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A finite element Galerkin/least-squares method for computation of multicomponent compressible–incompressible flows

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ABSTRACT

The space–time Galerkin/least-squares finite element method with discontinuity capturing (ST-GLSDC), developed by Hughes and collaborators [Shakib et al. A new finite element formulation for computational fluid dynamics: X. The compressible Euler and Navier–Stokes equations. Comput Methods Appl Mech Eng 1991;89:141–219], allows to study both compressible and incompressible single-fluid one-component flows. It is effective in the stabilization of the numerical solution without introducing excessive overdiffusion. In this work the development by Hauke and Hughes [A comparative study of different sets of variables for solving compressible and incompressible flows. Comput Methods Appl Mech Eng 1998;153:1–44] to pressure primitive variables is extended to single-fluid multicomponent compressible and incompressible flows of gas–liquid mixtures at local mechanical and chemical equilibrium. The stabilized algorithm is implemented in a parallel C++ library, which is tested on several benchmarks. The solution of the system of equations for the conservation of mass of each component, and of momentum and energy of the global mixture, requires the introduction of mass fractions as primitive variables to describe mixture composition. The weak formulation, the stabilization parameters, and the time-marching algorithm are rewritten in terms of the expanded set of variables, keeping similarity with the formulation in pressure variables.

1. Introduction

Flows of compressible–incompressible, multicomponent multiphase fluid mixtures are of common interest in theoretical, geophysical, and industrial CFD [1,2].

The computation of incompressible and compressible fluid dynamics generally requires completely different numerical approaches; only a few stabilized finite element formulations for compressible–incompressible flows have been developed. The compressible formulation in augmented conservation variables [3], derived from the streamline-upwind/Petrov–Galerkin techniques [4–6], properly computes the incompressible limit. The characteristic-based split procedure with Taylor-Galerkin/pressure-correction scheme, suitable for both compressible and incompressible regime [7,8], combines the methods [9–11] for compressible flows.

The Galerkin/least-squares formulation adds the least-squares term as a weighted residual. It was first introduced for compressible single-fluid flows [12], subsequently recast in entropy variables, supplemented with a shock-capturing operator and with a full space–time discretization to obtain the space–time Galerkin/least-squares formulation with discontinuity-capturing operator (ST-GLSDC) [13]. A compressible entropy formulation for multicomponent mixtures of ideal and perfect gases was also developed [14,15].

The single-fluid ST-GLSDC method and other slight variants were successfully applied to incompressible flows [16,17] and are well behaved in the incompressible limit in the context of primitive or entropy variables [18,19]. The unified approach by [18,19] is the development of ST-GLSDC to handle the whole spectrum of compressible–incompressible regimes, employing the same set of variables.

The stability, accuracy, and convergence of ST-GLSDC are well established, so that this method is a reliable basis for the present formulation. The ST-GLSDC also allows accessory techniques such as domain decomposition, local time-stepping and linear solution algorithms, and can be efficiently solved with a GMRES developed for the non-symmetric linear systems arising from the discretization [20]. The feasibility of computational improvements in accuracy and speed is a practical requirement for the simulation of multicomponent flows where the number of unknowns increases drastically as components are added.

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Nomenclature

$\boldsymbol{b}$	body force vector per unit mass
c	mixture sound velocity
$d = 1, 2$ or 3	number of spatial dimensions
e	specific internal energy of mixture
e_t	specific total energy of mixture
$\mathscr{F}$	source vector
$\boldsymbol{F}^{\text{adv}}$	advective flux vector
$\boldsymbol{F}^{\text{diff}}$	diffusive flux vector
g	partial specific Gibbs free energy of mixture
g_k	partial specific Gibbs free energy of component k
g_k^π	partial specific Gibbs free energy of component k in phase π
h	specific enthalpy of mixture
J_i^k	mass diffusion flux of component k in ith direction
k	specific kinetic energy of mixture
$\boldsymbol{K}_{ij}$	diffusivity matrices
M	Mach number
$\mathscr{M}$	molar mass of mixture
$\mathscr{M}_k$	molar mass of component k
n	number of components
p	pressure
$\text{Pr} = \frac{\mu}{\rho\kappa}$	Prandtl number
q_i	diffusive heat flux in ith direction
r	heat source per unit mass
R_k	specific gas constant of component k
$\text{Re} = \frac{\rho u L}{\mu}$	Reynolds number
$\boldsymbol{S}$	source matrix
$\text{Sc} = \frac{\mu}{\rho\mathscr{D}}$	Schmidt number
t	time
T	temperature
$\boldsymbol{u}$	velocity vector
$\boldsymbol{U}$	conservative variables vector
$\boldsymbol{V}$	entropy variables vector
x_k	mixture molar fraction of component k
x_k^π	mixture molar fraction of component k in phase π
y_k	mixture mass fraction of component k
y_k^π	mixture mass fraction of component k in phase π
$\boldsymbol{y} = (y_1, \ldots, y_n)$	vector of mass fraction of components
$\boldsymbol{Y}$	primitive variables vector
δ_{ij}	kronecker delta
η_k^π	mass fraction of component k in phase π with respect to component k
κ	thermal conductivity
μ	first viscosity coefficient of mixture
ν^h	discontinuity capturing operator
ξ_k^π	molar fraction of component k in phase π with respect to phase π
ρ	mixture density
τ	viscous stress tensor
τ_U	intrinsic time-scale matrix for conservation formulation
τ_V	intrinsic time-scale matrix for entropy formulation
τ_Y	intrinsic time-scale matrix for primitive formulation
$()_k$	kth component
$()_i$	ith spatial direction
$()^\pi$	phase π
$()_{\rho y_k}$	index for the ρy_k conservative variable entry
$()_{\rho\boldsymbol{y}}$	indexes for the $\rho y_1, \ldots, \rho y_n$ conservative variable entries
$()_{\rho u_i}$	index for the ρu_i conservative variable entry
$()_{\rho\boldsymbol{u}}$	indexes for the $\rho\boldsymbol{u}$ conservative variable entries
$()_{\rho e_t}$	index for the ρe_t conservative variable entry
$()_{\frac{\boldsymbol{g}-k}{T}}$	indexes for the $\frac{g_1-k}{T}, \ldots, \frac{g_n-k}{T}$ entropy variable entries
$()_{\frac{\boldsymbol{u}}{T}}$	indexes for the $\frac{\boldsymbol{u}}{T}$ entropy variable entries
$()_{-\frac{1}{T}}$	index for the $\frac{1}{T}$ entropy variable entry
$()_{\boldsymbol{y}}$	partial derivatives with respect to $y_1, \ldots, y_{n-1}$ primitive variables
$()_{,p}$	partial derivative with respect to p primitive variable
$()_{,\boldsymbol{u}}$	partial derivatives with respect to u_1, u_2, u_3 primitive variables
$()_{,T}$	partial derivative with respect to T primitive variable
$()_{,i}$	partial derivative with respect to the ith spatial direction
$()_{,t}$	partial derivative with respect to time

The formulation presented in this paper extends from single-fluid flows to multiphase multicomponent homogeneous gas–liquid mixture flows at mechanical and chemical local equilibrium the ST-GLSDC method [19] employing primitive variables, and generalizes to primitive variables and fluids with general equations of state the multicomponent entropy method [14]. The weak formulation, the stabilization parameters, and the algorithmic implementation at elemental level are written in order to solve the conservation equations for the mass of each component rather than for the fluid mass, along with the conservation equations for momentum and energy of the mixture as a whole. The additional terms due to increased degrees of freedom in the formulation are derived within the weak formulation. The expressions for the stabilization parameters of the original ST-GLSDC, namely the τ parameter and the discontinuity capturing operator, are replaced with analogous ones accounting for the mixture components, keeping dimensional consistency and simplicity. The criterion followed in this extension is to keep the robustness of the original method maintaining a reasonable computing effort.

Several finite element methods have been developed for multicomponent and/or multiphase flows. Some of them deal with particular subjects such as diffusion or sintering of phases, others are restricted to incompressible flows with the SUPG formulation [21–25]. The method proposed in this work allows the solution of both compressible and incompressible large number of problems such as shock wave interaction with contact discontinuities, evolution of internal interfaces, bubbly flows with evaporation or gas dissolution.

2. Physical model

The model considers a compressible–incompressible multicomponent multiphase mixture at mechanical, thermal and chemical local equilibrium. Components can be in gaseous or liquid state, and undergo instantaneous phase change. Chemical reactions resulting in component production or consumption are not allowed to occur. Gas–liquid mixtures may contain a continuous and a dispersed phase, or phases separated by internal interfaces.

The governing equations are mass conservation of each component, and momentum and energy conservation of the mixture as a whole:

$$(\rho y_k)_{,t} + (\rho u_i y_k)_{,i} = -J^k_{i,i} \quad \text{for } k = 1, \ldots, n \tag{1}$$

$$(\rho u_j)_{,t} + (\rho u_i u_j + p\delta_{ij})_{,i} = (\tau_{ji})_{,i} + \rho b_j \quad \text{for } j = 1, \ldots, d \tag{2}$$

$$(\rho e_t)_{,t} + (\rho u_i e_t + p u_i)_{,i} = \left(\tau_{ij}u_j - q_i - \sum_{k=1}^{n} J_i^k h_k\right)_{,i} + \rho(b_i u_i + r) \tag{3}$$

where all symbols are defined in the Nomenclature or the Appendixes. Indexes after an inferior comma represent variables with respect to which partial differentiation is computed; the summation convention on repeated indexes is applied throughout. The mixture