High-Order Methods for Multi-Physics Multi-Material ALE in BLAST

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Introduction

BLAST is a multiphysics Arbitrary Lagrangian-Eulerian (ALE) code based on high-order finite elements. We improve its remap phase by a new Flux-Corrected Transport (FCT) algorithm that removes instabilities resulting from using high-order (above Q_3) polynomials. We also introduce a new point-based closure model that improves material evolution in mixed cells during the Lagrangian phase. Finally we present our new radiation-diffusion module.

Non-oscillatory high order FCT remap

After the Lagrangian and the remesh phases, our remap must transition a high-order FE function η between two meshes with the same topology. For this we solve the advection equation $d\eta/d\tau = \vec{u}\cdot\nabla\eta$, where $\vec{u}$ is mesh velocity and τ is transition pseudotime. We use FCT to preserve the bounds at each time step.

$$M\frac{d\eta}{d\tau} = K\eta\,, \quad \min_{N_i}\eta_j^n := \eta_i^{max} \le \eta_i^{n+1} \le \eta_i^{min} := \max_{N_i}\eta_j^n$$

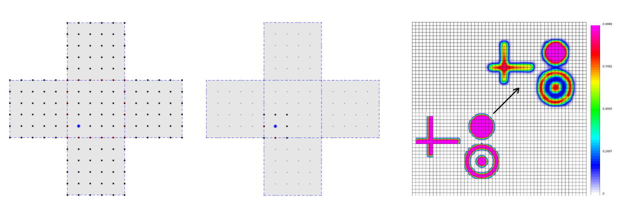
Above Q_3, standard FCT causes oscillations and excessive diffusion, because it is based on the full sparsity pattern of the transport operator. New approach:

- We localize the bounds by including into N_i only the i's neighbors. This restricts the range of admissible values (less room for oscillations).
- Element-based FCT - having η^{min}, η^{max} and the high-order solution η^H, we limit each degree of freedom (instead of each flux contribution) to $\eta_i^* = \min(\eta_i^{max}, \max(\eta_i^H, \eta_i^{min}))$. This yields some mass error in the cell.
- Cell-based mass redistribution - using the low-order solution η^L (NOTE: η^L and η^H have the same mass on K), which has the correct mass and is in (non-restricted) bounds by default, we interpolate to the new solution:

$$m_i(\eta_i^{n+1} - \eta_i^L) = f_i\,, \quad f_i = f_i^* - \lambda z_i\,, \quad f_i^* = m_i(\eta_i^* - \eta_i^L)\,, \quad \lambda = \sum_{i\in K} f_i^* \Big/ \sum_{i\in K} z_i$$

Here $\sum_{i\in K} f_i = 0$ gives conservation; z_i is based on the local mass violation $|\eta_i^* - \eta_i^H|$ and is chosen in a way s.t. η_i^{n+1} is between η_i^L and η_i^*.

Advection of a Q_{11} jump function: Standard FCT with full and local bounds; Element-based FCT with full and local bounds. Maximum values: 1, 0.9748, 0.9996, 0.9999.



Stencils defining the full and local bounds; Advection of Q_5 discontinuous shapes (60 remaps).

A new closure model algorithm for high-order FE

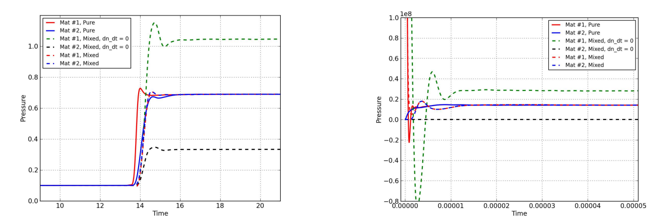
Lagrangian methods must handle cells containing multiple materials. We introduce a new variable $\beta_k = dV_k/dV$ that controls the evolution of the material indicator functions $\eta_k = V_k/V$. These β_k are defined through the bulk modulus relation $dp = -\kappa dV/V$ and a pointwise pressure equilibration argument:

$$(\beta_k - \eta_k)\nabla\cdot\vec{v} = \frac{1}{\Delta\tau}\frac{\eta_k}{\kappa_k}(\bar{p}_k^{n+1} - p^*) = \nabla\cdot\vec{v}\left(-\eta_k + \frac{\eta_k}{\kappa_k}\Big/\sum_i\frac{\eta_i}{\kappa_i}\right) + \frac{1}{\Delta\tau}\frac{\eta_k}{\kappa_k}(p_k^n - p^{**})$$

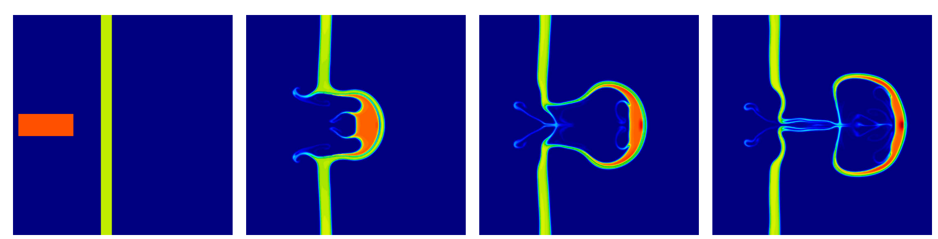
Here $\Delta\tau = c_1\min_k(h/c_{s,k})$ is equilibration time scale, $\bar{p}_k^{n+1}$ is a pressure prediction for the case of constant volume fractions, p^* is equilibrium pressure at time $t+\Delta\tau$, and p^{**} is an average pressure at time t. All η_k and β_k are defined at integration points and they are not FE functions. Each integration point relaxes its pressures towards an equilibrium value with time scale $\Delta\tau > \Delta t$; this is not an instantaneous equilibration process. Then we evolve the system:

$$\frac{d\eta_k}{dt} = (\beta_k - \eta_k)\nabla\cdot\vec{v}\,, \quad \rho\frac{d\vec{v}}{dt} = -\nabla\cdot\sigma\,, \quad \eta_k\rho_k\frac{de_k}{dt} = (\eta_k\sigma_k + (\beta_k - \eta_k)c_2\sigma^*) : \nabla\vec{v}$$

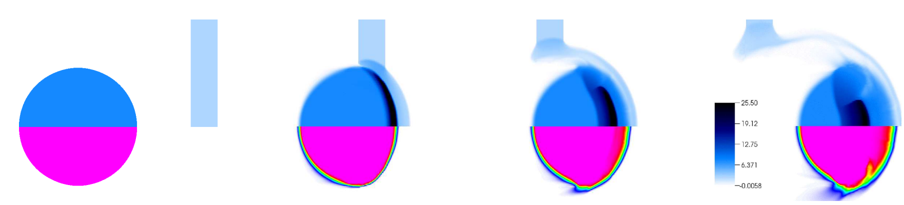
This is a continuous model applicable to any space discretization and time integration. It involves no interface reconstruction. The red terms correspond to volume and energy redistribution due to the closure model adjustments.



Left: Two gases with different compressibility, initially at equilibrium, are hit by a shock wave. Right: A more challenging shock tube containing water ($\rho_0 = 10^9$) and air ($\rho_0 = 10^4$). Both plots show pressure histories at the middle integration point of the mixed cell.



Gas impactor ($v_0 = 2km/s, \rho_0 = 20g/cm^3, \gamma = 50$) hits a gas wall ($\rho_0 = 15g/cm^3, \gamma = 5/3$). Background is gas ($\rho_0 = 1g/cm^3, \gamma = 1.4$). Q_2Q_1 ALE simulation with Q_2 materials, 160x160.



Steel ball ($v_0 = 30km/s, \rho_0 = 7.81g/cm^3$) hits an aluminum wall ($\rho_0 = 2.702g/cm^3$). Background is gas ($\rho_0 = 1e^{-3}g/cm^3, \gamma = 1.2$). Q_3Q_2 ALE simulation with Q_2 materials, NURBS mesh. We show total density (top half) and the material indicator of the steel ball (bottom half).

Single energy group, multi-material radiation diffusion

The explicit hydrodynamics terms are coupled to implicit radiation diffusion:

$$\eta_k\rho_k\frac{\partial e_k}{\partial t} = \eta_k\sigma_k : \nabla\vec{v} + \eta_k\, c\,\sigma_{p,k}(E - B(T(e_k)))\,,$$

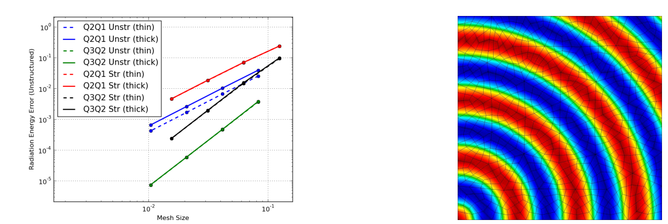
$$\frac{\partial E}{\partial t} + \nabla\cdot\vec{F} = -\sum_k\left(\eta_k\, c\,\sigma_{p,k}(E - B(T(e_k)))\right) - E\nabla\cdot\vec{v} + S\,,$$

$$\frac{1}{3}\nabla E = -\sum_k \eta_k\frac{\sigma_{r,k}}{c}\vec{F}\,, \quad c\mathcal{A}E - \mathcal{B}\vec{n}\cdot\vec{F} = \mathcal{C} \quad \text{on } \partial\Omega\,.$$

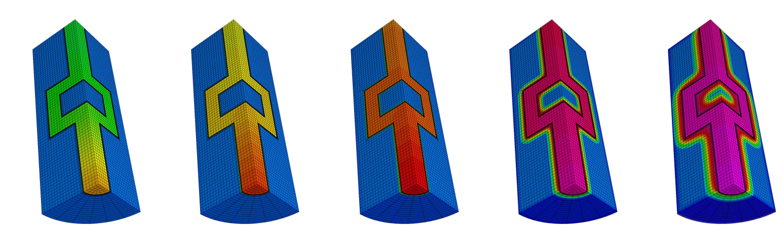
Our discretization in space uses high-order H^1, L^2 and $H(div)$ spaces. We define a generic implicit time step, $k = \mathcal{F}(y^n + \Delta t k)$; $k = (\ldots k_{e_k}\ldots, k_E)$ and use Newton's method to solve the resulting non-linear, implicit system: $k^n = k^{n-1} - [\partial\mathcal{N}(k^{n-1})]^{-1}\mathcal{N}(k^{n-1})$; $k = (\ldots k_{e_k}\ldots, k_E, \vec{F})$.

$$\partial\mathcal{N}(k) = \begin{bmatrix} \ddots & & \mathbf{0} & \vdots & \vdots \\ & L_{\rho_k} + \partial H_k & & -c\Delta t L_{\sigma_k} & 0 \\ \mathbf{0} & & \ddots & \vdots & \vdots \\ \ldots & -\partial H_k & \ldots & L + c\Delta t\sum_k L_{\sigma_k} & D \\ \ldots & 0 & \ldots & \frac{1}{3}\Delta t D^T & \frac{1}{c}R_\sigma + \frac{1}{3}R_n \end{bmatrix}$$

Schur complements (elimination) lead to a global $H(div)$ system for $\vec{F}$. Back-substitution is done by solving local L^2 problems.



Convergence rates for a manufactured smooth solution (left) and profile of the smooth radiation energy (right). Optimal rates are obtained on structured and unstructured meshes for different FE spaces, in both thin ($\sigma = 4$) and thick ($\sigma = 4e^4$) regimes.



Propagation of a radiation field in a pipe with complex shape and discontinuities in opacity. We consider a pipe with a very thin ($\sigma_a = 0.2$) material surrounded by very thick ($\sigma_a = 200.0$) material on the outside. A heating source is located at the bottom of the thin material. This is a Q_2Q_1 simulation with RT_1 radiation flux.

Conclusions and future work

This work allows us to remap arbitrary high-order spaces and run more challenging multi-material problems.We continue work on radiation hydrodynamics and *synchronized* FCT remap.

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