LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

Advanced multidomain method for multiphase flow interaction with Lagrangian structural meshes

Y. Kanarska, S. Schofield, T. Dunn, B. Liu, C. Noble

November 30, 2017

1   **Advanced multi-domain method for multiphase flow interaction with Lagrangian**

2   **structural meshes**

3

4   Yuliya Kanarska[1], Samuel Schofield, Timothy Dunn, Benjamin Liu, Charles Noble

5   Lawrence Livermore National Laboratory

6   [1]kanarska1@llnl.gov

7

9

10 **ABSTRACT**

11

12 Multiphase flow with particulates has emerged as a topic of fundamental fluid and continuum

13 mechanics interest in many applications including national security applications. For more

14 efficient simulation workflows, the utilization of a separate background multiphase flow mesh

15 and foreground Lagrangian structural meshes is greatly beneficial. We propose a multi-domain

16 coupling method for multiphase Godunov compressible high-speed flow interacting with an ALE

17 structure on a different mesh. Along with cell centered updates in ghost points similar to ghost

18 fluid methods we use additional modifications of the solid states at faces in such a way that

19 resulting solution of the Riemann problem at each face satisfies the boundary interface

20 conditions. Due to variation in targets and potentially dense particulate phases, the embedded

21 grid coupling methodology needs to be stable across a wide range of fluid/structure density ratios

22 as well as both dense and dilute particle regimes. We are developing multiphase extensions of

23 the Banks, et. al. (2011) interface conditions that are appropriate for the wide range of multi-

24 phase flow conditions. Several examples demonstrate applicability of the method for multiphase

25 flow interaction with dynamic deformable Lagrangian structural meshes.

26

27 **1. Introduction**

28

29 In the research community, there has been significant progress in numerical methods for fluid-

30 structure interaction with high speed flows (Pember aet al., 1995, Peskin et al., 2002, Ghias et al.,

31 2007, Tipton et al. 2011, Puso et al., 2012). However, little work has been done on the consistent

32   coupling of multiphase compressible flow with Lagrange structural meshes. To provide a more

33   productive capability with rapid analysis turnaround, the utilization of separate background

34   multiphase flow meshes and foreground Lagrangian structural meshes is greatly beneficial. A

35   solid model used for structural or thermo-mechanical calculations can be used almost "as is" in

36   the dynamic calculation. These targets often have very unstructured meshes making the creation

37   of a globally conformal mesh that ties the structure to the finely, reasonably uniform, zoned

38   mesh required for the turbulent high-speed flow calculation extremely challenging. The

39   embedded mesh approach has much more flexibility and is clearly preferred, however, there are

40   significant challenges in extending the numerical methods used for embedded boundaries to

41   multiphase formulations that are currently used for multiphase blast. There has been significant

42   progress in numerical methods for fluid-structure interaction with high speed flows including the

43   ghost fluid method (Fedkiw, 2002, Ghias 2007, Tipton et al., 2011), cut cell method (Pember et

44   al., 1998), immersed boundary method (Peskin, 2002), Lagrange multiplier method (Pusso et al.,

45   2012). The primary difficulty of standard embedded grid schemes is that traditional discrete

46   interface conditions often result in numerical instability. Due to variation in target and potentially

47   dense particulate phases, the embedded grid coupling methodology needs to be stable across a

48   wide range of fluid/structure density ratios, something only few coupling methods have (Banks

49   et al., 2011).

50   The proposed approach is the extension of the ghost fluid method to couple Eulerian

51   multiphase to ALE Lagrangian solid dynamics including interaction of multiphase particles with

52   the foreground mesh. We have combined a number of ideas from the recent literature including

53   ghost-fluid and embedded interface methods. Some unique features of this work include

54   development of a multiphase (and even multiple EOS) extension of the Banks, et. al. (2011)

55   interface conditions that is appropriate to couple multiphase fluid with Lagrangian structures

56   across wide range of material properties. In addition to the ghost cell updates we modify the left

57   and right Riemann states similar to Gorsse et al., (2011) in such a way that resulting solution of

58   the Riemann problem at each face satisfies the boundary interface conditions. These

59   modifications allow achieving higher accuracy of the resulting scheme.

60   The paper is organized as follows: In section 2 a short description of our multi-domain approach

61   is presented. The multiphase solver equations and algorithm are briefly described in section 3.

62   The low Mach number corrections to the standard compressible flows are presented in section 4.

63 Section 5 outlines the explicit Lagrangian hydrodynamic equations and solver. The mesh

64 intersection and element categorization is described in Section 6. The interface conditions used

65 are detailed in section 7 and the coupling technique is described in section 8. Verification,

66 validation, and numerical simulations are discussed in section 9. Conclusions and future work

67 are given in the last section.

68

69 ## 2. Multi-domain partitioned approach

70

71 ALE3D code is a multi-physics numerical simulation software tool utilizing arbitrary-

72 Lagrangian-Eulerian (ALE) techniques (Noble et al., 2017). It has different physical solvers and

73 mesh generation techniques. The goal of our multi-domain multi-physics coupling approach is to

74 couple different solvers in ALE3D that operate on different domains and meshes. However, the

75 technique described in this paper can be adopted for other multiphysics codes as well. Each

76 domain and its associated simulation solver and mesh are isolated and communicate with other

77 domains only through surfaces. A problem can be decomposed into domains on which an

78 appropriate solver is chosen, for instance a rigid body solver coupled with an explicit time

79 stepping compressible flow solver or a thermal-mechanical solid model can be coupled with an

80 incompressible flow model. This approach is often referred to as "partitioned" and has many

81 advantages including low memory requirements, low computational cost, and high parallel

82 efficiency. There is no need to solve globally coupled systems of equations, which can be

83 problematic particularly during parallel execution. Since the coupling occurs only through

84 surfaces, well tested single physics solvers can be used, with each solver remaining separate and

85 operating on its own domain. This will also enable different fluid and/or solid solvers to be

86 exchanged with minimal effort. In a numerical scheme, there are many ways that velocity- and

87 stress-continuity can be enforced in the discrete approximation. Banks et al., (2011) performed a

88 normal mode stability analysis of the linearized problem to investigate the stability of different

89 numerical interface conditions for a model problem approximated by upwind type finite

90 difference schemes. Their analysis shows that depending on the ratio of densities between the

91 solid and the fluid, some numerical interface conditions are stable up to the maximal Courant–

92 Friedrich–Levy (CFL)-limit, while other numerical interface conditions suffer from a severe

93 reduction of the stable CFL-limit. They also proposed a new interface condition which is

94 obtained as a simplified characteristic boundary condition (described in Section 7), that is proved

95 to not suffer from any reduction of the stable CFL-limit.

96 In this paper, we are extending and applying these conditions for coupling multiphase fluid with

97 Lagrange structures. We describe the coupling technique with application to the finite volume

98 multiphase solver described in section 3 and finite element Lagrange hydro solver described in

99 section 4.

100

101 **3. Multiphase flow equations**

102

103 The multiphase solver is based on the finite volume method using the discrete equation model

104 (DEM) and allows description of multiple multiphase species, including dense particles

105 (Chinnaya et al., 2003, Dunn, 2011). In this model, each phase has its own velocity and

106 thermodynamic state (pressure, temperature, etc.). The presence of multiple velocities requires a

107 modification to the standard single-phase ALE integration. The multiphase model handles these

108 complications by integrating discrete equations for volume fraction α (can vary between 0 and

109 1), density ρ, momentum ρu, and total energy ρE of each species. Considering two-phase gas-

110 particle flow, this model is described by a system of seven partial differential equations:

111 conservations of mass, momentum, and energy for each phase, plus an additional equation for

112 the evolution of volume fraction. For one-dimensional flow, these equations are given as:

113

114 $$\frac{\partial \alpha_c}{\partial t} = -V^I \frac{\partial \alpha_c}{\partial x} \tag{1}$$

115 $$\frac{\partial \alpha_c \rho_c}{\partial t} + \frac{\partial \alpha_c \rho_c u_c}{\partial x} = 0 \tag{2}$$

116 $$\frac{\partial \alpha_c \rho_c u_c}{\partial t} + \frac{\partial (\alpha_c \rho_c u_c^2 + \alpha_c P_c)}{\partial x} = P^I \frac{\partial \alpha_c}{\partial x} + F^I \tag{3}$$

117 $$\frac{\partial \alpha_c \rho_c E_c}{\partial t} + \frac{\partial (\alpha_c \rho_c u_c E_c + \alpha_c u_c P_c)}{\partial x} = P^I V^I \frac{\partial \alpha_c}{\partial x} + F^I V^I + Q^I \tag{4}$$

118 $$\frac{\partial \alpha_d}{\partial t} = V^I \frac{\partial \alpha_c}{\partial x} \tag{5}$$

119 $$\frac{\partial \alpha_d \rho_d}{\partial t} + \frac{\partial \alpha_d \rho_d u_d}{\partial x} = 0 \tag{6}$$

120 $$\frac{\partial \alpha_d \rho_d u_d}{\partial t} + \frac{\partial (\alpha_d \rho_d u_d^2 + \alpha_d P_d)}{\partial x} = -P^I \frac{\partial \alpha_c}{\partial x} - F^I \tag{7}$$

121 $$\frac{\partial \alpha_d \rho_d E_d}{\partial t} + \frac{\partial (\alpha_d \rho_d u_d E_d + \alpha_d u_d P_d)}{\partial x} = -P^I V^I \frac{\partial \alpha_c}{\partial x} - F^I V^I - Q^I \tag{8}$$

122

123   where the subscripts *c* and *d* indicate properties of the carrier phase or discrete particle phase

124   respectively. For simplicity we present 1D equations, whereas the numerical code operates on

125   3D grids.   Details of the model equations and solution can be found in Saurel & Abgrall (1999)

126   and Dunn (2011). The left sides of the equations represent the hydrodynamic response of the

127   material, whereas the right-hand-side represents the non-conservative interaction between

128   phases. These non-conservative terms account for momentum and energy transfer from one

129   phase to the other due to various mechanisms such as drag F^I and heat transfer Q^I. The equations

130   are solved indirectly using the Discrete Equation Method (DEM) of Chinnayya et al. (2004). The

131   key idea is to discretize the multiphase mixture at the microscopic level and then to average the

132   discrete equations. It provides a new discrete model as well as the numerical method. The DEM

133   implicitly defines the values for the interface pressure P^I and interface velocity V^I and

134   evaluation of these terms can be found in Chinnaya et al. (2004) and Dunn (2011). The resulting

135   DEM equations are discretized using an Eulerian-based Godunov finite volume method with

136   mesh motion. The convective and mesh motion integral terms are evaluated as surface fluxes.

137   The DEM prescribes that these fluxes are computed at each inter-phase contact as well as

138   contacts between different phases. The current formulation uses the Artificial Upstream Flux

139   vector Splitting (AUFS) scheme of Sun & Takayama (2003) by default to compute the flux. It

140   should be noted, that the numerical method presented here can be applied to any finite volume

141   multiphase solver, but DEM method is chosen here since it has already existed in ALE3D code.

142

143   **4. Low Mach correction.**

144

145   It is known that low Mach features are heavily dampened in the standard compressible numerical

146   schemes. Venkatesewaran and Merkle (1998) and Thornber et al. (2008a) demonstrated that the

147   leading order kinetic energy dissipation rate in a finite volume Godunov scheme increases as

148   Mach number *M* decreases. In the particular case of the MUSCL advection scheme with a van

149   Leer limiter it was shown that the leading order kinetic energy dissipation rate can be written as

150      $\epsilon = \frac{\Delta x^2}{12} u u_x u_{xx} + \frac{\Delta x^3}{24} (3 u_{xx}^2 + (2C - 3) u_x u_{xxx})$ (9)

151

152 where u and a are the velocity normal to the cell interface and speed of sound, respectively, C is

153 the Courant–Friedrich–Levy (CFL) number and Δx is the cell length. Therefore, the dissipation is

154 proportional to the speed of sound and the magnitude of the velocity derivatives squared at

155 leading order. It was demonstrated that the increase in dissipation at low Mach numbers is not

156 physical, but is a property of the discrete system. Thornber et al., (2008) proposed a simple

157 modification of the reconstruction process within finite volume schemes to allow significantly

158 improved resolution of low Mach number perturbations for use in mixed

159 compressible/incompressible flows. The idea of the method is to modify left u_L and right states

160 u_R computed using standard compressible solver as

161 $$u_{LM,L} = \frac{u_L + u_R}{2} + z \frac{u_L - u_R}{2} \tag{10}$$

162 $$u_{LM,R} = \frac{u_L + u_R}{2} + z \frac{u_R - u_L}{2} \tag{11}$$

163 where $z = \min\left(M_{local}, 1\right)$ and $M_{local} = \max\left(M_L, M_R\right)$.

164 We implemented this correction in the DEM multiphase solver. It will be shown in example 9.1

165 in Section 9 that such modifications prevent the numerical suppression of low Mach number

166 flow instabilities.

167

168 **5. Lagrangian hydrodynamic equations**

169

170 The arbitrary Lagrangian-Eulerian hydrodynamic solver solves the equations of motion in the

171 Lagrange frame and accomplishes advection numerically by calculating fluxes between the

172 Lagrange mesh and its relaxed or Eulerian mesh. Compressible flow modeling is accomplished

173 via the addition of an artificial viscosity term to the momentum equation. The equations of

174 motion and the energy equation are discretized using the finite element method

175 The momentum equations are

176 $$\frac{\partial \sigma_{\alpha\beta}}{\partial x_\beta} + \rho f_\alpha = \rho \ddot{x}_\alpha \tag{12}$$

177 where $\sigma_{\alpha\beta}$ is the Cauchy stress, ρ is the density, and f is the body force density and x_α is the

178 displacement.

179 Mass conservation is stated as

180 $$\rho V = \rho_0 \tag{13}$$

181 where V is the relative volume and ρ_0 is the reference density.

182   The energy equation is

183    $\dot{E} = V s_{\alpha\beta} \dot{\epsilon}_{\alpha\beta} - (p + q)\dot{V}$ (14)

184   which is integrated in time and used for the equation-of-state (EOS) evaluations and a

185   global energy balance. The deviatoric stresses are

186    $s_{\alpha\beta} = \sigma_{\alpha\beta} - (p + q)\, \delta_{\alpha\beta}$ (15)

187   where p is pressure and defined as

188    $p = -\frac{1}{3}\sigma_{\lambda\lambda} - q$ (16)

189   q is the artificial viscosity, $\delta_{\alpha\beta}$ is the Kronecker delta, and $\dot{\epsilon}_{\alpha\beta}$ is the strain rate tensor.

190   As most hydrocodes, we split the stress into the pressure which comes from the EOS and the

191   deviatoric stress which is obtained in an incremental form using the Jaumann rate and a

192   traditional Wilkins type plasticity treatment. Details of the numerical solution procedure can be

193   found in Noble et al., (2017).

194

195   **6. Mesh intersection and element categorization**

196

197   At each cycle, the intersection of the exterior boundary of the foreground mesh with the

198   background mesh is computed.   The result of the calculation is a set of interface segments,

199   which are portions of the exterior faces of the foreground mesh clipped to the background mesh

200   cell in which they are contained. For each segment the outward normal, segment center, and

201   segment area are computed and stored (Figure 2). For efficient identification of ghost cells of the

202   background grid, underlying the foreground mesh and its boundary, a distance function φ is

203   used. The signed distance to the interface segment is evaluated at each node of the element φ_N

204   and at the element center φ_C. Based on those signed distances, the elements are categorized as

205   fluid (all $\varphi_N > 0$ and t $\varphi_C > 0$), fluid-cut (some $\varphi_N < 0$ and $\varphi_C > 0$), solid-cut (some $\varphi_N < 0$

206   and $\varphi_C < 0$), and ghost (all $\varphi_N < 0$ and $\varphi_C < 0$) elements. For categorization, the foreground

207   is deemed to be the "solid" and the background the "fluid", although properly the foreground

208   ALE solver can also be fluid, that is materials without strength. Element categorization

209   according to the signed distance is presented in Table 1. An example for a circular interface is

210   shown in Figure 3. The element categorizations are used to update solution. The fluid-cut cells

211   are treated as any other cells in the multiphase solver. Fluid-cut and fluid elements are used to

212 enforce boundary conditions at the interface. The solutions for ghost and solid-cut elements are

213 updated using specified interface conditions. In addition, the element categorization is used to

214 define which fluxes at the faces need to be modified. It will be shown in section 8 that in addition

215 to the cell-center update, similar to the most ghost fluid methods, we modify the solid side of the

216 Riemann problem at the faces which result in better accuracy of the coupling scheme.

217

218 **Table 1. Element categorization according to the signed distance.**

φ_C	φ_N	Element category	Description
$\varphi_C > 0$	All $\varphi_N > 0$	Fluid	Element outside the interface
$\varphi_C > 0$	Some $\varphi_N < 0$	Fluid-cut	Element cut by interface
$\varphi_C < 0$	Some $\varphi_N < 0$	Solid-cut	Element cut by interface
$\varphi_C < 0$	All $\varphi_N < 0$	Ghost	Element inside the interface

219

220 **7. Interface conditions**

221

222 Standard fluid structure interaction (FSI) conditions are usually formulated as follows: (1) the

223 fluid velocity is forced to be equal to the solid velocity and (2) solid boundary conditions include

224 pressure boundary conditions taken from the fluid. However, Banks et al. (2011) showed that

225 such approximation may lead to numerical instabilities if the solid and fluid have similar

226 densities, which could be the case of multiphase dense particles. In the recent articles (Banks et

227 al., 2011 and Banks et al., 2014), a stable interface projection scheme was developed for the

228 problem of coupling a compressible and incompressible fluid with stress and velocity state

229 (σ_L, u_L) and a deformable elastic solid states (σ_R, u_R) of arbitrary density ρ_L and ρ_R. These

230 conditions can be summarized as

231 $$n^T u_I = \frac{\epsilon_L}{\epsilon_R + \epsilon_L} n^T u_R + \frac{\epsilon_R}{\epsilon_R + \epsilon_L} n^T u_L + \frac{1}{\epsilon_R + \epsilon_L} n^T (\sigma_R n - \sigma_L n), \tag{17}$$

232 $$t^T u_I = \frac{\epsilon_L}{\epsilon_R + \epsilon_L} t^T u_R + \frac{\epsilon_R}{\epsilon_R + \epsilon_L} t^T u_L + \frac{1}{\epsilon_R + \epsilon_L} t^T (\sigma_R n - \sigma_L n), \tag{18}$$

233 $$n^T \sigma_I n = \frac{\epsilon_L}{\epsilon_R + \epsilon_L} n^T \sigma_L n + \frac{\epsilon_R}{\epsilon_R + \epsilon_L} n^T \sigma_R n + \frac{1}{\epsilon_R + \epsilon_L} n^T (u_R - u_L), \tag{19}$$

234 $$t^T \sigma_I n = \frac{\epsilon_L}{\epsilon_R + \epsilon_L} t^T \sigma_L n + \frac{\epsilon_R}{\epsilon_R + \epsilon_L} t^T \sigma_R n + \frac{1}{\epsilon_R + \epsilon_L} t^T (u_R - u_L), \tag{20}$$

235 where impedances are $\epsilon_{L,R} = 1/c\rho_{L,R}$, $\boldsymbol{n}$ is a unit normal to the interface and t is the outward

236 vector tangent to the interface (there are two tangential mutually orthogonal vectors in 3D). It

237 was shown by Banks et al., (2011) that the last term in these equations can be dropped because

238 they are approximations to the interface coupling conditions of no jump in stress or velocity.

239 Also, they mention that they could be kept if one desired. Such conditions proved to be stable for

240 the entire range fluid/solid density ratios including the difficult regime of light solids coupled to

241 heavy fluids. Such a stable coupling has been elusive in the literature and lays the groundwork

242 for other coupling regimes. We used such conditions to develop a coupling scheme for each pair

243 of multiphase variables and Lagrange hydro variables. Those averaged values are later

244 extrapolated to both multiphase solver and Lagrange hydro as shown in the next section.

245

246   **8. Coupling scheme**

247

248 In this section, the numerical algorithm of solving the multiphase equations and Lagrange hydro

249 equations on the coupled meshes is presented. The numerical solution is derived as multi-stage

250 procedure illustrated in Figure 4 as follows

251

252 *Step1: Advance Lagrange hydro*

253 Solve the ALE Lagrange hydro equations to advance the solution from time step *n* to *n+1*. The

254 interface pressure and velocity computed at the end of previous time step are applied as the

255 boundary conditions to the Lagrange mesh. There are several options for the averaging

256 techniques to derive the interface pressure. The first option is to use volume averaging of the

257 pressures for each species at the interface. The second option is to use impedance averaging of

258 the species pressures. We are currently using the first option of averaging in this paper and will

259 consider other options later on. Once the averaged pressure is available the solution is advanced

260 using the standard Lagrange hydro approach described in Section 3.

261

262 *Step 2: Define interface conditions*

263 We update the interface position at time step *n+1*, create interface segments and categorize

264 elements. We calculate interface conditions at the mesh interface at *n+1* time step for each state

265 variable. For each segment, we find the closest fluid and solid elements and derive interface

266 conditions in the projection to normal. We use impedance-weighted conditions described in

267 Section 7. In the case of the frictionless compressible flow and slip boundary conditions between

268 solid and multiphase we use those interface conditions for hydrodynamic pressure p. As

269 suggested by Banks et al. (2011) we also dropped last terms. Each multiphase species has its own

270 interface conditions (p_I^i, u_I^i) based on the impedance averaging of species state (p_m^i, u_m^i) and

271 Lagrange hydro material (p_l, u_l) as

272 $$p_I^i = \frac{\epsilon_l p_l + \epsilon_m^i p_m^i}{\epsilon_m^i + \epsilon_l} \tag{21}$$

273 $$u_I^i = \frac{\epsilon_l u_m^i + \epsilon_m^i u_l}{\epsilon_m^i + \epsilon_l} \tag{22}$$

274 This interface values are used to update multiphase variables in ghost and solid-cut regions as

275 described at the next steps.

276

277 *Step 3: First order ghost update*

278 Since ghost zones can be uncovered at the next time step due to the mesh motion we need to

279 update those values. We use first order neighbors and interface values derived at Step 2. First, we

280 project a ghost fluid grid point of interest onto the fluid–structure interface and determine its

281 reflection (image point) with respect to the interface segment containing that ghost fluid grid

282 point (cell 0 in Figure 4, Step 3). Since an image point usually falls in the physical fluid domain,

283 the fluid state variables at this point are computed by interpolation, using available first order

284 neighbors (cells 1, 2 and 3 in Figure 4, Step 3). Then, the multiphase velocity state vector for

285 each species at the ghost fluid grid point is computed as follows. The fluid velocity vector (or its

286 normal component in the case of slip boundary conditions) is obtained by linearly extrapolating

287 the interpolated fluid velocity vector at the image point and the structural velocity vector at the

288 projection point. The values of the remaining primary fluid variables (mass, pressure, internal

289 energy and volume fractions) at the ghost fluid grid point are set to the interpolated values at the

290 image fluid grid point. This step is somewhat similar to the ghost fluid methods (e.g. Ghias et al.,

291 2007). However, to improve accuracy of the method, additional modifications to the face

292 variables are done at the Step 5. This step is also necessary in the case of moving objects. When

293 a cell changes from a ghost cell to a fluid cell, ghost values become a fluid and further evolved as

294 any other fluid data.

295

296 *Step 4: Find states of the Riemann problem in multiphase solver*

297 At this step, we find the left and right states of the Riemann problem for multiphase fluid

298 variables using standard MUSCL reconstruction scheme for each multiphase species as $U_+ =$

299 $(\alpha_+, \rho_+, u_+, p_+)$ and $U_- = (\alpha_-, \rho_-, u_-, p_-)$. We will further assume that the solid side

300 corresponds to U_+ and fluid side corresponds to U_-.

301

302 *Step 5: Second order interface update*

303 Extrapolate interface conditions defined at Step 2 to the faces using first and second order

304 neighbor elements (Figure 4). We update here the face states for the cell 0 (see Step 5 in Figure

305 4). In particular, the value of u_* is determined by the following formula

306 $$(\boldsymbol{u_*} \cdot \boldsymbol{n_I}) = (\boldsymbol{u_I} \cdot \boldsymbol{n_I}) + (\tfrac{1}{2} - d)s \qquad (23)$$

307 $$(\boldsymbol{u_*} \cdot \boldsymbol{\tau_I}) = (\boldsymbol{u_-} \cdot \boldsymbol{\tau_I}) \qquad (24)$$

308 where d is the distance between interface point I and cell center 1 (Step 5 in Figure 4). Interface

309 point I is evaluated as the intersection of the boundary of the foreground grid with the line

310 connecting the cell centers 0 and 1 (Step 5 in Figure 4). Slope s for velocity field is computed

311 using d-weighted slope computation as in Gorsse et al., (2012) as

312 $$s = \boldsymbol{u_I} \cdot \boldsymbol{n_I} - \boldsymbol{u_1} \cdot \boldsymbol{n_I} + \frac{1-d}{1+d}(\boldsymbol{u_I} \cdot \boldsymbol{n_I} - \boldsymbol{u_2} \cdot \boldsymbol{n_I}), \qquad (25)$$

313 where $\boldsymbol{u_I}$ is the interface velocity computed at the previous step, $\boldsymbol{u_1}$ is the velocity of the cell 1

314 and $\boldsymbol{u_2}$ is the velocity of the cell 2 (Step 5 in Figure 4). Computing slope in this way allows

315 avoiding instability when the cell center 1 is close to the interface I. If the slope limiter is needed

316 the limiter slope is defined as $s_{limiter} = minmod(s, s_2)$, where

317 $$s_2 = \boldsymbol{u_1} \cdot \boldsymbol{n_I} - \boldsymbol{u_2} \cdot \boldsymbol{n_I} \qquad (26)$$

318 Interface pressure is assumed to be equal to the interface pressure computed at the previous step

319 as $p_* = p^I$. As a result of this procedure we will have interpolated interface values (u_*, p_*) to be

320 used at the next step.

321

322 *Step 6: Modify Riemann states*

323 At this step, we modify the solid side of the Riemann problem for each multiphase species using

324 extrapolated face interface values defined at the previous step as $U_+ = (\alpha_-, \rho_-, -u_- + 2u_*, p_*)$

11

325 Modified in this way the solution of Riemann problem at the faces satisfies exactly the boundary

326 interface conditions at the faces. With states on either side of the interface in this way, the exact

327 solution to the Riemann problem is symmetric about the path of the interface in *x-t* plane. When

328 velocity of the fluid side state u_- is less than interface velocity u_*, the solution consists of two

329 rarefactions. When velocity the fluid side state u_- is greater than the interface velocity u_*, the

330 solution consists of two shock waves.

331

332 *Step 7: Advance multiphase solution*

333 The Artificially Upstream Flux-vector Splitting (AUFS) (Sun and Takayama, JCP, 2003)

334 Riemann solver is used to advance the solution on the background multiphase flow mesh. This

335 step completes the coupling scheme at time n+1.

336

337 **9. Numerical results**

338

339 In this section, we demonstrate the effectiveness of the presented coupling method for dynamic

340 Lagrange hydro interfaces and their interaction with multiphase fluid across the entire range of

341 material parameters for both single and multiple phases. All gases in the considered problem are

342 modeled as ideal gases with adiabatic exponent $\gamma = 1.4$. Since the multiphase solver is explicit

343 we use CFL number 0.4 in all examples.

344

345 *9.1 Low Mach example*

346

347 In this example, we demonstrate applicability of the underlying multiphase flow for subsonic

348 flow applications. In this case, an initial subsonic flow that moves from the left to right with

349 Mach number 0.05 interacts with a step-like structure (Figure 5). We did simulations with an

350 original compressible scheme for multiphase flow and modified scheme with the Low Mach

351 correction described in Section 4. We used a 2D configuration with 640 by 320 mesh resolution.

352 The vorticity field in both simulations is presented in Figure 5. We can see that the original

353 scheme heavily damps the Low Mach instabilities at the interfaces. The low Mach correction

354 reduces the dissipation allowing the scheme to capture the interfacial instabilities.

355

356   *9.2 Advection with uniform velocity*

357

358   Here we present a test when the solid object moves diagonally with the same velocity as the

359   surrounding fluid. In this case, there should be no artificial flows generated if the interface

360   conditions and ghosts, fluid-cut and solid-cut elements are updated correctly. Mesh resolution

361   was 13x13. Figure 6 shows the initial velocity and the velocity after 200 cycles. It is unchanged

362   and there is no artificial flow generated. Therefore, we conclude that the method proposed in this

363   paper has been implemented correctly.

364

365   *9.3 Piston problem*

366

367   The initial problem consists of a gamma law gas on the left and right and a solid piston in the

368   center. The problem setup is similar to what was used in Dunn et al., (2011). Initially, the gas on

369   the left is at a higher pressure than the gas on the right, resulting in a pressure force pushing the

370   piston to the right. As the piston moves, the volume on the left increases causing a decrease in

371   the pressure on the left. At the same time, the volume on the right decreases causing an increase

372   in the pressure on the right. Eventually, the pressure on the right becomes greater than the

373   pressure on the left causing the piston to decelerate and then get pushed to the left. Thus, the

374   pressure force causes the piston to travel back and forth in a cyclic fashion. The initial geometry

375   for this problem is shown in Figure 7. We used a 3D configuration with 40x8x8 mesh resolution.

376   The problem consists of a rigid piston separating two gases. The piston is modeled using

377   properties similar to steel, resulting in an essentially rigid material. This problem uses a one-

378   dimensional geometry. It is modeled using a two-dimensional mesh with a single zone in the y

379   direction and symmetry boundary conditions on the sides, resulting in a pseudo-1D flow in the x

380   direction. The problem has a domain length of 4 with the origin (x = 0) at the center. The

381   piston's length is 1. Initially, the gas on the left has a length of 1 and the right gas has a length of

382   2. Thus, the initial volume of the gas on the right is twice the volume of the gas on the left.

383   Therefore, the pressure in the left gas is initially twice that of the right gas.

384   We did several simulations by varying piston/gas density ratios and used a standard FSI coupling

385   conditions and impedance averaged interface conditions presented in Section 7. Figure 7 shows

386   the results of simulation for 100 piston/air mass ratio and 0.01 piston/air ratio. In the last case the

387 piston was simulated as a low density fluid. Figure 7c shows that the spurious waves are

388 generated for a piston problem without impedance conditions at low solid/fluid density ratios,

389 whereas the solution is smooth if we use impedance coupling conditions. In addition, the second

390 order coupling scheme, as expected, appears more accurate at all range of density ratios. Since

391 the motion of the piston is governed by Newton's second law it can be shown (Dunn, 2011) that

392 it is described by equation

393

394 $$\frac{d^2x}{dt^2} = \frac{p_*A}{m_{sol}}\left[\left(\frac{V_*}{V_*+Ax}\right)^{\gamma} - \left(\frac{V_*}{V_*-Ax}\right)^{\gamma}\right],$$ (27)

395

396 where x is the center of mass of the piston, p_* and V_* are the pressure and volume at equilibrium,

397 A is the frontal area of the piston equal to 1 here, m_{sol} is the mass of the piston. Figure 7b shows

398 results of comparisons with the analytical solution. The second order coupling scheme with

399 impedance coupling conditions match very well the analytical solution.

400

401 *9.4 Modified Sod problem*

402

403 To demonstrate that the proposed coupling technique is applicable and stable when both

404 foreground and background solvers have similar properties the method has been applied to the

405 Sod shock tube test case. The initial conditions are $(\rho, u, p)_L = (1, -0.5, 1)$, $(\rho, u, p)_R =$

406 $(0.125, 0, 0.1)$, where the initial discontinuity is placed at x=0.5 and the foreground grid with

407 gamma law gas was initially placed at x=0.6 (Figure 8a). The background domain of size 1x1

408 was discretized using 128x128 mesh resolution. The foreground domain of initial length 0.25

409 was discretized with 32x32 mesh resolution. Figure 8 shows the pressure, density and velocity

410 profiles in both background and foreground regions. The foreground grid is allowed to move and

411 it deforms and propagates with the shock wave. The pressure, density and velocity are similar on

412 both meshes, but they are sharper for the foreground mesh since this mesh moves with the shock

413 wave and have little numerical dissipation. In this example, the background and foreground

414 solvers have similar properties (gamma law gases in this example). Therefore, this example

415 demonstrates that the proposed coupling technique is stable and capable reproducing

416 discontinuities at the interfaces between domains with similar material properties.

417

9.5 Shock wave interaction with Lagrange structure

419

420 This is a validation test of the multiphase model for a simulation of a shock wave impacting a

421 steel panel. The test is designed to test fluid-structure interaction for a transient compressible

422 flow. A two-dimensional planar geometry was used in the calculations. The problem dimensions

423 are given in Figure 9a. A thin steel plate is placed at the center of a rectangular domain. An

424 initial high-pressure, high temperature region (p=10^1 Mbar, T=3000 K) of radius 10 cm is placed

425 at x= 25 cm. The surrounding gas has atmospheric air conditions (p=1^{-6} Mbar, T=300 K). This

426 initial pressure and temperature jump generates a shock, which impacts the panel and induces

427 flexure of the plate. The thickness of the plate is 10 cm. The background mesh has resolution

428 50x50 cells. The steel panel (foreground mesh) is discretized using 5x25 cells. The plate is

429 modeled using the Lagrangian structural model for steel while the air is modeled as a single-

430 phase material using the multiphase method. No analytic solution is available for this test.

431 Therefore, we compare results of the simulations with conforming grid simulations that are done

432 with the same initial conditions and resolution. In the last case, the conforming grid stretches and

433 deforms as the plate moves whereas in the first case the background mesh remains uniform.

434 Figure 9 shows snapshots of velocity field in both simulations at time 0.2 s (embedded approach

435 – Figure 9c, conforming grid – Figure 9d) and 0.65 s (embedded approach – Figure 9e,

436 conforming grid – Figure 9f). Figure 9b shows comparison of the averaged velocity in the plate

437 in both simulations. We see that results obtained using two different techniques agree very well.

438 Therefore, we conclude that the multiphase-flow algorithm appears to be coupled to the

439 Lagrangian structure properly for this problem.

440

9.6 Shock wave with tungsten particles interaction with Lagrange structure

442

443 This last example demonstrates interaction of a shock wave that consists of tungsten particles

444 with a solid structure. The setup is similar to the previous example but now the initial high-

445 pressure region consists of tungsten particles (10% volume fractions) and air (90% volume

446 fraction). Figure 9 shows reflection of the tungsten particles from the structure once they interact

447 with a plate. Several drag models are available to parametrize air-particles coupling terms. For

448   this particular simulation, we used Akhatov drag model (Akhatov and Vainshtein 1984). The

449   background mesh has resolution 120x120x120 cells. The steel target (foreground mesh) is

450   discretized using 40x40x10 cells. As flow with the tungsten particles reaches the target, the steel

451   panel starts to deform and solid stresses inside the steel target are developed (Figure 10). These

452   results demonstrate that the coupling algorithms used in the current approach are appropriate for

453   modeling the interaction between multiphase particles and Lagrange structures.

454

455   **10. Conclusions**

456

457   A numerical technique to couple an Eulerian multiphase flow solver with Lagrangian

458   hydrodynamics has been developed. The primary purpose is to allow simulations using different

459   solvers operating on different domains and meshes. A number of algorithmic ideas are combined

460   to design a coupling technique in such a way that coupling occurs only through interfaces,

461   allowing simulation codes to remain separate. Some unique features of this work included

462   development of multiphase interface conditions that are appropriate for the multi-phase flow

463   conditions across the entire range of material parameters. In addition to the cell centered updates

464   in ghost points similar to the ghost fluid methods we use additional modifications of the solid

465   states at the faces in such a way that resulting solution of the Riemann problem at the faces

466   satisfies the boundary interface conditions and approves accuracy of the scheme. The ability of

467   the new coupling technique to reproduce complex features of the interaction of multiphase flow

468   with Lagrange structures is presented on several examples. These examples demonstrate the

469   efficiency and potential of the present technique to simulate interaction of the multiphase blast

470   with deformable tragets.

471

472   **Acknowledgment**

477

16

References

1. Akhatov, I. S. & Vainshtein, P. B. 1984 Transition of porous explosive combustion into detonation. *Combustion Explosion And Shock Waves* **20** (1), 63–69.

2. Banks, J. W., Sjogreen, B. A normal mode stability analysis of numerical interface conditions for fluid/structure interaction. *Comm. In Comp. Physics*, **10**(2):279-304, 2011

3. Banks, J. W., Henshaw, W. D. , Schwendeman, D. W., An analysis of a new stable partitioned algorithm for FSI problems. Part I: Incompressible flow and elastic solids, *J. of Comp. Physics*, 269:108–137, 2014.

4. Chinnayya A., E. Daniel, and R. Saurel. 2004. Modelling detonation waves in heterogeneous energetic materials. Journal of Computational Physics, 196(2):490–538.

5. Dunn, T.A. "A cell-centered multiphase ALE scheme with structural coupling", Ph.D. dissertation, University of California, Davis, 2011.

6. Fedkiw, R. P. Coupling an Eulerian fluid calculation to a Lagrangian solid calculation with the ghost fluid method. *J. of Comp. Physics*, **175**:200-224, 2002.

7. Ghias R., Mittal R., Dong H. A sharp interface immersed boundary method for compressible viscous flows. *J. of Comp. Physics,* **2225:** 528-553, 2007.

8. Gorsse, Y., Iollo A., Telib, H., Weynans, L. A simple second order Cartesian scheme for compressible Euler flows. *J. of Comp. Physics,* **231:** 7780-7794, 2012.

9. Noble et al., 2017. ALE3D: An Arbitrary Lagrangian-Eulerian Multi-Physics Code. Technical Report, Lawrence Livermore National Laborartory, LLNL-TR—732040

10. Pember R. B., Bell J. B., Colella P., Crutchfield W. Y., Welcome M. L. An adaptive Cartesian grid method for unsteady compressible flow in irregular regions. *J. Comput. Phys* 120, 1995, 278–304

11. Peskin C. S. The immersed boundary method *Acta Numerica*, 11, 2002, 479-517.

12. Puso, M., Sanders, J., Settgast, R. and Liu, B., "An embedded mesh method in a multiple material ALE," *Computer Methods in Applied Mechanics and Engineering*, 245, 273-289 (2012).

13. R. Saurel and R. Abgrall. A multiphase godunov method for compressible multifluid and multiphase flows. *J. of Comp. Physics*, 150(2):425–467, 1999.

508 14. M. Sun and K. Takayama. An artificially upstream flux vector splitting scheme for the
509   Euler equations. J. *of Comp. Physics*, 189(1):305–329, July 2003.

510 15. Thornber B., D. Drikakis, R.J.R. Williams, D. Youngs. On entropy generation and
511   dissipation of kinetic energy in high-resolution shock-capturing schemes. J. Comp.
512   Phys., 227 (2008), 4853-4872.

513 16. Thornber B., A. Mosedale, D. Drikakis, D. Youngs, R.J.R. Williams. An improved
514   reconstruction method for compressible flows with low Mach number features. J. Comp.
515   Phys., 227 (2008), 4873-4894

516 17. Tipton D. G., M. A. Christon, M. S. Ingber. Coupled fluid-solid interaction under shock
517   wave loading. Int. J. For Numer. Methods in Fluids, 67, 2011, 848-884.

518 18. Venkateswaran, S., Merkle, C.L., 1998. Evaluation of artificial dissipation models and
519   their relationship to the accuracy of Euler and Navier–Stokes computations. In: Lecture
520   Notes in Physics. 16th Int. Conf. on Numer. Methods in Comp. Physics, vol. 4(12). pp.
521   427–432.

522

523
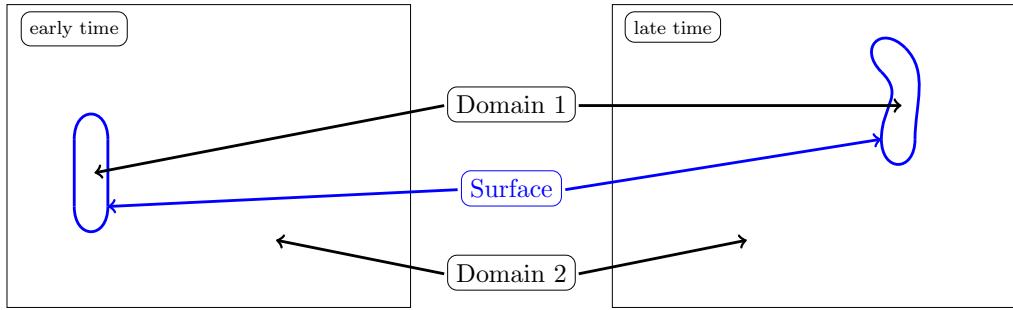
Figure 1. A cartoon depicting the evolution of a multi-domain problem.
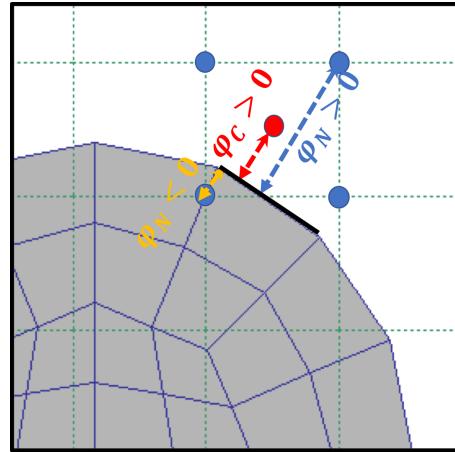
Figure 2. An example of signed distances evaluation for the nodes and the cell center.
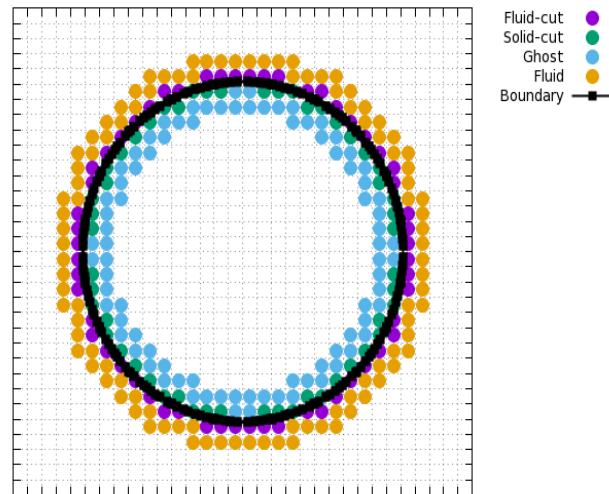
Figure 3. An example of circular foreground Lagrangian boundary and the background mesh element categories that participate in coupling.
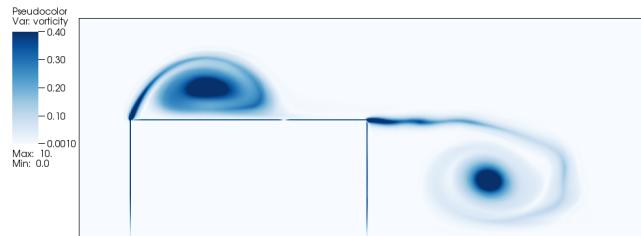
531

532
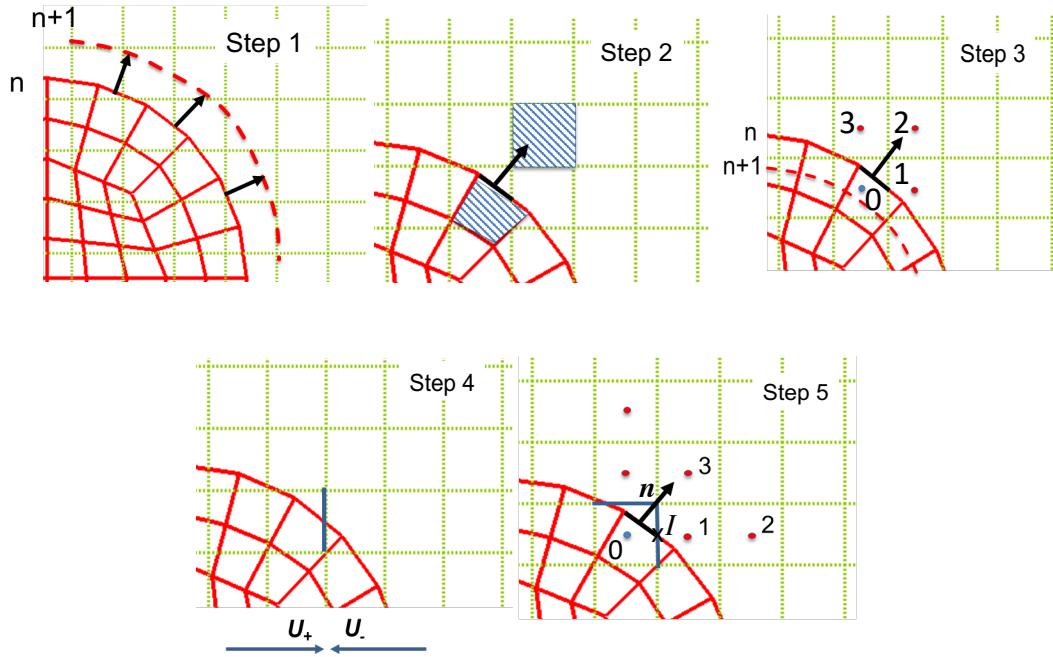
533

534

535   Figure 4. Illustration of the multi-step coupling algorithm for the multiphase solver operated on

536   the background grid (green) and Lagrange hydro operated on the foreground grid (red).

537

538
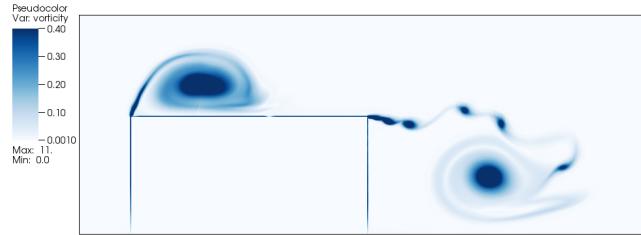
539   (a)

540   (b)

541   Figure 5. Results of the interaction of subsonic flow with a step solid structure. The calculated

542   voriticity using the modified low Mach scheme is shown in (a) and the standard compressible

543   scheme results are shown in (b). The low Mach number features presented in (a) are heavily

544   damped by the standard compressible numerical scheme (b).

545

546
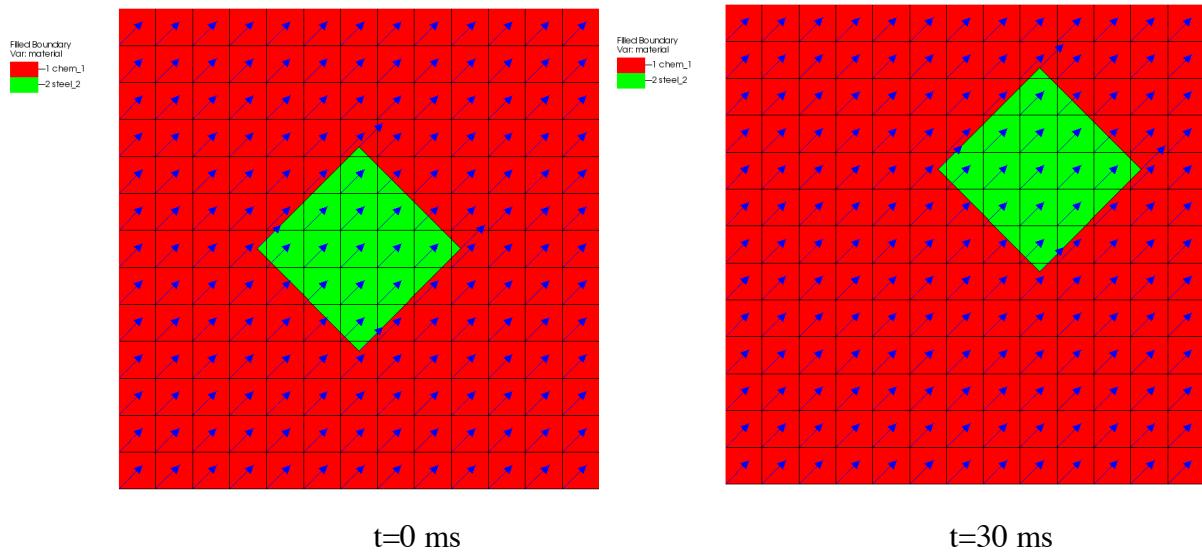
547   t=0 ms   t=30 ms

548   Figure 6. Advection of the Lagrangian object moving with the matching velocity of the fluid. As

549   expected, no artificial flows are generated. Therefore, the interface conditions are implemented

550   correctly.

21

551
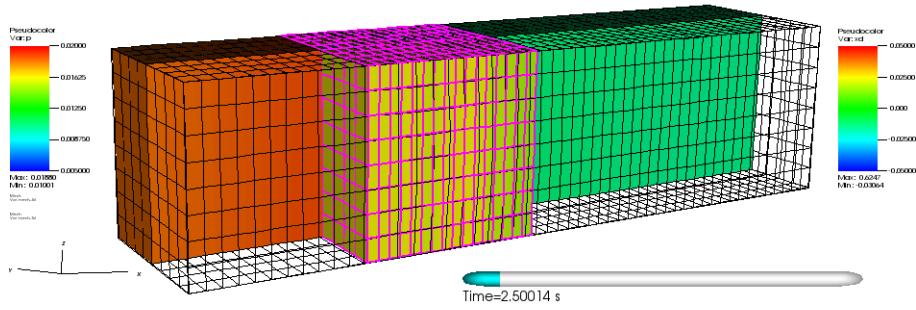
552   (a)

553
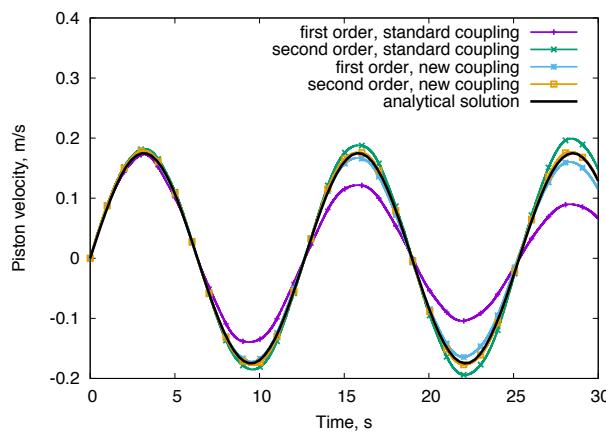
554   (b)

555
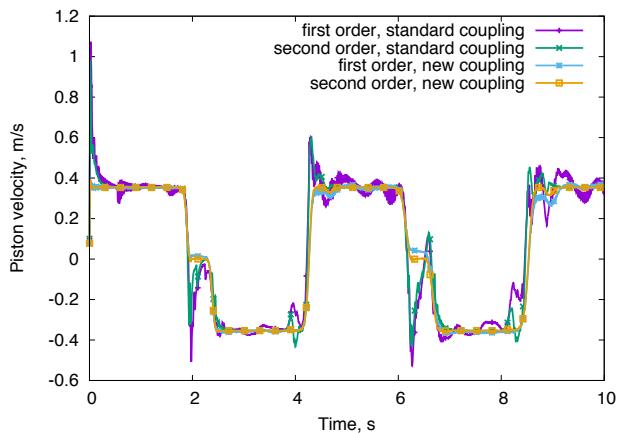

556   (c)

557   Figure 7. Pressure driven piston calculation showing the importance of numerical boundary and

558   coupling methods at different solid/fluid density ratios. A high-pressure gas on the left pushes a

559   solid piston to the right (a). The piston velocity is shown for solid/fluid density ratios of 100

560   along with the analytical solution (b) and solid/fluid density ratios of 0.01 (c). Without the

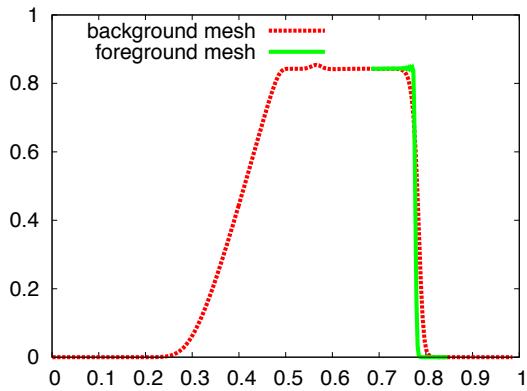561   impedance based interface conditions, spurious waves are generated.

562

(a)

(b)

563

564

(c)

(d)

565

566
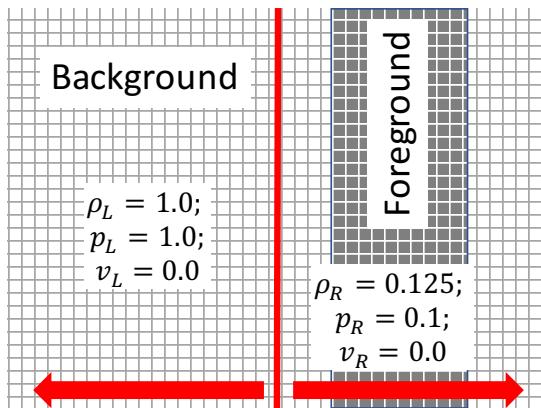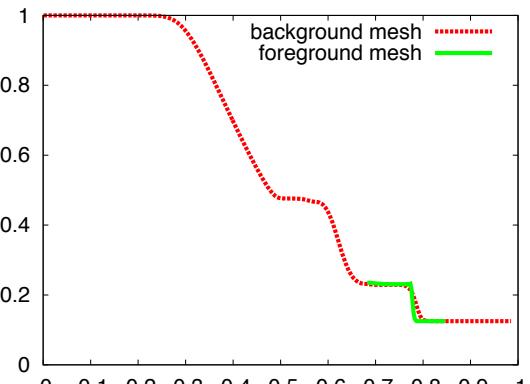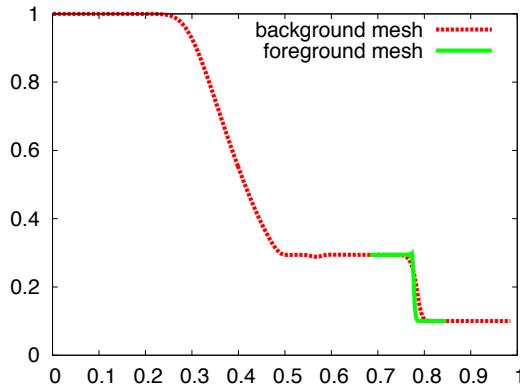
Figure 8. Results from the modified Sod shock tube test case problem for coupled meshes. A foreground mesh is initially placed at the right (a). Both background and foreground material is gamma-low air therefore impedance-averaged conditions are important in this example. As shock propagates to the right, foreground mesh moves. Density (b), pressure (c) and velocity (d) at time t=0.15 in both background solvers and foreground solvers are shown.

567

568

569

570

571

572

573
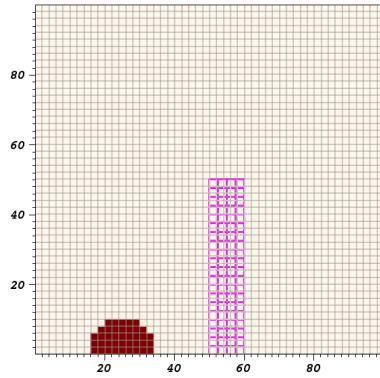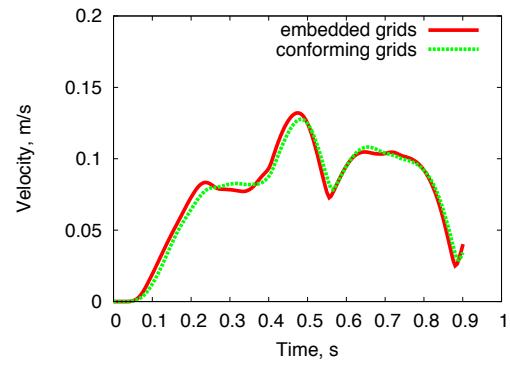
574
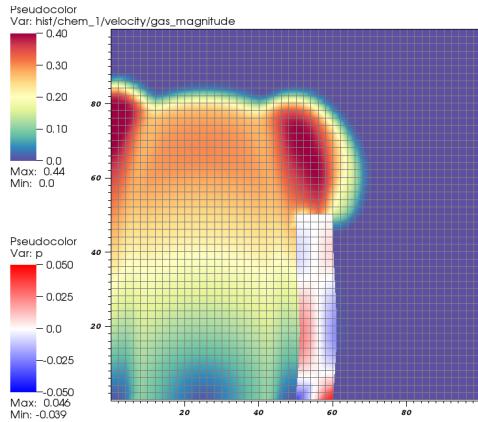575   (a)   (b)
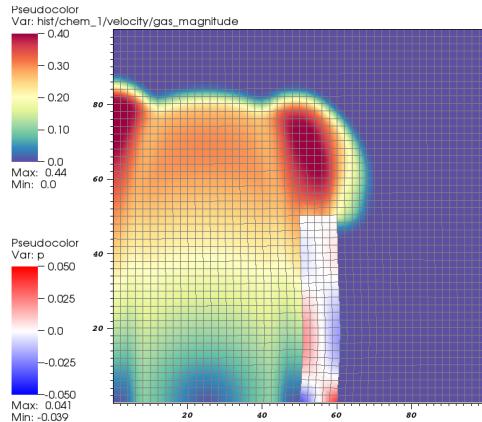

576
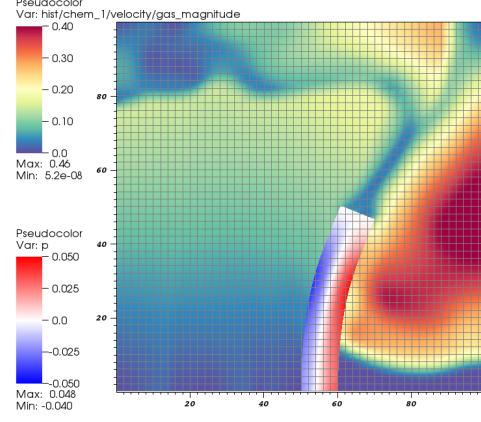577   (c)   (d)
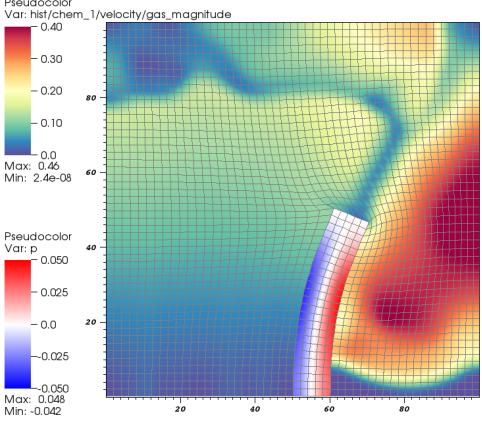

578
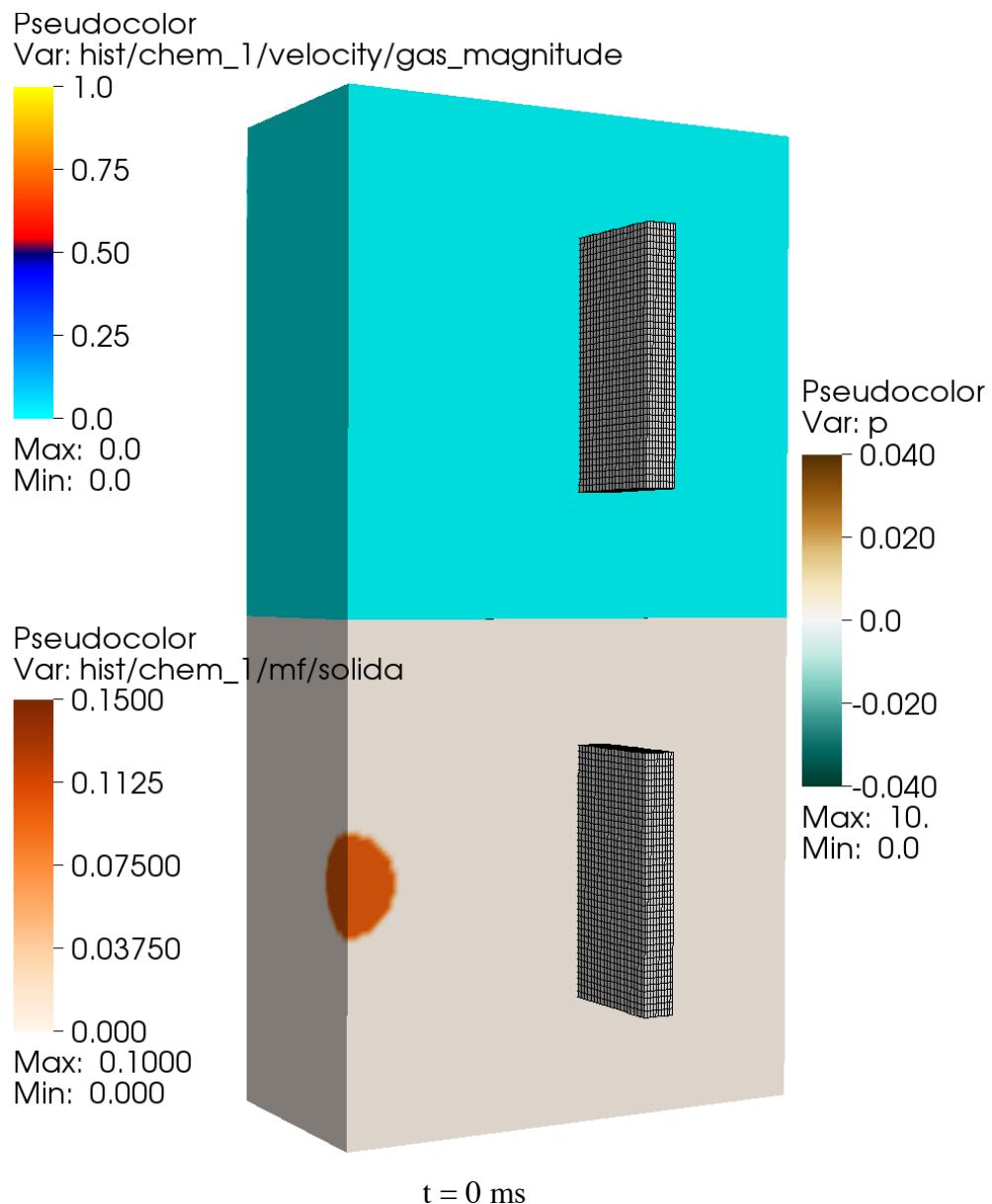579   (e)   (f)
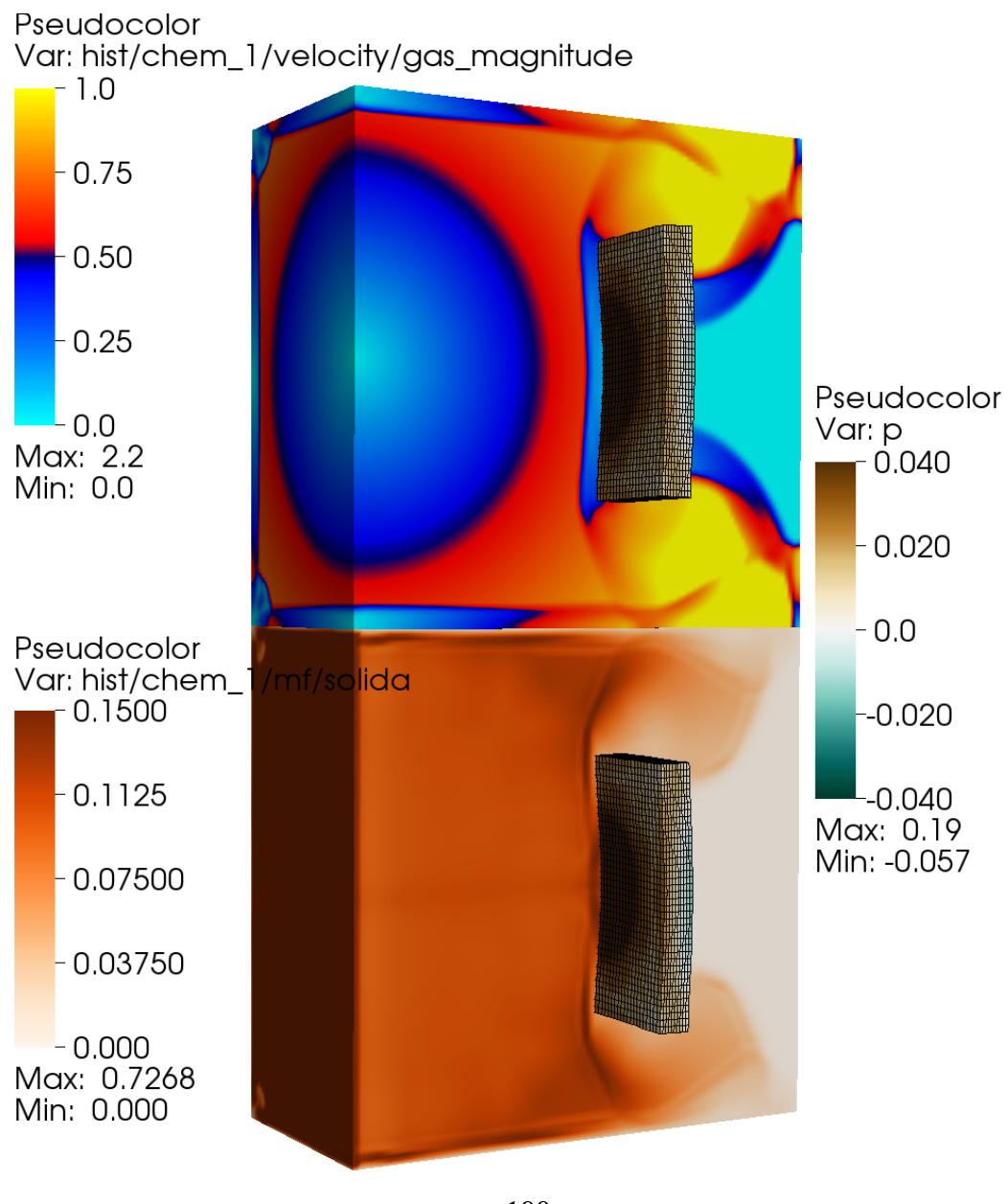
580   Figure 9. Comparison of shock wave interaction with a Lagrange deformable structure. The

581   initial pill of high-pressure air is located on the left (a). Simulations are done with the embedded

582   grids method presented in this work and compared to a conformal mesh method. Velocity field

583   comparison are presented for time 0.17 s (embedded grid (c) and conformal mesh –(d) and a time

584   0.67 s (embedded grid (e) and conforming mesh (f).

24

Pseudocolor
Var: hist/chem_1/velocity/gas_magnitude

- 1.0
- 0.75
- 0.50
- 0.25
- 0.0

Max: 0.0
Min: 0.0

Pseudocolor
Var: p

- 0.040
- 0.020
- 0.0
- -0.020
- -0.040

Max: 10.
Min: 0.0

Pseudocolor
Var: hist/chem_1/mf/solida

- 0.1500
- 0.1125
- 0.07500
- 0.03750
- 0.000

Max: 0.1000
Min: 0.000

t = 0 ms

Pseudocolor
Var: hist/chem_1/velocity/gas_magnitude
— 1.0

— 0.75

— 0.50

— 0.25

— 0.0
Max: 2.2
Min: 0.0

Pseudocolor
Var: p
— 0.040

— 0.020

— 0.0

— -0.020

— -0.040
Max: 0.19
Min: -0.057

Pseudocolor
Var: hist/chem_1/mf/solida
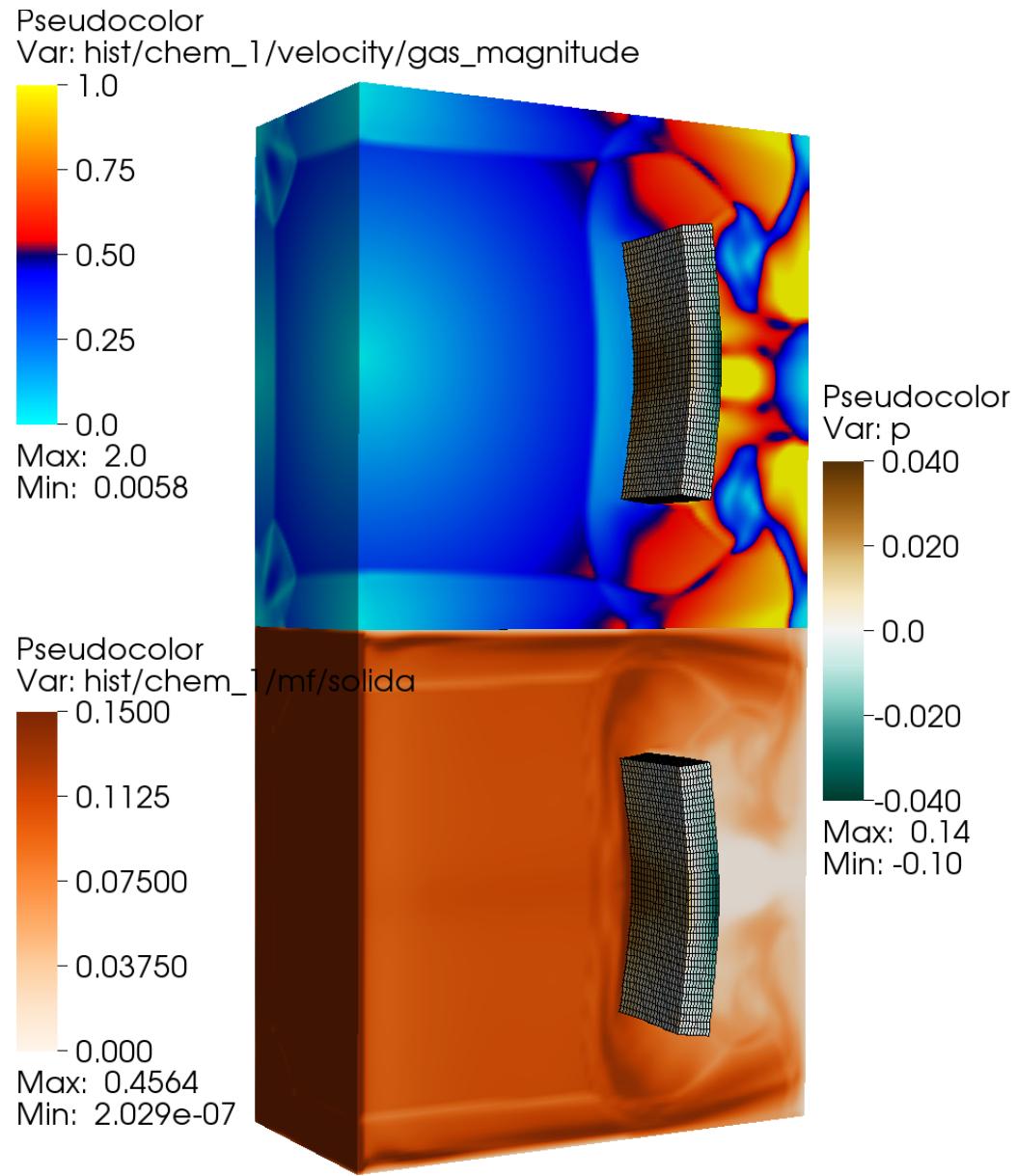— 0.1500

— 0.1125

— 0.07500

— 0.03750

— 0.000
Max: 0.7268
Min: 0.000

588
589

t = 100 ms

T=150 ms

Figure 10. A blast wave that consists of tungsten particles (10% volume fraction) and air (90% volume fraction) interacts with a solid structure. Once particles reach the wall they are reflected. The velocity field in the air phase is shown in the upper panels and the particle mass fraction is shown in the lower panels. Also shown are stresses developed inside the steel plate due to the interaction with the shock wave.