

COMPUTER & COMPUTATIONAL
SCIENCES



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

Mark A. Christon
Continuum Dynamics, CCS-2
Los Alamos National Laboratory

14th International Conference on
Finite Elements in Flow Problems

March 26 - 28, 2007



LAUR-07-1832





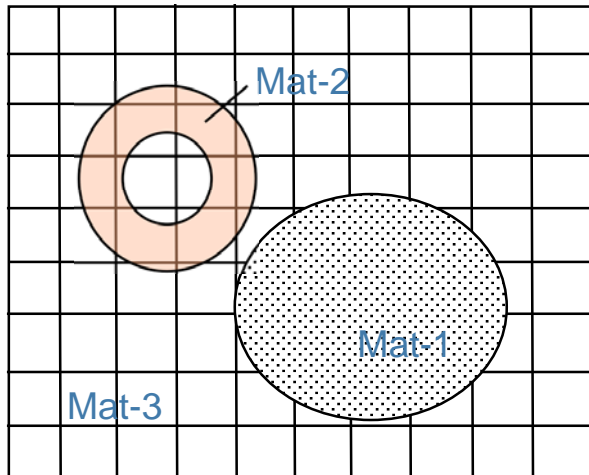
Overview

- ❑ 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



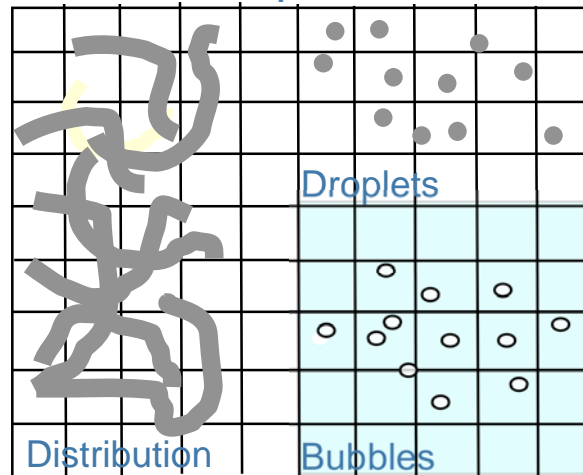
Multifluid, multimaterial and hybrid problems span a spectrum of flow regimes

Multimaterial/Multifluid



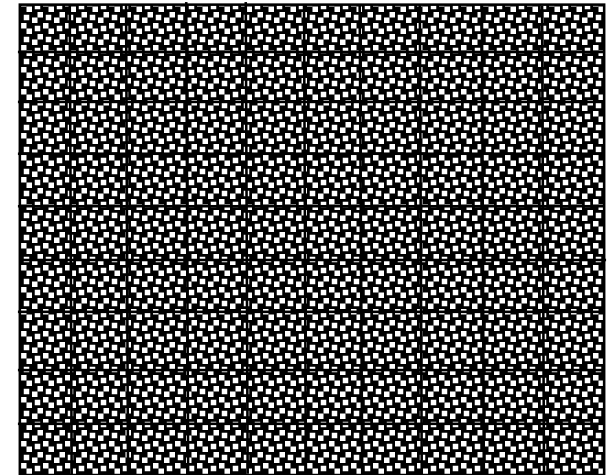
- Materials are immiscible
- Modest number of sharp interfaces are represented numerically
- Typically relies on the “mean-strain” approximation -- Each material has a unique stress and energy
- Incorporates treatment of void
- Sub-cell pressure equilibrium can be enforced, but it can be expensive to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



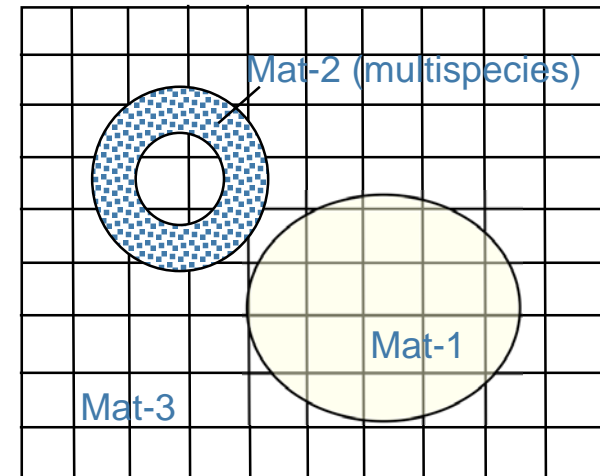
- Components are completely miscible from a continuum view
- Typically applied to gases or materials at high temperatures, i.e., plasmas
- Use pressure-temperature equilibrium, i.e., Amagat model for gases
- Extensible to a carrier material with stress deviator and advective transport of multiple species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

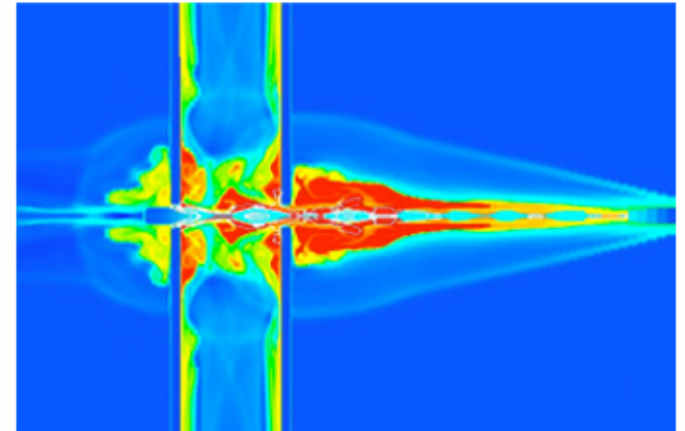
- ◆ Multiphase materials, represented via homogenization, may be used in the multimaterial formulation, e.g., embedded rebar
- ◆ State variables for multiphase (homogenized) materials can not mix with single phase materials or multispecies materials

□ 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

