha} \rho^{\alpha}\left(c_d^{\alpha}\right)^2 V^{\alpha}}{\sum_{\alpha} \rho^{\alpha}V^{\alpha}}}$$

Volume fractions remain constant during the Lagrangian phase

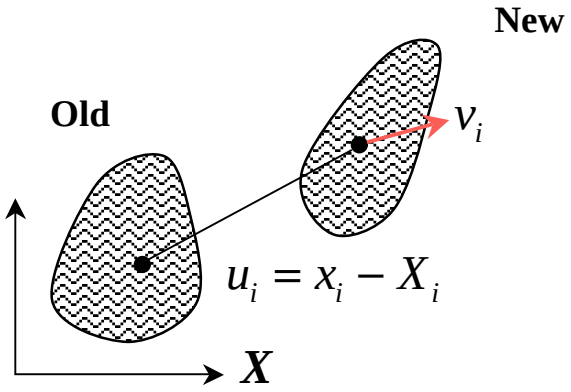
- Volumetric strain is applied uniformly to each material

$$m = \sum_{\alpha} m^{\alpha} = const. \quad \text{and} \quad m^{\alpha} = \rho^{\alpha} \mathcal{F}^{\alpha} V = const.$$

$$\text{Apply Volumetric Strain Uniformly}: \ \rho^{\alpha}_{new} = \rho^{\alpha}_{old} \frac{V_{old}}{V_{new}}$$

$$\left(\rho^{\alpha}_{old} \frac{V_{old}}{V_{new}} \right) \mathcal{F}^{\alpha}_{new} V_{new} = \rho^{\alpha}_{old} \mathcal{F}^{\alpha}_{old} V_{old} \ \Rightarrow \ \mathcal{F}^{\alpha}_{new} = \mathcal{F}^{\alpha}_{old}$$

$$\therefore \mathcal{F}^{\alpha} = const. \quad \forall \alpha$$

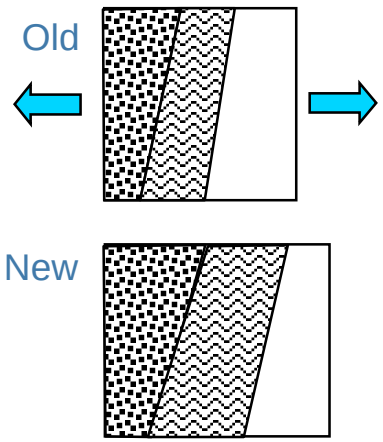


- Special cases can affect the volume fractions and energies
  - Void compression, aka, void collapse
  - Partitioning volumetric strain among materials

Void treatment preferentially compresses void in multimaterial elements

- 4-cases to consider -- strain field is not modified

Case-1: Expansion

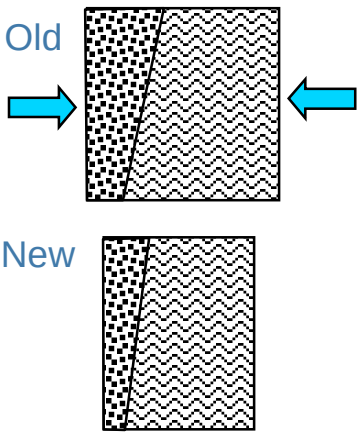


$$\mathcal{F}^{\alpha}_{new} = \mathcal{F}^{\alpha}_{old}$$

$$\beta^{\alpha} = \frac{\mathcal{F}^{\alpha}_{old} V_{old}}{\mathcal{F}^{\alpha}_{new} V_{new}} = \frac{V_{old}}{V_{new}} = \beta$$

$$\rho^{\alpha}_{new} = \rho^{\alpha}_{old} \beta \quad \forall \alpha$$

Case-2: No Void

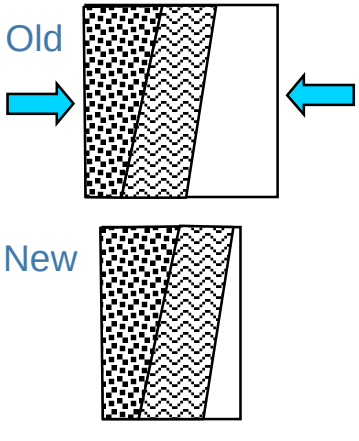


$$\mathcal{F}^{void}_{new} = 1 - (1 - \mathcal{F}^{void}_{old}) \left\{ \frac{V_{old}}{V_{new}} \right\}$$

$$\mathcal{F}^{\alpha}_{new} = \mathcal{F}^{\alpha}_{old} \left\{ \frac{V_{old}}{V_{new}} \right\} \quad \forall \alpha$$

$$\rho^{\alpha}_{new} = \rho^{\alpha}_{old}$$

Case-3: Sufficient Void

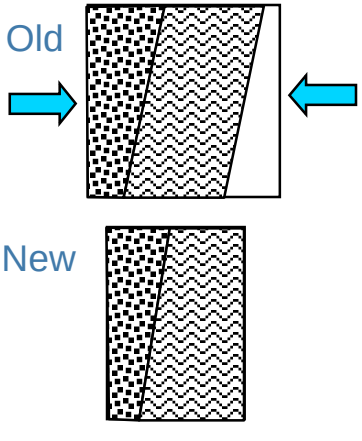


$$\mathcal{F}^{void}_{new} = 0$$

$$\mathcal{F}^{\alpha}_{new} = \frac{\mathcal{F}^{\alpha}_{old}}{\left(1 - \mathcal{F}^{void}_{old}\right)}$$

$$\rho^{\alpha}_{new} = \rho^{\alpha}_{old} \left\{ \frac{V_{old}}{V_{new}} \right\} \left(1 - \mathcal{F}^{void}_{old}\right) \quad \forall \alpha$$

Case-4: Void Closes



The single-velocity mixture model permits multiple approaches to pressure equilibrium – all have limitations …

- Pressure equilibrium
  - Can be non-physical for explicit computation of high-rate events since pressure equilibrium typically requires waves to transit a cell many times
  - Tensile failure mechanisms are inhibited in the presence of void
- Pressure and temperature equilibrium
  - Same limitations as pressure equilibrium model
  - Implies that thermal conductivity is infinite for finite-rate problems
  - Leads to artificial heating/cooling when multimaterial cells contain solids and gases
- Mean strain-rate (implies pressure equilibrium)
  - Can lead to high artificially high stresses/pressures when multimaterial cells contain solids and gases
  - **Most widely used model** – generally reported to give "surprisingly good" results (e.g., see McGlaun, 1992, Benson, 1992, etc.)

Multimaterial pressure equilibration modifies the volume fractions

- Case-1: Pair-wise pressure equilibrium $\left(\bar{p} = p^{\alpha} \text{ since } \sum \mathcal{F}^{\alpha} = 1\right)$

$$\begin{Bmatrix} p^1 - p^2 \\ p^2 - p^3 \\ \vdots \\ p^{Nmat-1} - p^{Nmat} \\ \sum_{\alpha=0}^{Nmat} \mathcal{F}^{\alpha} - 1 \end{Bmatrix} = 0$$

Newton's Method

$$\left.\frac{\partial p^{\alpha}}{\partial \mathcal{F}^{\alpha}} = V^{\alpha} \frac{\partial p^{\alpha}}{\partial V^{\alpha}}\right|_{s} = -K^{\alpha}$$

$$\begin{bmatrix} K^1 & -K^2 & 0 & \cdots & 0 \\ 0 & K^2 & -K^3 & & \\ \vdots & & \ddots & \ddots & \\ 0 & & & K^{Nmat-1} & -K^{Nmat} \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \begin{Bmatrix} \delta\mathcal{F}^1 \\ \delta\mathcal{F}^2 \\ \vdots \\ \delta\mathcal{F}^{Nmat-1} \\ \delta\mathcal{F}^{Nmat} \end{Bmatrix} = - \begin{Bmatrix} p^1 - p^2 \\ p^2 - p^3 \\ \vdots \\ p^{Nmat-1} - p^{Nmat} \\ \sum_{\alpha=0}^{Nmat} \mathcal{F}^{\alpha} - 1 \end{Bmatrix}$$

- Case-2: Mean pressure equilibrium $\left(\bar{p} = p^{\alpha} \text{ where } \bar{p} = \sum \mathcal{F}^{\alpha} p^{\alpha}\right)$

$$\begin{Bmatrix} p^1 - \bar{p} \\ p^2 - \bar{p} \\ \vdots \\ p^{Nmat} - \bar{p} \\ \sum_{\alpha=0}^{Nmat} \mathcal{F}^{\alpha} - 1 \end{Bmatrix} = 0$$

Newton's Method

$$\begin{bmatrix} -K^1 & 0 & .... & & 0 \\ 0 & -K^2 & & & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & & & -K^{Nmat} & 0 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \begin{Bmatrix} \delta\mathcal{F}^1 \\ \delta\mathcal{F}^2 \\ \vdots \\ \delta\mathcal{F}^{Nmat} \\ \delta\mathcal{F}^0 \end{Bmatrix} = - \begin{Bmatrix} p^1 - \bar{p} \\ p^2 - \bar{p} \\ \vdots \\ p^{Nmat} - \bar{p} \\ \sum_{\alpha=0}^{Nmat} \mathcal{F}^{\alpha} - 1 \end{Bmatrix}$$

- Case-3 (*most typical*): Single relaxation pass using Case-2
  - Mitigates large pressures in cells with small material volume fraction

The multispecies mixture EOS closure problem enforces pressure-temperature equilibrium

- The mixture EOS closure problem requires finding the equilibrium mixture pressure and temperature such that

$$e = \sum_i Y_i \hat{e}_i \qquad 1 \le i \le Nspec$$

$$v = \frac{1}{\rho} = \sum_i \frac{Y_i}{\hat{\rho}_i} = \sum_i Y_i \hat{v}_i$$

- Recall that e, ρ are found from the state update

$$e^{\alpha}\Big|_{t+\Delta t} = e^{\alpha}\Big|_{t} + \left\{ \frac{1}{\rho^{\alpha}\Big|_{t+\Delta t/2}} \right\} \left[\frac{\left(\sigma_{ij}^{\alpha}\Big|_{t} + \sigma_{ij}^{\alpha}\Big|_{t+\Delta t} \right)}{2} \right] \Delta\varepsilon_{ij}\Big|_{t+\Delta t}$$

Multispecies Mixture Relations

$$\rho^{\alpha} = \sum_i \rho_i, \qquad 1 \le i \le Nspec$$

$$\hat{\rho}_i = \hat{\rho}_i(p,T), \quad \hat{e}_i = \hat{e}_i(p,T)$$

$$f_i = \frac{V_i}{V^{\alpha}} \qquad Note: f_i \neq F^{\alpha}$$

$$Y_i = \frac{m_i}{m} = \frac{\rho_i}{\rho} \Rightarrow \sum_i Y_i = 1 \text{ and } \sum_i f_i = 1$$

$$\hat{e}_i = \hat{e}_i(p,T)$$

$$e = \sum_i \frac{m_i}{m} \hat{e}_i(p,T) = \sum_i Y_i \hat{e}_i(p,T)$$

$$v = \frac{1}{\rho} = \sum_i \frac{Y_i}{\hat{\rho}_i(p,T)}$$

- The specific depend on the details of the underlying EOS

Solving the pressure-temperature EOS closure problem for the multispecies model

- For an EOS written in terms of $v = v(p,T),\ e = e(p,T)$

$$\{F\} = \begin{Bmatrix} e - \sum_i Y_i \hat{e}_i \\ v - \sum_i Y_i \hat{v}_i \end{Bmatrix} = \mathbf{0} \quad \Rightarrow \text{Newton's Method} \quad \begin{bmatrix} -\sum_i Y_i \frac{\partial \hat{e}_i}{\partial T} & -\sum_i Y_i \frac{\partial \hat{e}_i}{\partial p} \\ -\sum_i Y_i \frac{\partial \hat{v}_i}{\partial T} & \left[v - \sum_i Y_i \hat{v}_i - p \sum_i Y_i \frac{\partial \hat{v}_i}{\partial p} \right] \end{bmatrix} \begin{Bmatrix} \delta T \\ \delta p \end{Bmatrix} = - \begin{Bmatrix} e - \sum_i Y_i \hat{e}_i \\ v - \sum_i \frac{Y_i}{\hat{\rho}_i} \end{Bmatrix}$$

- Consider limiting case of ideal gases (or γ-Law gases)

$$\hat{e}_i = C_{v_i} T \qquad T_{ref} = 0 \quad \textit{for convenience}$$

$$\hat{v}_i = \frac{(\gamma_i - 1) C_{v_i} T}{p}$$

- Leads to lower-triangular Jacobian

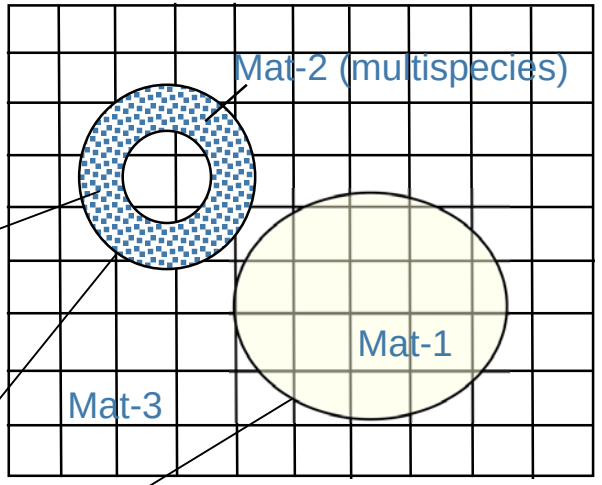
$$\begin{bmatrix} -\bar{C}_v & 0 \\ -\bar{R} & v \end{bmatrix} \begin{Bmatrix} \delta T \\ \delta p \end{Bmatrix} = - \begin{Bmatrix} \left[e - \bar{C}_v T \right] \\ \left[pv - \bar{R} T \right] \end{Bmatrix} \qquad \textit{mixture quantities} \quad \begin{cases} \bar{C}_v = \sum_i Y_i C_{v_i} \\ \bar{R} = \sum_i Y_i (\gamma_i - 1) C_{v_i} \end{cases}$$

- Solution algorithm is self-starting, and only a single pass required for constant specific heat, ratio of specific heats

The hybrid subgrid model permits multispecies regions in multimaterial/multifluid problems

- All "materials" are treated as immiscible with separating, sharp interfaces
- P-T equilibrium enforced for each multispecies region (locally miscible)

$$\begin{bmatrix} -\sum_i Y_i \frac{\partial \hat{e}_i}{\partial T} & -\sum_i Y_i \frac{\partial \hat{e}_i}{\partial p} \\ -\sum_i Y_i \frac{\partial \hat{v}_i}{\partial T} & \left[v - \sum_i Y_i \hat{v}_i - p \sum_i Y_i \frac{\partial \hat{v}_i}{\partial p} \right] \end{bmatrix} \begin{Bmatrix} \delta T \\ \delta p \end{Bmatrix} = - \begin{Bmatrix} e - \sum_i Y_i \hat{e}_i \\ v - \sum_i \frac{Y_i}{\hat{\rho}_i} \end{Bmatrix}$$



- Pressure equilibrium enforced between immiscible regions

$$\begin{bmatrix} -K^1 & 0 & .... & & 0 \\ 0 & -K^2 & & & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & & & -K^{Nmat} & 0 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \begin{Bmatrix} \delta \mathcal{F}^1 \\ \delta \mathcal{F}^2 \\ \vdots \\ \delta \mathcal{F}^{Nmat} \\ \delta \mathcal{F}^0 \end{Bmatrix} = - \begin{Bmatrix} p^1 - \bar{p} \\ p^2 - \bar{p} \\ \vdots \\ p^{Nmat} - \bar{p} \\ \sum_{\alpha=0}^{Nmat} \mathcal{F}^\alpha - 1 \end{Bmatrix}$$

Overall nonlinear solver must permit backup, restart strategies for outer-iteration

Summary & Future Directions

- Interface treatment remains a pacing technology for multifluid/multimaterial problems -- desirable to have:
  - Physics-based interfaces rather than numerics-based interfaces, e.g., material-order independence
  - Ability to transition from sharp to diffuse or permeable interfaces
- There are a number of methods to achieve pressure equilibrium
  - Computational cost considerations have favored simple relaxation schemes (*or none at all*)
  - Nonlinearity of EOS and/or discrete nature of tabular EOS may result in situations where Newton's method does not converge
    - Backup strategy relies on a simple bisection method
    - Quality of bulk moduli may also affect convergence rates
- Single-velocity mixture models are inadequate for some problems
  - Over-arching approach to span miscible - to - immiscible regimes is now available
  - Ad-hoc extensions, e.g., for void compression, can prevent rigorous code verification

Backup Slides

The Multimaterial Formulation with the Mean Strain-Rate Mixture model

Assumptions:

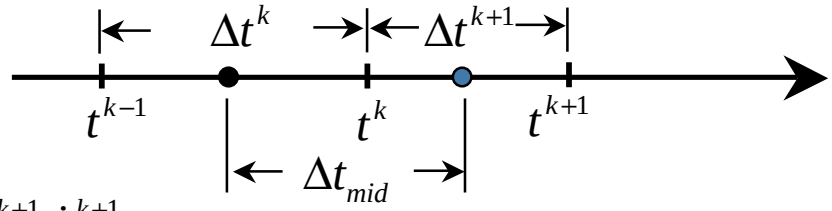
- Each material experiences the mean strain-rate of the cell
  - May extend to partitioned strain-rates
  - Can extend to consider contact mixture theory (see Benson, 2005)
- A single velocity field is used for all materials
- Volume fractions remain constant over the Lagrangian step except when void-compression or strain-partitioning is active
- Virtual work for the element is the volume-fraction weighted sum of the work for the individual materials
- Internal work = external work at the cell level by construction, i.e., it is a "compatible" discretization
- Sound-speed in a multimaterial cell is bounded by the single-material sound-speed thus stability is no worse than the single-material case

The Multimaterial Eulerian Solution Algorithm

The multimaterial Eulerian solution algorithm is broken into three distinct phases

1. Lagrangian step
2. Remesh procedure (accounts for prescribed mesh movement)
3. Remap (advection) variables
    1. Compute volume fluxes for affected elements
    2. Advect element variables in volume coordinates
    3. Advect nodal variables in volume coordinates (typically none)
    4. Interface reconstruction for multi-material, affected elements
    5. Advect material variables in volume/mass coordinates
    6. Advect nodal fields (velocity) for affected nodes
    7. Post-advection update of EOS/Constitutive models as necessary

Time Integration – Lagrangian Phase



$$\Delta t_{mid} = \tfrac{1}{2}\left(\Delta t^k + \Delta t^{k+1}\right)$$

1. Update mean velocity $\dot{\boldsymbol{u}}^{k+\frac{1}{2}} = \dot{\boldsymbol{u}}^{k-\frac{1}{2}} + \Delta t_{mid}\, \ddot{\boldsymbol{u}}^k$
2. Calculate incremental displacement $\Delta \boldsymbol{u}^{k+1} = \Delta t^{k+1}\, \dot{\boldsymbol{u}}^{k+1}$
   Update displacement $\boldsymbol{u}^{k+1} = \boldsymbol{u}^k + \Delta \boldsymbol{u}^{k+1}$
3. Update internal state ρ, σ_{ij}, e^{k+1}; Calculate forces $\left\{\boldsymbol{F}^{ext} - \boldsymbol{F}^{int}\right\}$;
   Perform penalty-based contact
4. Solve for acceleration $\ddot{\boldsymbol{u}}^{k+1} = M_L^{-1}\left\{\boldsymbol{F}^{ext} - \boldsymbol{F}^{int}\right\}$
5. Enforce constraints on acceleration
6. Perform constraint-based contact
7. Calculate "state velocities"
8. Enforce constraints on state velocities
9. Repeat 1-8 until designated termination

Artificial Bulk Viscosity

Multimaterial bulk viscosity uses volume-averaged density, sound-speed

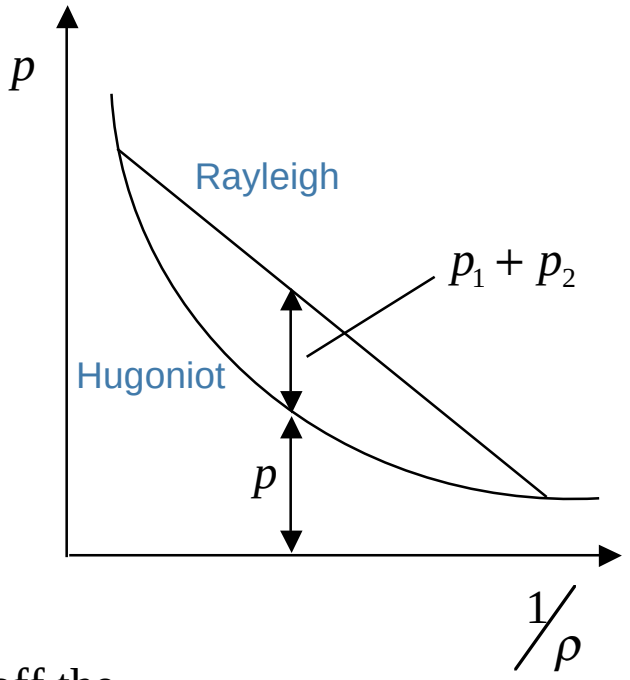
- Relies on uniform volumetric strain to produce a bulk element-level pressure
- Follows current implementation and segregates linear and quadratic terms

$$Linear: \; p_1 = b_1 \overline{\rho} \overline{c}_d L^{\varepsilon} \dot{\varepsilon}_v$$

$$Quadratic: \; p_2 = \overline{\rho} \left(b_2 L^{\varepsilon} \right)^2 \left| \dot{\varepsilon}_v \right| \min(0, \dot{\varepsilon}_v)$$

$$\overline{c}_d = \sum_{\alpha} F^{\alpha} c_d^{\alpha} \quad or \quad \overline{c}_d = \sqrt{\frac{\sum_{\alpha} \rho^{\alpha} \left(c_d^{\alpha} \right)^2 V^{\alpha}}{\sum_{\alpha} \rho^{\alpha} V^{\alpha}}}$$

$$Defaults: \; b_1 = 0.06, \quad b_2 = 1.2$$



- Strong shock calculations may require shutting off the default linear term in order to obtain correct isentropic expansions

Artificial Bulk Viscosity (cont.)

Limiting case of void cells:

$$\mathcal{F}^{void} \to 1$$

$$\overline{c}_d = \sum_\alpha F^\alpha c_d^\alpha = 0$$

$$\overline{\rho} = \sum_\alpha F^\alpha \rho^\alpha = 0$$

$$p_1 = b_1 \overline{\rho} \overline{c}_d L^\varepsilon \dot{\varepsilon}_v = 0$$

$$p_2 = \overline{\rho} \left(b_2 L^\varepsilon \right)^2 \left| \dot{\varepsilon}_v \right| \min(0, \dot{\varepsilon}_v) = 0$$

Volume averaged sound-speed yields correct limiting behavior for bulk viscosity

Benson's Average – 1-Material & Void

$$\left(\overline{c}_d\right)^2 = \frac{\sum_\alpha \rho^\alpha \left(c_d^\alpha\right)^2 V^\alpha}{\sum_\alpha \rho^\alpha V^\alpha} = \frac{\sum_\alpha \rho^\alpha \left(c_d^\alpha\right)^2 F^\alpha}{\sum_\alpha \rho^\alpha F^\alpha}$$

$$\lim_{\mathcal{F}^1 \to 0} \frac{\rho^1 \left(c_d^1\right)^2 F^1}{\rho^1 F^1} = \left(c_d^1\right)^2 \quad \Rightarrow \overline{c}_d = c_d^1$$

Provides poor behavior in the limit of void cells … so use volume averaged sound speed

Limitations for Pressure and Temperature Equilibrium Mixture Models

Pressure equilibrium model

- Can be non-physical for many wave propagation problems since pressure equilibrium typically requires waves to transit an element many times
  - May be reasonable when elements are small enough to admit stress equilibration on the wave propagation time-scale
- Tensile failure mechanisms are inhibited in the presence of void

Pressure and temperature equilibrium model

- Same limitations as pressure equilibrium model
- Implies that thermal conductivity is infinite for finite-rate problems
- Leads to artificial heating/cooling when multimaterial elements contain solids and gases
- P-T equilibrium formulation closely follows the multispecies P-T equilibrium formulation

Multimaterial Pressure Equilibrium

The general pressure equilibration problem is highly nonlinear, difficult to solve, and requires sophisticated (and sometimes expensive) algorithms to achieve a robust implementation

- Pressure equilibration modifies the volume fractions during the Lagrangian phase
- Full-blown pressure equilibrium avoids the need for a void compression algorithm, but is unrealistic for wave propagation problems
- A limited number of "simplified" pressure equilibration iterations may be used to relax towards pressure equilibrium in an element
  - Can help to avoid calculating large pressures for small fragments that see large strain rates in nearly void cells
- Potential for violating energy conservation exists
- See "Computational methods in Lagrangian and Eulerian hydrocodes," D. J. Benson, CMAME, vol. 99, 1992 for more details

Pressure Equilibrium Summary

There are a number of methods to achieve pressure equilibrium

- Pressure equilibrium is an unrealistic assumption for most wave propagation problems
- Computational cost considerations favor simple updates schemes
- Quasi-static problems may require fully-coupled approach
- Nonlinearity of material models may result in some situations where Newton's method does not converge
  - Backup strategy relies on a simple bisection method
  - Quality of bulk moduli may also affect convergence rates
- Typical to use a single pressure relaxation step for most multimaterial problems in order to ameliorate the behavior of materials with small volume fractions subjected to large strains

Strain Partitioning Methods

For some problems it may be desirable to partition the strain among stiff and soft materials undergoing compression

- Can interact with void compression
- Energy conservation may be violated when strains are modified
- Can result in changes to volume fractions during the Lagrangian phase
- Will require carrying additional volumetric strain information for material model state updates and energy computations
- Two formulations are considered here
  - Series model with fixed volume fractions
  - Linearized model
- Strain adjustment methods will require limiters to avoid completely compressing material in a single step which will result in numerical instabilities

Strain Partitioning Methods

Strain partitioning is formulated with several constraints in mind

- Strain partitioning: $\varepsilon_{ij}^{\alpha} = \bar{\varepsilon}_{ij}^{'} + \varepsilon_{v}^{\alpha}\delta_{ij}$

  $\bar{\varepsilon}_{ij}^{'} \equiv$ mean deviatoric strain

- Mean Strain: $\bar{\varepsilon}_{ij} = \sum_{\alpha=1}^{Nmat} \mathcal{F}^{\alpha}\varepsilon_{ij}^{\alpha}$

  $\bar{\varepsilon}_{v} = \sum_{\alpha=1}^{Nmat} \mathcal{F}^{\alpha}\varepsilon_{v}^{\alpha}$

  Mean strain/stress definitions permit micro and macro virtual work statements to be equivalent, i.e., a consistent energy calculation

- Mean Stress: $\bar{\sigma}_{ij} = \sum_{\alpha=1}^{Nmat} \mathcal{F}^{\alpha}\sigma_{ij}^{\alpha}, \qquad \bar{p} = \sum_{\alpha=1}^{Nmat} \mathcal{F}^{\alpha}p^{\alpha}$

- Pressure Equilibrium: $p^{\alpha} = \bar{p} \quad \alpha = 1,\ldots,Nmat \quad (\text{No void pressure})$

$$\sum_{\alpha=1}^{Nmat} \mathcal{F}^{\alpha} = 1$$

Assumptions for the Multispecies Formulation

Assumptions:

- All constituents are in pressure-temperature equilibrium
  - For gases, this is the Amagat model
  - Each constituent has a separate density and energy that contributes to the mixture
- There is a single constitutive model, i.e., stress-strain relationship
  - Consititutive model may depend on the mixture constitutents, i.e., mass fractions present
  - Extended material state data required to store multispecies mass fractions
- Reaction chemistry, counter-diffusion processes, and mass sources/sinks can be included but are not discussed here in detail
- The multispecies formulation will be used in the overall multimaterial Eulerian framework
  - Use a single velocity field and a single strain field

Multispecies Model – Basic Relationships

- In the multimaterial sense, consider a given multispecies material -- "α"

  $\rho^{\alpha}, e^{\alpha}, \sigma_{ij}^{\alpha}, \mathcal{F}^{\alpha}, V^{\alpha}, \ldots$

  - "α" superscript is dropped for convenience
- "Cell" density for species-i: $\rho_i \quad 1 \le i \le Nspec$
- Multispecies mixture density: $\rho = \sum_i \rho_i$
- Micro density for species-i: $\hat{\rho}_i = \hat{\rho}_i(p,T)$
- Material volume for species-i: V_i

For γ-Law gases, requires EOS evaluation

- Species mass: $m_i = \rho_i V = \hat{\rho}_i V_i$
- Material mass and volume: $m = \rho V, \quad V = \sum_i V_i$
- Species volume fraction (in V^{α}): $f_i = \frac{V_i}{V} \qquad Note: \; f_i \neq \mathcal{F}^{\alpha}$
- Species mass fraction: $Y_i = \frac{m_i}{m} = \frac{\rho_i}{\rho} \;\Rightarrow\; \sum_i Y_i = 1 \text{ and } \sum_i f_i = 1$

Multispecies Model – Basic Relationships (cont.)

- Species-I specific internal energy: $\hat{e}_i = \hat{e}_i(p,T)$
- Material specific internal energy: $e = \sum_i \frac{m_i}{m} e_i(p,T) = \sum_i Y_i e_i(p,T)$
- Material specific volume: $v = \frac{1}{\rho} = \sum_i \frac{Y_i}{\hat{\rho}_i(p,T)}$
- Mole-fraction: $Z_i = \frac{n_i}{n}$ where $n_i = Y_i \bar{M}_i$, $n = \sum_i Y_i$, $\bar{M}_i \equiv$ molecular weight
- Viscosity via Wilke's formula
  - Based on Chapman-Enskog theory for multicomponent gas mixtures

$$\dot{S}_{ij} = \mu \frac{\partial v_i}{\partial x_j}$$

$$\mu = \sum_i \left[\frac{Z_i \mu_i}{\sum_j Z_j \Phi_{ij}} \right], \quad \Phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j} \right)^{-1/2} \left[1 + \left(\frac{\mu_i}{\mu_j} \right)^{1/2} \left(\frac{M_j}{M_i} \right)^{1/4} \right]^2$$

Density-Temperature EOS

For an EOS written in terms of (ρ, T)

- A constraint on each species is added such that $p = p_i \quad \forall i$
- Result is a nonlinear system

$$\{F\} = \begin{Bmatrix} p - p_i \\ \vdots \\ e - \sum_i Y_i \hat{e}_i \\ \\ v - \sum_i \frac{Y_i}{\hat{\rho}_i} \end{Bmatrix} = \mathbf{0}$$

- Solve using Newton's method $\left[\frac{\partial F_i}{\partial a_j}\right]\{\Delta a_j\} = -\{F\}$
- Leads to an (Nspec+2) x (Nspec+2) system with block-diagonal structure

Density-Temperature EOS (cont.)

$$\begin{bmatrix} -\frac{\partial p_1}{\partial v_1} & & -\frac{\partial p_1}{\partial T} & & -1 \\ & -\frac{\partial p_1}{\partial v_1} & -\frac{\partial p_2}{\partial T} & & -1 \\ & & \ddots & \vdots & \vdots \\ -Y_1\frac{\partial \hat{e}_1}{\partial v_1} & -Y_2\frac{\partial \hat{e}_2}{\partial v_1} & \cdots & -\sum_i Y_i\frac{\partial \hat{e}_i}{\partial T} & 0 \\ -Y_1 & -Y_2 & \cdots & 0 & 0 \end{bmatrix} \begin{Bmatrix} \delta v_1 \\ \delta v_2 \\ \vdots \\ \delta T \\ \delta p \end{Bmatrix} = -\begin{Bmatrix} p - p_1 \\ p - p_2 \\ \vdots \\ e - \sum_i Y_i \hat{e}_i \\ v - \sum_i \frac{Y_i}{\hat{\rho}_i} \end{Bmatrix}$$

- Matrix structure scales as (Nspec+2), but permits a simple reduction of final 2-equations followed by a back-substitution
- Solution algorithm is not self-starting at t=0
- Non-smooth EOS data may result in a breakdown of convergence