New Developments in Particle-Based Method for Blast Simulation of Explosives

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Outline of the talk

- Problem statement
- Kinematic Analysis of convected particle domain interpolation method (CPDI)
- **Multi Point Query Interpolator** (MPQ)
- Conclusions
Kinematics: Motivation

Simple 1D detonation simulation in Uintah software showed that particles that have been converted from solid to gas have very different values of F depending on the interpolation scheme used.

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GIMP
CPDI
Frozen CPDI
F Frozen CPDI, Cent. Diff
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Picture by Professor Guilkey
Kinematics: Motivation

Picture provided by David Austin
1D Analysis of Deformation Gradient

- Central difference

\[ F_{p}^{n+1} = F_{p}^{n} + \frac{\Delta t}{8r_0} \left[ \left( S_{i+1}(c_3) + S_{i+1}(c_4) \right) v_{i+1}^{n+1} + \left( S_{i}(c_3) + S_{i}(c_4) - S_{i}(c_1) - S_{i}(c_2) \right) v_{i}^{n+1} \right] \]

\[-\frac{\Delta t}{8r_0} \left( S_{i-1}(c_1) + S_{i+1}(c_2) \right) v_{i-1}^{n+1} \]

- CPDI

\[ F_{p}^{n+1} = F_{p}^{n} + \frac{\Delta t}{2r_0} \left[ S_{i+1}(c_3) v_{i+1}^{n+1} + \left( S_{i}(c_3) - S_{i}(c_2) \right) v_{i}^{n+1} - S_{i-1}(c_2) v_{i+1}^{n+1} \right] \]
Kinematics: Problem statement

• Current algorithms for updating the deformation gradient produce results that are often grossly inconsistent with the update of particle positions.
  • Problems involving very large and rapidly changing velocity gradients.
  • Implementation of Boundary conditions.
Large and rapidly changing velocity gradients

Real displacement

SPQ

Proposed MPQ
Validation: Method of manufactured solutions

- Verification of a numerical solver for some PDE.
- You manufacture an arbitrary solution for the PDE.
- The solution is substitute back into the PDE along with consistent initial and boundary conditions to determine analytically a forcing function.
- This forcing function reproduces exactly the manufactured solution.
- The forcing function is used in the numerical solver and the solution is compared with the manufactured solution.
Validation: 1D Adiabatic Gas Expansion

• Time varying constructed displacement field

\[ u = \beta t X \quad x = X + u \]

• Deformation gradient, acceleration and velocity

\[ F = \frac{\partial x}{\partial X} = 1 + \beta t \quad a = \ddot{u} = 0 \quad v = \frac{\partial x}{\partial t} = \beta X \]

• Governing equation and constitutive model

\[ -\frac{\partial P}{\partial x} + \rho b = \rho a \quad P = P_0 (F)^{-\gamma} - P_{ATM} \]

• Body forces

\[ b = \frac{1}{\rho \partial x} \frac{\partial P}{\partial x} = 0 \]
Analysis of SPQ

\[ m_i^0 a_i^0 = f_{\text{ext}}^0 + f_{\text{int}}^0 = 0 \Rightarrow a_i^0 = 0 \]

\[ v_i^1 = v_i^0 + a_i^0 \Delta t = v_i^0 \]

- Interpolation to the particles

\[ v_p^1 = v_p^0 + \sum_i \phi_{ip} a_i^0 \Delta t = v_p^0 = \text{MS} \]
Analysis of SPQ

- Interpolation to the particles in boundary cells

\[ \nabla v_{p1}^1 = \nabla v_{p2}^1 = \nabla v_{p5}^1 = \nabla v_{p6}^1 = \frac{5}{8} \beta \neq MS = \beta \]

Error of 37.5%

- Interpolation to the particles in inner cell

\[ \nabla v_{p3}^1 = \nabla v_{p4}^1 = \beta \neq MS = \beta \]

No Error
Analysis of SPQ

\[ \nabla v_{p}^{n+1} = \sum_{i} \nabla \phi_{ip} v_{i}^{n+1} \]

Lack of Symmetry in Boundary Cells

\[ F_{p}^{n+1} = (1 + \nabla v_{p}^{n+1} \Delta t)F_{p}^{n} = (1 + \nabla v_{p}^{n+1} \Delta t)(1 + \nabla v_{p}^{n} \Delta t)(1 + \nabla v_{p}^{1} \Delta t)F_{p}^{0} \]

- Update of stresses \( \sigma \) depends on updates of \( F \).

\[ \sigma = P_0 F - P_{ATM} \]
Analysis of SPQ

Deformation gradient at time 0.005

50000 times steps

β = 10000
Analysis of SPQ

Stress in particles at time 0.005

50000 times steps

\[ \beta = 10000 \]
Analysis of SPQ

Velocity at particles center at time 0.005

50000 times steps

SPQ
Manufacturesd Solution
Analysis of SPQ

Current position at time 0.005

50000 times steps

- SPQ
- Manufactured Solution
Analysis of SPQ

Aceleration at particles at time 0.0049999

49999 times steps

Acceleration

0

-2

-4

-6

-8

0.5

1

1.5

2

X0

Particle corners
Particle center
Analysis of SPQ

- Updates of position and velocity of particles are not consistent with updates of deformation gradients.

\[ v_{p}^{n+1} = v_{p}^{n} + \sum_{i} \phi_{ip} a_{i}^{n} \Delta t \]

\[ x_{p}^{n+1} = x_{p}^{n} + \sum_{i} \phi_{ip} v_{i}^{n+1} \Delta t \]

\[ a_{i}^{n} = \frac{f_{ext_{i}}^{n} + f_{int_{i}}^{n}}{m_{i}^{n}} \]

\[ f_{int_{i}}^{n} = -\sum_{p} \nabla \phi_{ip} \sigma_{p}^{n} V_{p} \]

\[ F_{p}^{n+1} = (1 + \nabla v_{p}^{n+1} \Delta t) F_{p}^{n} = (1 + \nabla v_{p}^{n+1} \Delta t)(1 + \nabla v_{p}^{n} \Delta t)...(1 + \nabla v_{p}^{1} \Delta t) F_{p}^{0} \]
Effects of increasing the velocity gradient

Deformation gradient at time 0.00125

12500 times steps

\[ \beta = 10^6 \]
Effects of increasing the velocity gradient

Velocity at particles center at time 0.00125

12500 times steps

$\beta = 10^6$
Effects of increasing the velocity gradient

Current position at time 0.00125

12500 times steps

$\beta = 10^6$
Effects of increasing the velocity gradient

Stress in particles at time 0.00125

- **SPQ**
- **Manufactured Solution**

12500 times steps

\[ \beta = 10^6 \]
Discrepancies between velocity, position and deformation gradient of particles

• Condition for not separation of adjacent domains of particles

\[ x_{p+1}^n - x_p^n = \left( F_{p+1}^n + F_p^n \right) r_0 \]
Discrepancies between velocity, position and deformation gradient of particles

- At large velocity gradients, domains of particles start separating from each other?
  \[ x_{p+1}^n - x_p^n \neq (F_{p+1}^n + F_p^n) r_0 \]

\[
\left( x_{p+1}^n - x_p^n \right)_\text{true} + \delta_{x\text{ error}} = \left( F_{p+1}^n + F_p^n \right)_\text{true} r_0 + \delta_{F\text{ error}}
\]

\[
\delta_{x\text{ error}} = \delta_{F\text{ error}}
\]
Effects of increasing the velocity gradient

Deformed domain at time = 0.00125
Multi Point Query Method (MPQ)

Interpolate position and velocity from nodes to particle’s corners

\[
\phi_i v_{i}^{n+1} = n_{pc}^{n+1}
\]

\[
x_{pc}^{n+1} = x_{pc}^{n} + v_{pc}^{n+1} \Delta t
\]
Algorithm of Multi Point Query (MPQ)

Update deformation gradient

$$F_{p}^{n+1} = \frac{2r^{n+1}}{2r_{0}}$$

2r

2r₀ Initial length of particle’s domain
Deformation gradient at time 0.00125

12500 times steps

\[ \beta = 10^6 \]
Velocity at particles corners at time 0.00125

- SPQ
- Manufactured Solution

12500 times steps

$\beta = 10^6$
Implementation of artificial cells

- Solve the lack of symmetry for $\nabla \phi_{ip}$

Time=0

Artificial Cell  Boundary Cell  Interior Cells

- Velocity of particles in the artificial cell are extrapolated from particles in the boundary cell at time 0
MPQ: Implemented Artificial Cells

Deformation gradient at time 0.00125

- MPQ
- Manufactured Solution
SPQ: Artificial cells implemented

Deformation gradient at time 0.00125

12500 times steps

\( \beta = 10^6 \)
MPQ: Artificial cells implemented

Deformation gradient at time 0.00125

\[ 2r_0 = 1 \]

12500 times steps

\[ \beta = 10^6 \]
Kinematics: Conclusions

- **SPQ:**
  - Error in the update of deformation gradient:
    - Introduce through \( \nabla \phi_{ip} \)
    - Products of errors over time.
  - Update of stress through constitutive model:
    Depends on sensitivity to deformation gradient.

- **MPM:**
  - Central difference scheme to update deformation gradient.
    - \( F \) is consistent with the Manufactured solution.
    - \( F \) shows no discrepancies with updates of position and velocity of particles.
    - Artificial cells
THANK YOU
Simulations: Deformation Gradient

Deformation gradient at the center of particles at time 0.0001

$F_{\text{Manufactured Solution}} = 1 + \beta t$

$F_{\text{Boundary Particles}} = 1 + \frac{5}{8} \beta t$
Algorithm of Multi Point Query (MPQ)

Map velocity and mass from particles' center to nodes
Map internal and external forces from particle’s domain to nodes

\[
m_i^n = \sum_p \phi_{ip} m_p
\]

\[
v_i^n = \frac{\sum_p \phi_{ip} m_p v_p^n}{m_i^n}
\]
Algorithm of Multi Point Query (MPQ)

Solve for acceleration of nodes and update velocity of nodes

\[ a_i^n = \frac{f_i^{\text{int}} + f_i^{\text{ext}}}{m_i} \]

\[ v_i^{n+1} = v_i^n + a_i^n \Delta t \]
Algorithm of Multi Point Query (MPQ)

Update position and velocity of particle center (same as SPQ)
Update stress using constitutive model

\[ v_p^{n+1} = v_p^n + \sum_i \phi_{ip} a_i^n \Delta t \]

\[ x_p^{n+1} = x_p^n + \sum_i \phi_{ip} v_i^{n+1} \Delta t \]
Simulations: Deformation Gradient

Deformation gradient at the center of particles at time 0.0001

- MPQ
- Manufactured Solution
Simulations: Velocity at the center of particles

Velocity at center of particles at time 0.0001
Simulations: Position at the center of particles

Current position at the center of particles at time 0.0001

- **MPQ**
- **Manufactured Solution**