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

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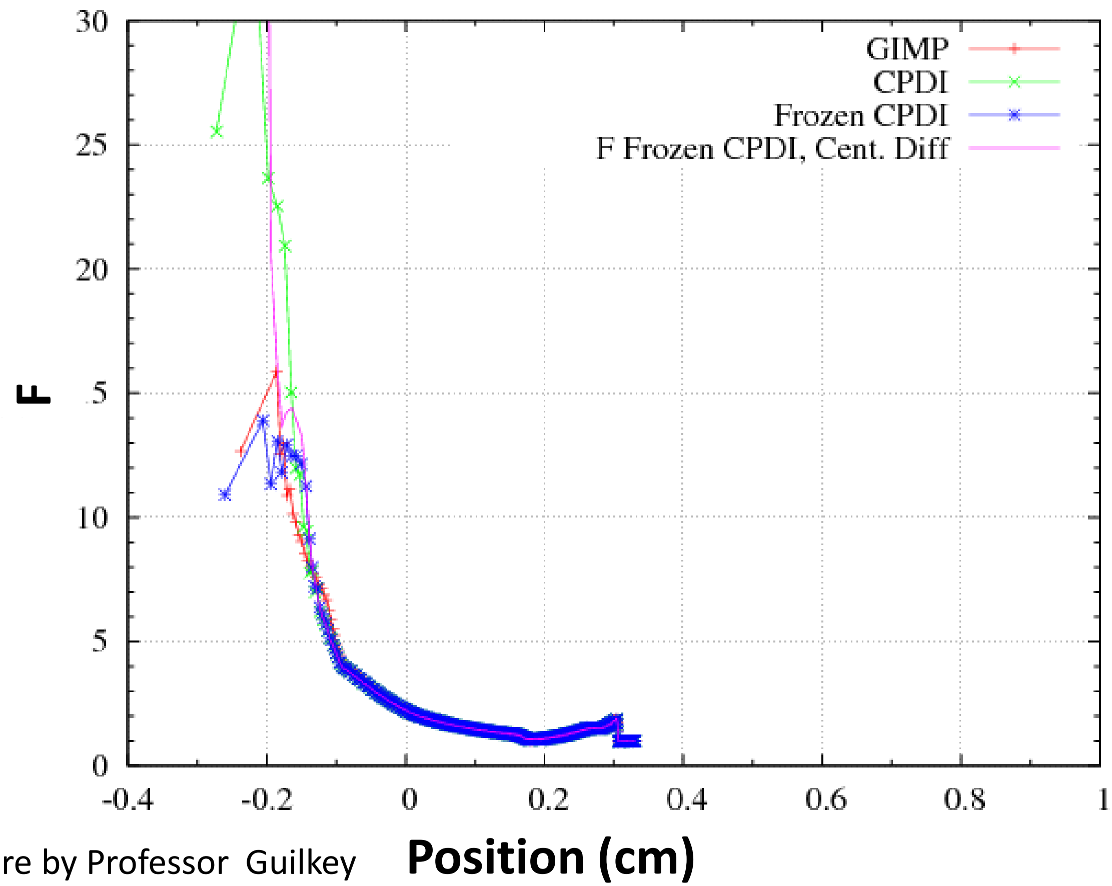
Outline of the talk

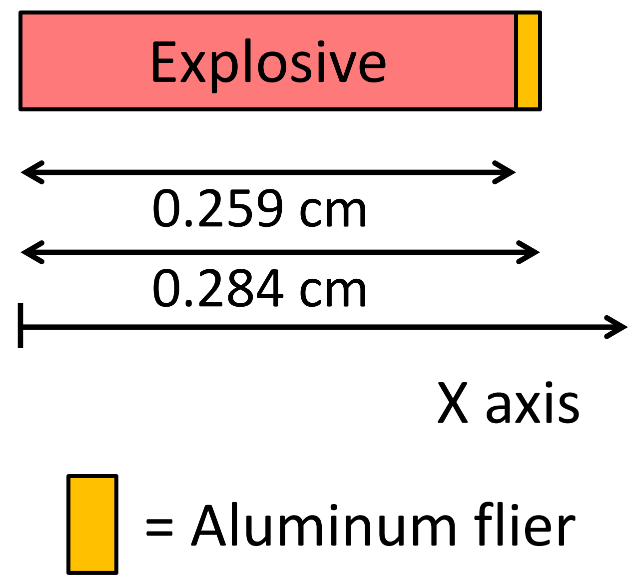
- Problem statement
- Kinematic Analysis of convected particle domain interpolation method (CPDI)
- **M**ulti **P**oint **Q**uery Interpolator (MPQ)
- Conclusions

Kinematics: Motivation

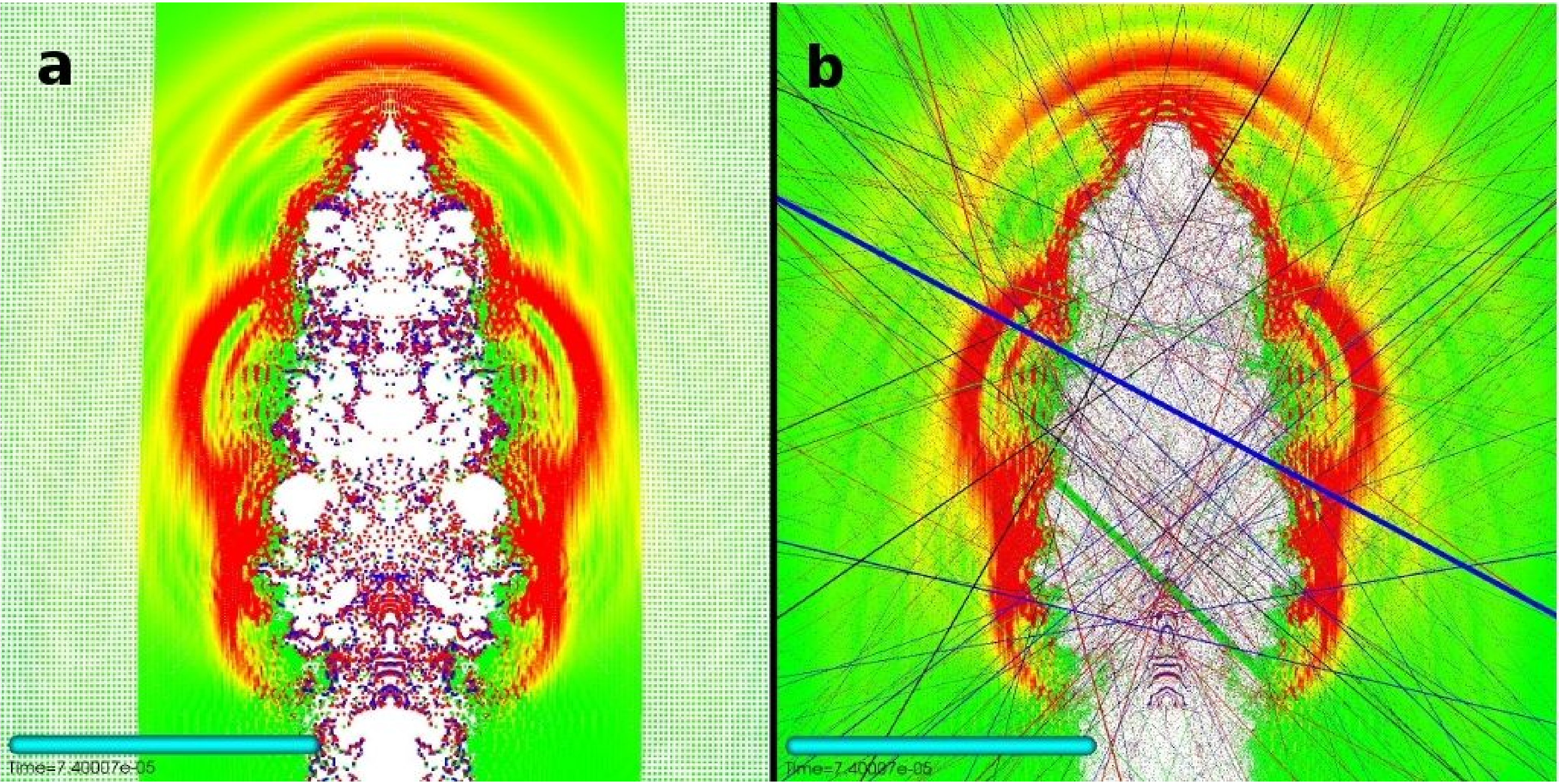
Simple 1D detonation simulation in Uintah software showed that particles that have been converted from solid to gas have very different values of F depending on the interpolation scheme used.



Picture by Professor Guilkey

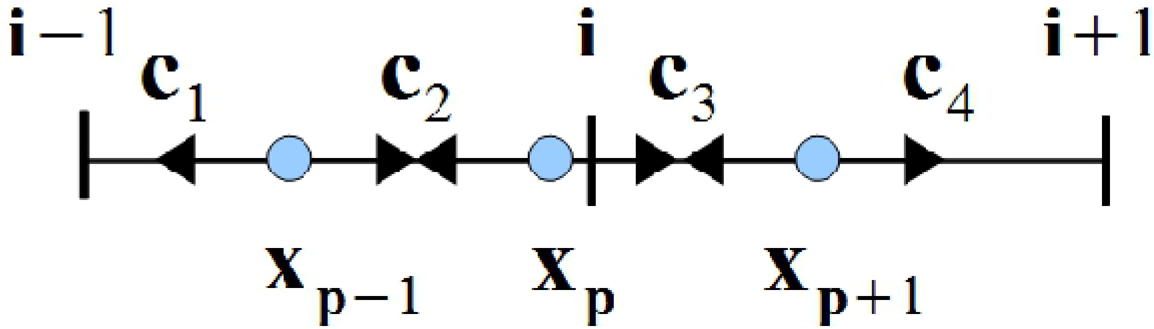


Kinematics: Motivation



Picture provided by David Austin

1D Analysis of Deformation Gradient



- Central difference

$$F_p^{n+1} = F_p^{n} + \frac{\Delta t}{8r_0}\Big[\big(S_{i+1}(c_3) + S_{i+1}(c_4)\big)v_{i+1}^{n+1} + \big(S_i(c_3) + S_i(c_4) - S_i(c_1) - S_i(c_2)\big)v_i^{n+1}\Big]$$

$$-\frac{\Delta t}{8r_0}\big(S_{i-1}(c_1) + S_{i+1}(c_2)\big)v_{i-1}^{n+1}$$

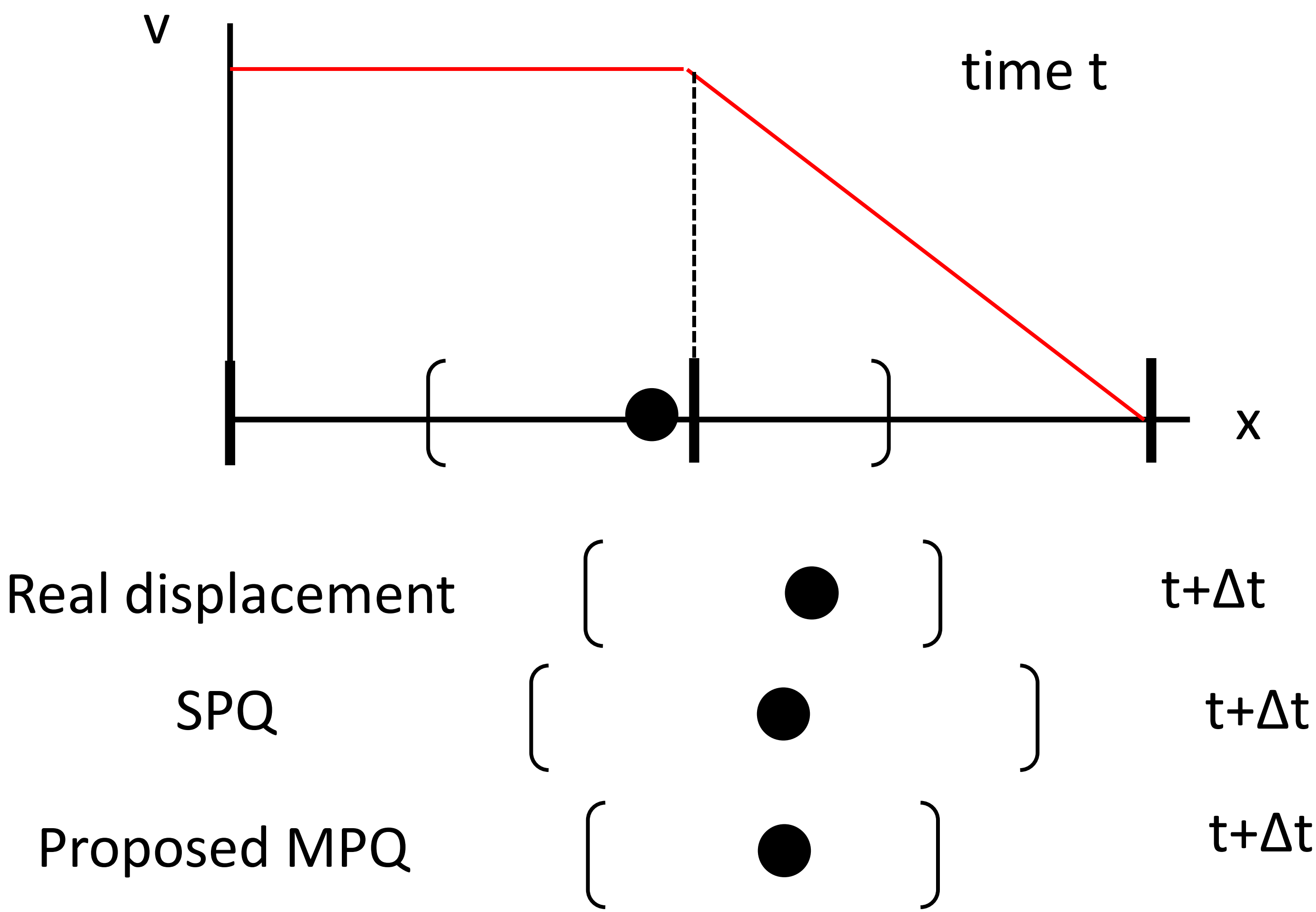
- CPDI

$$F_p^{n+1} = F_p^{n} + \frac{\Delta t}{2r_0}\Big[S_{i+1}(c_3)v_{i+1}^{n+1} + \big(S_i(c_3) - S_i(c_2)\big)v_i^{n+1} - S_{i-1}(c_2)v_{i+1}^{n+1}\Big]$$

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



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

$$u = \beta t X \qquad x = X + u$$

- Deformation gradient, acceleration and velocity

$$F = \frac{\partial x}{\partial X} = 1 + \beta t \qquad a = \ddot{u} = 0 \qquad v = \frac{\partial x}{\partial t} = \beta X$$

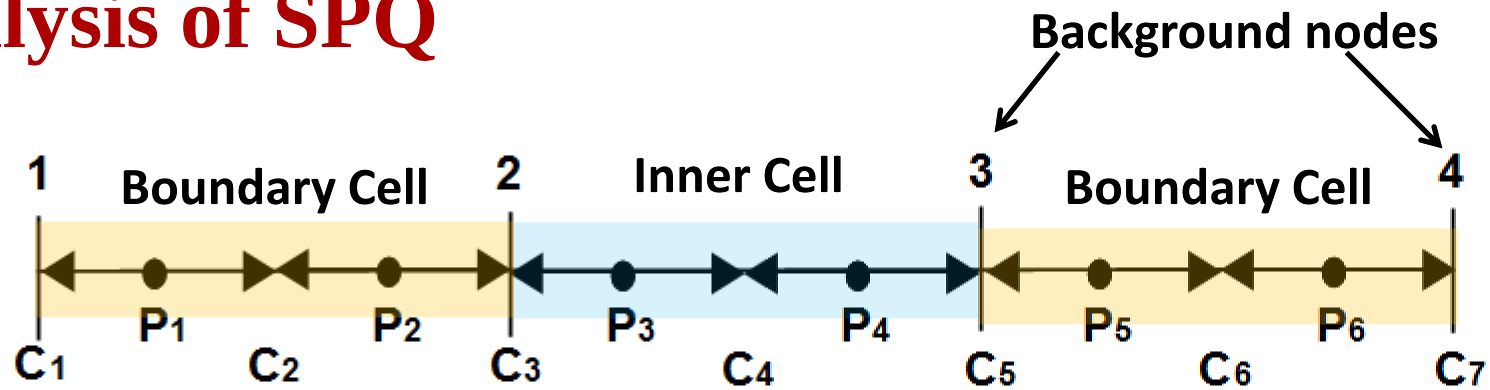
- Governing equation and constitutive model

$$-\frac{\partial P}{\partial x} + \rho b = \rho a \qquad P = P_0 \left(F \right)^{-\gamma} - P_{ATM}$$

- Body forces

$$b = \frac{1}{\rho} \frac{\partial P}{\partial x} = 0$$

Analysis of SPQ



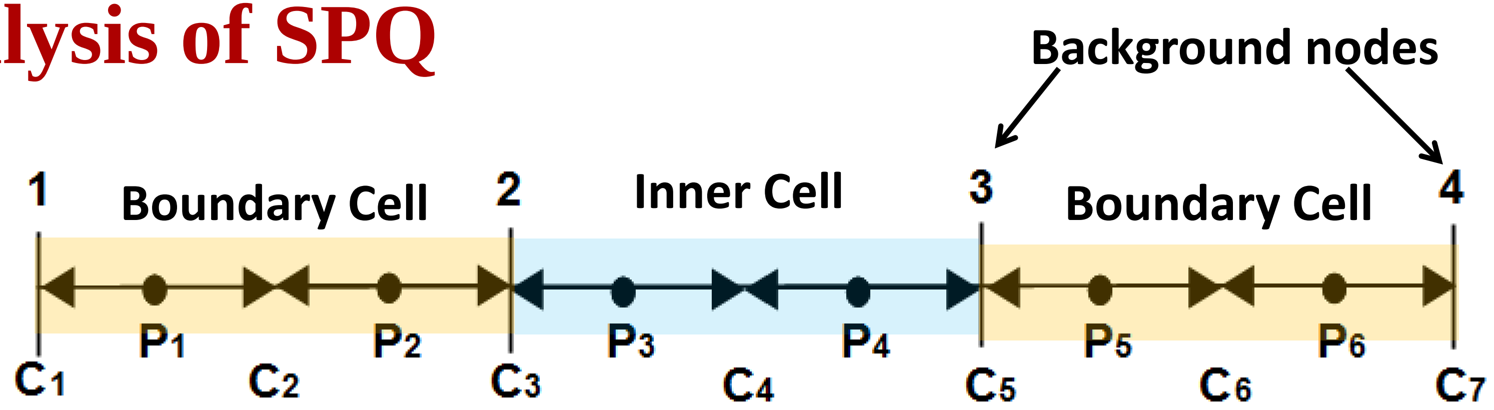
$$m_i^0 a_i^0 = f_{\mathrm{ext}_i}^0 + f_{\mathrm{int}_i}^0 = 0 \Rightarrow a_i^0 = 0$$

$$v_i^1 = v_i^0 + a_i^0 \Delta t = v_i^0$$

- **Interpolation to the particles**

$$v_p^1 = v_p^0 + \sum_i \phi_{ip} a_i^0 \Delta t = v_p^0 = \mathrm{MS}$$

Analysis of SPQ



- **Interpolation to the particles in boundary cells**

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

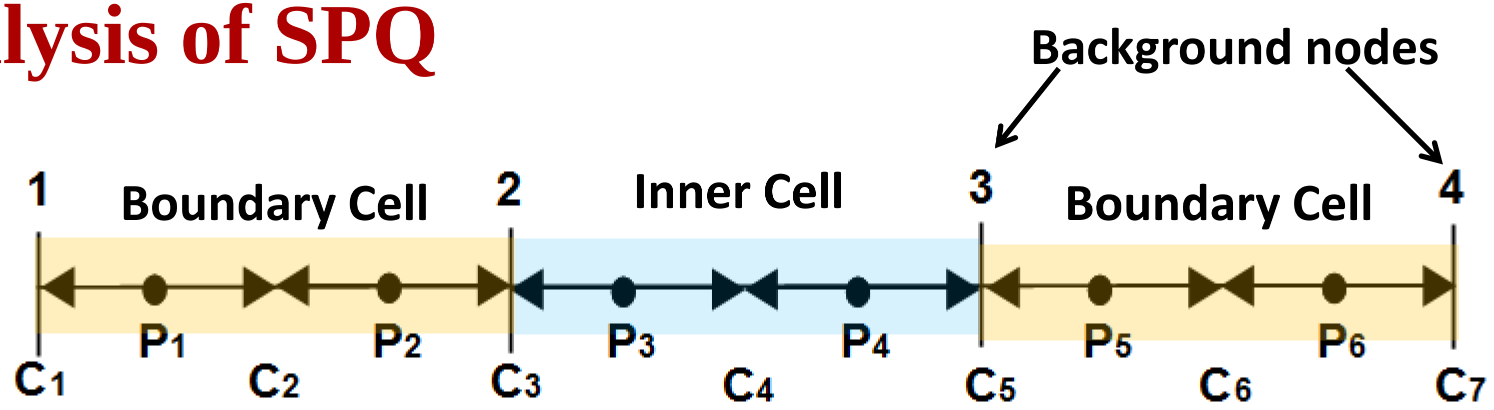
Error of 37.5%

- **Interpolation to the particles in inner cell**

$$\nabla v_{p3}^{1} = \nabla v_{p4}^{1} = \beta \neq \mathrm{MS}= \beta$$

No Error

Analysis of SPQ



$$\nabla v_p^{n+1} = \sum_i \nabla \phi_{ip} v_i^{n+1}$$

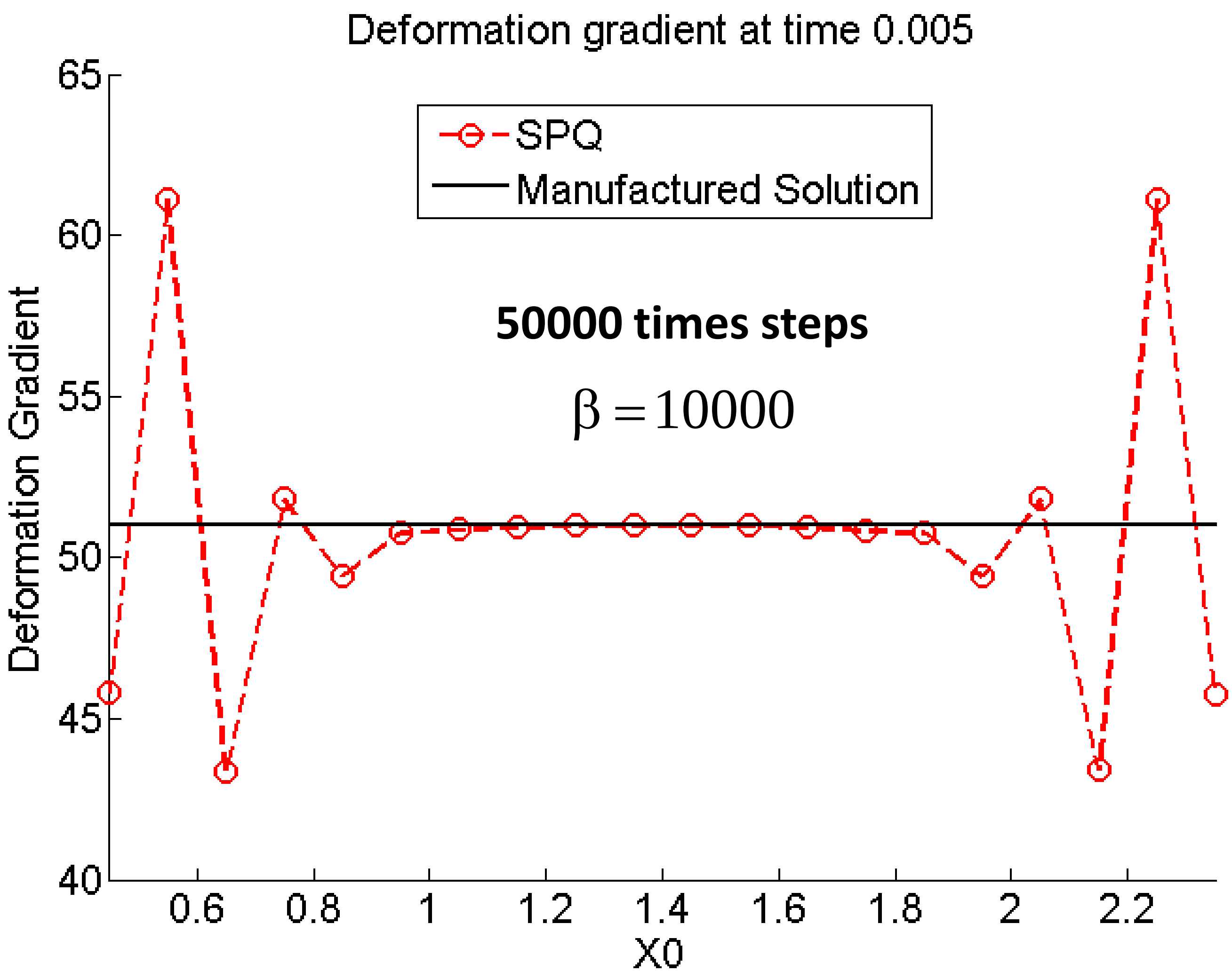
Lack of Symmetry in Boundary Cells

$$F_p^{n+1} = (1+\nabla v_p^{n+1}\Delta t)F_p^n = (1+\nabla v_p^{n+1}\Delta t)(1+\nabla v_p^n \Delta t)\ldots(1+\nabla v_p^1 \Delta t)\, F_p^0$$

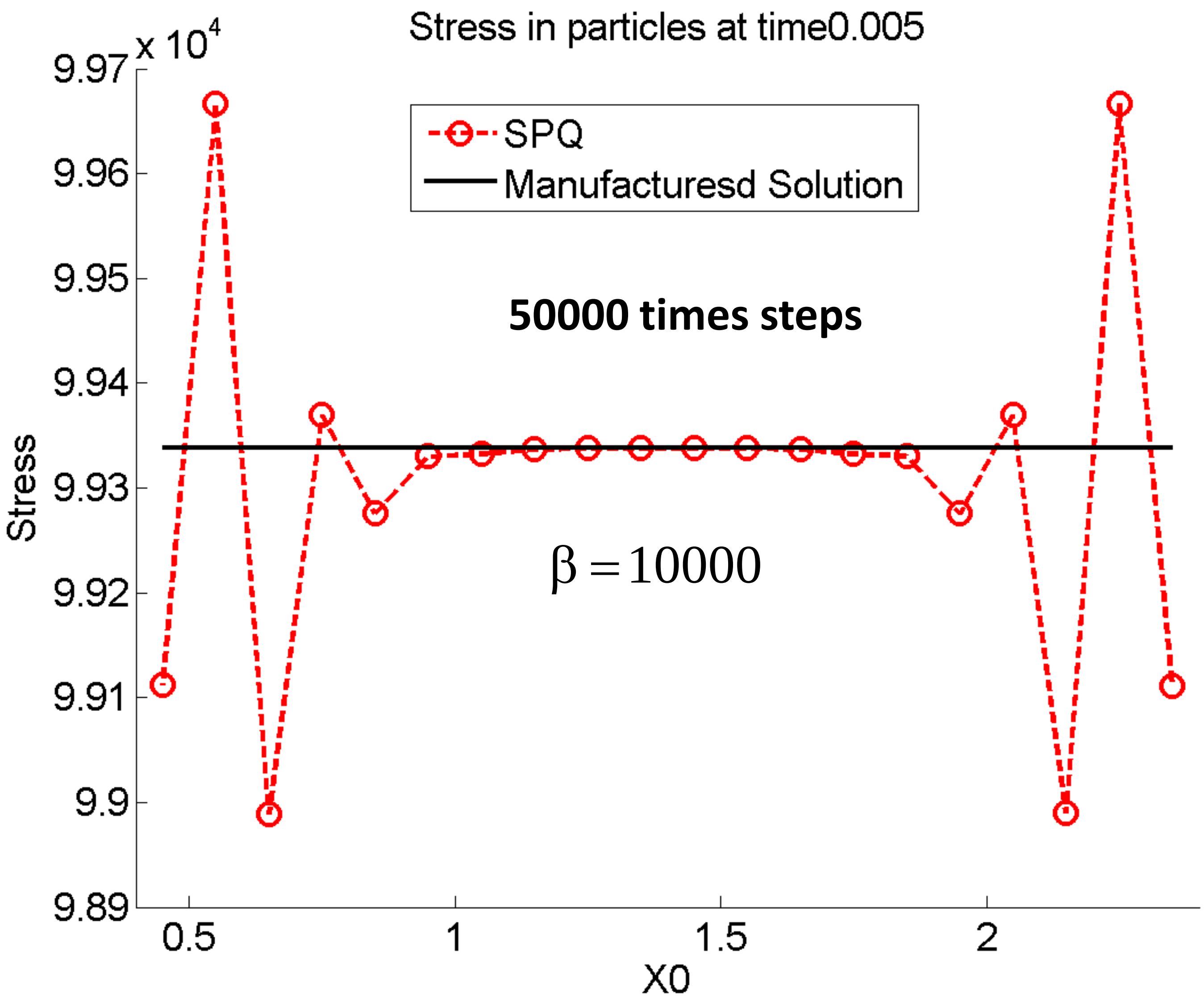
- Update of stresses σ depends on updates of F.

$$\sigma = P_0 F - P_{ATM}$$

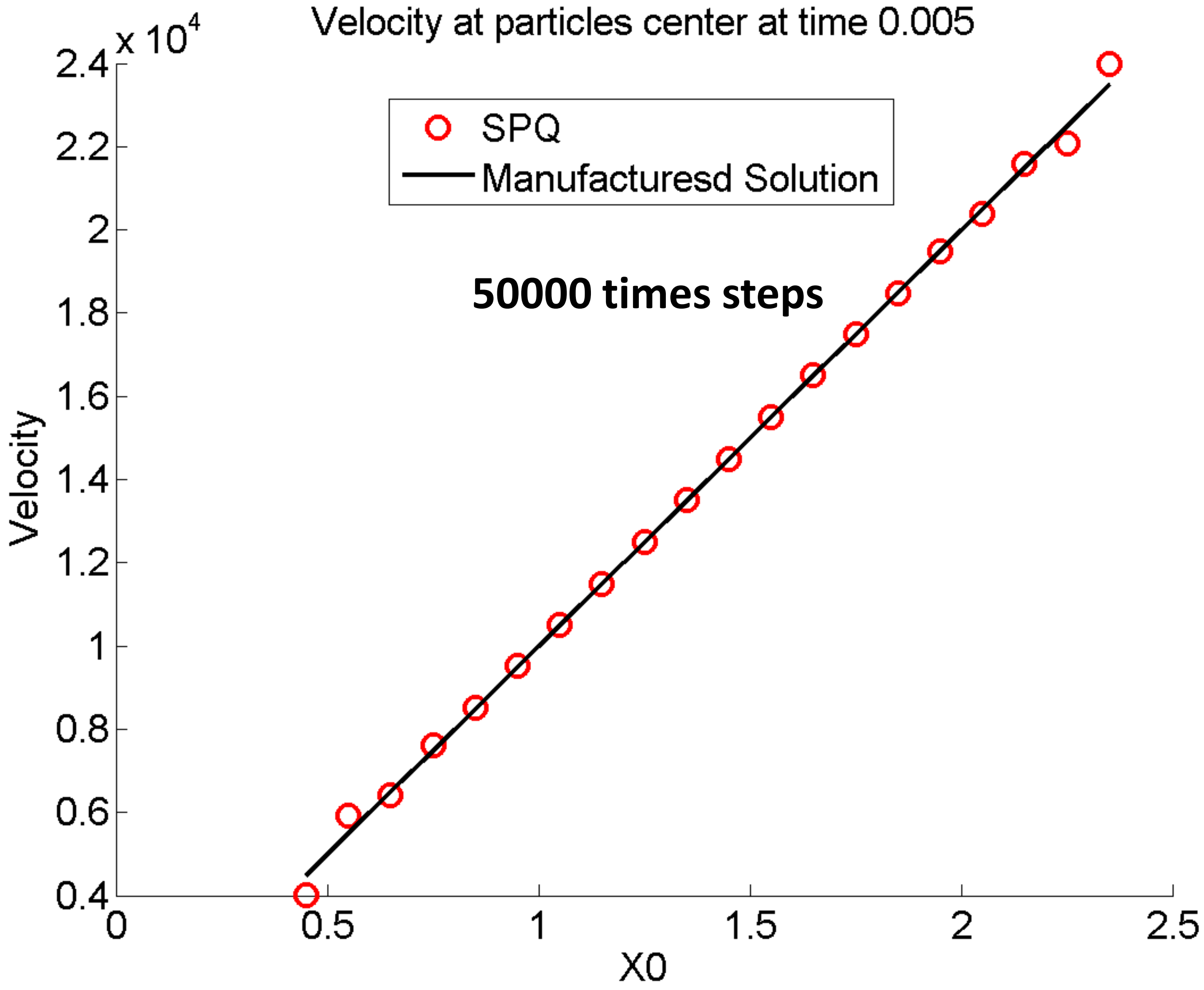
Analysis of SPQ



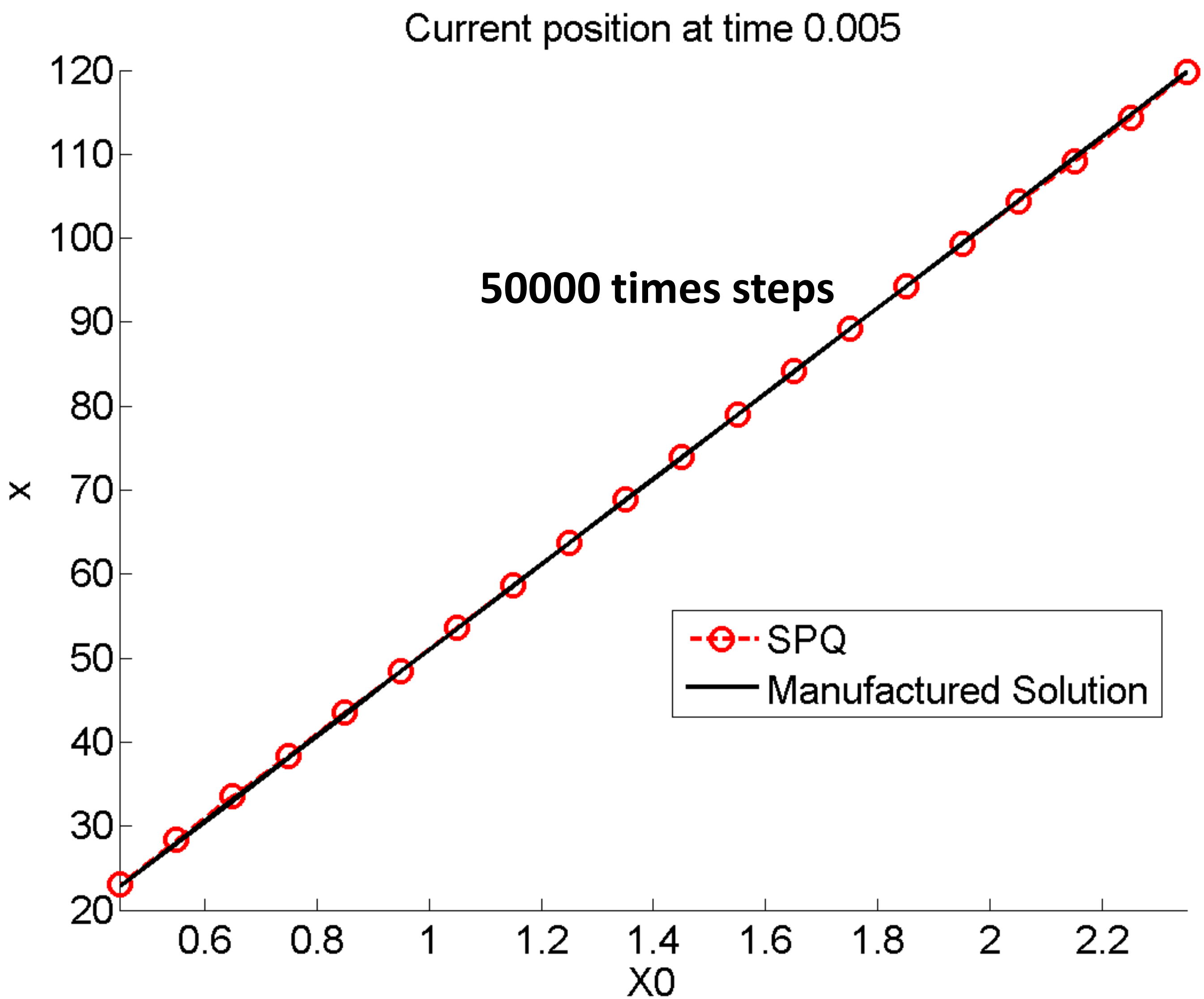
Analysis of SPQ



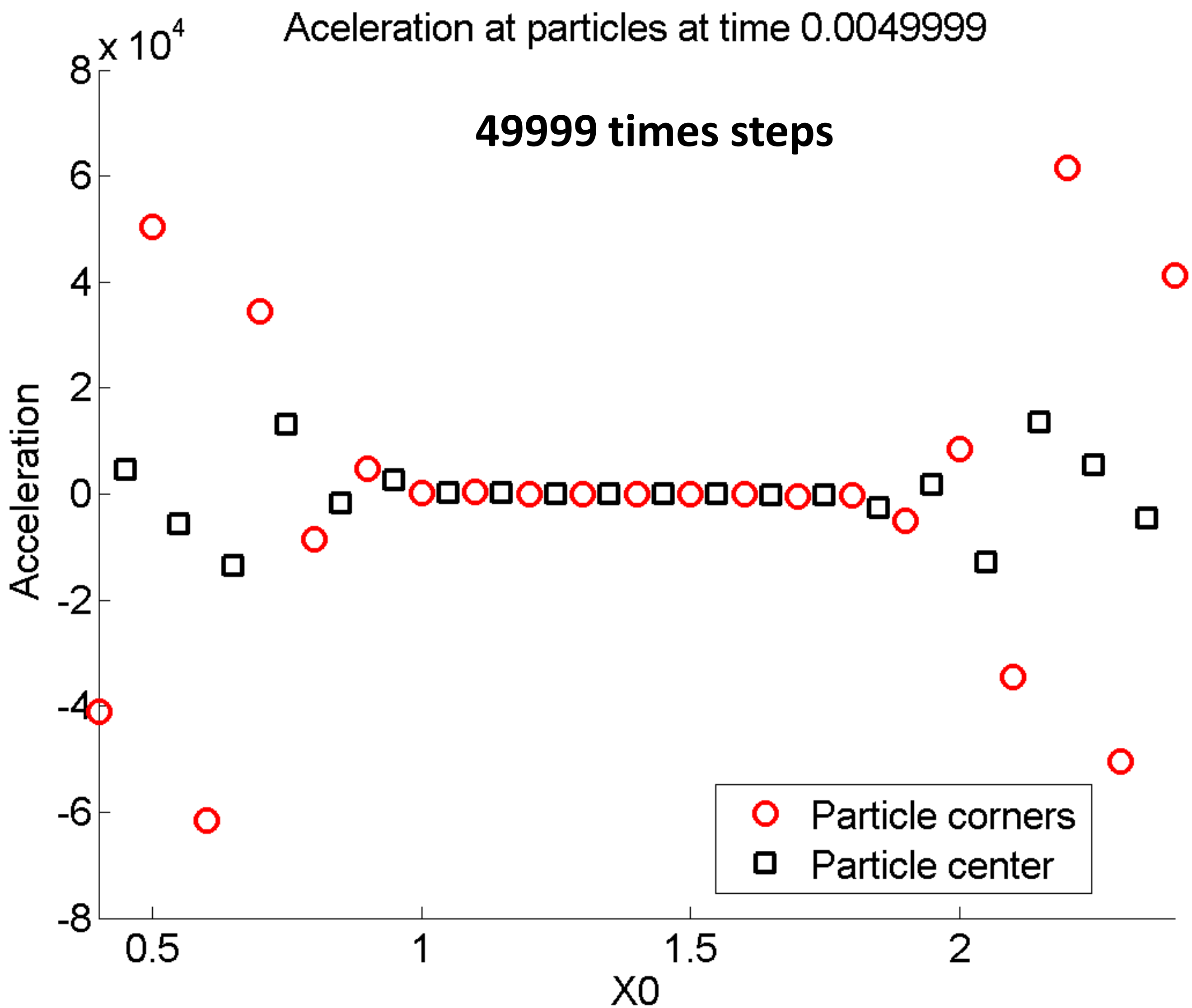
Analysis of SPQ



Analysis of SPQ



Analysis of SPQ



Analysis of SPQ

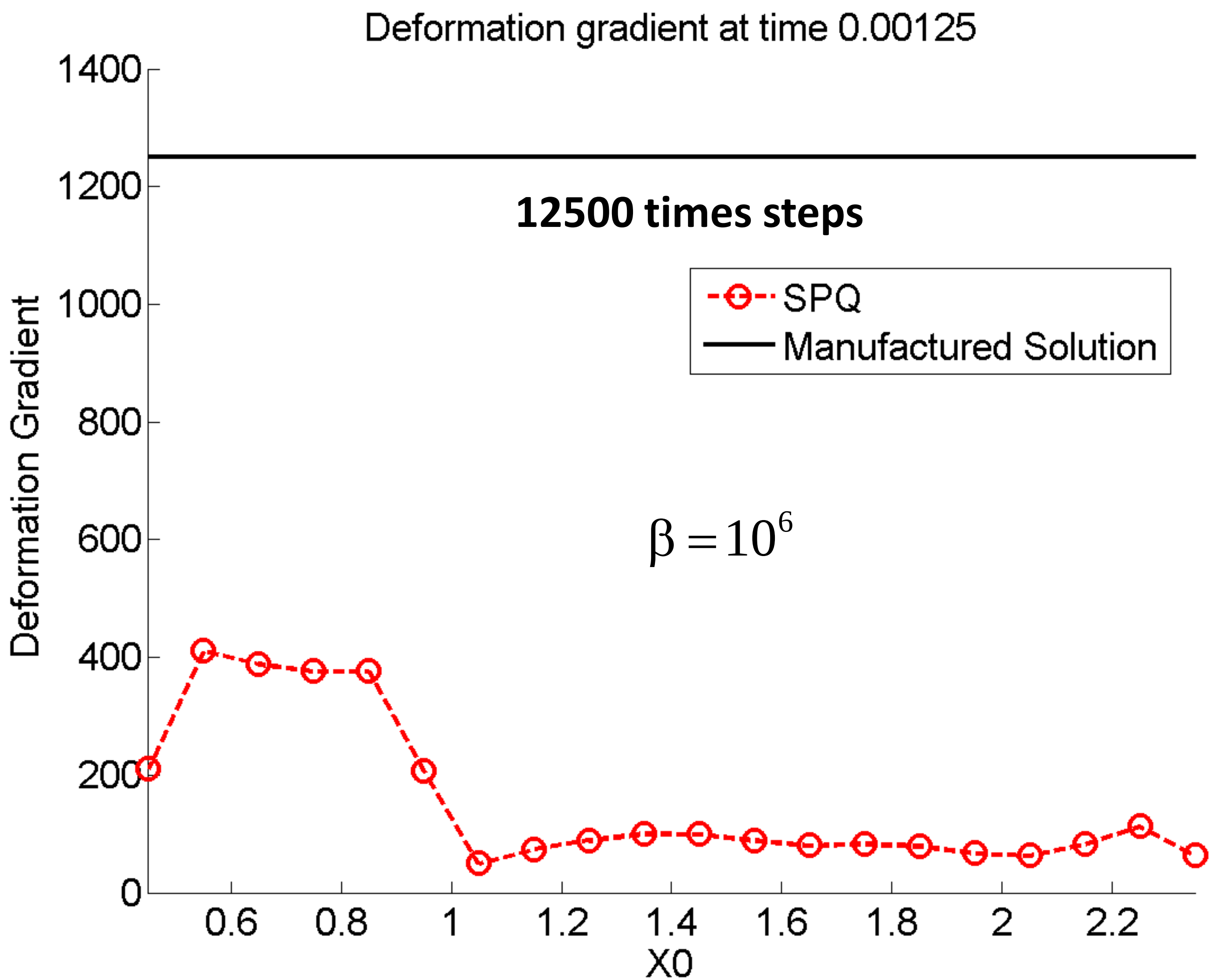
- **Updates of position and velocity of particles are not consistent with updates of deformation gradients.**

$$v_p^{n+1} = v_p^n + \sum_i \phi_{ip} a_i^n \Delta t \qquad x_p^{n+1} = x_p^n + \sum_i \phi_{ip} v_i^{n+1} \Delta t$$

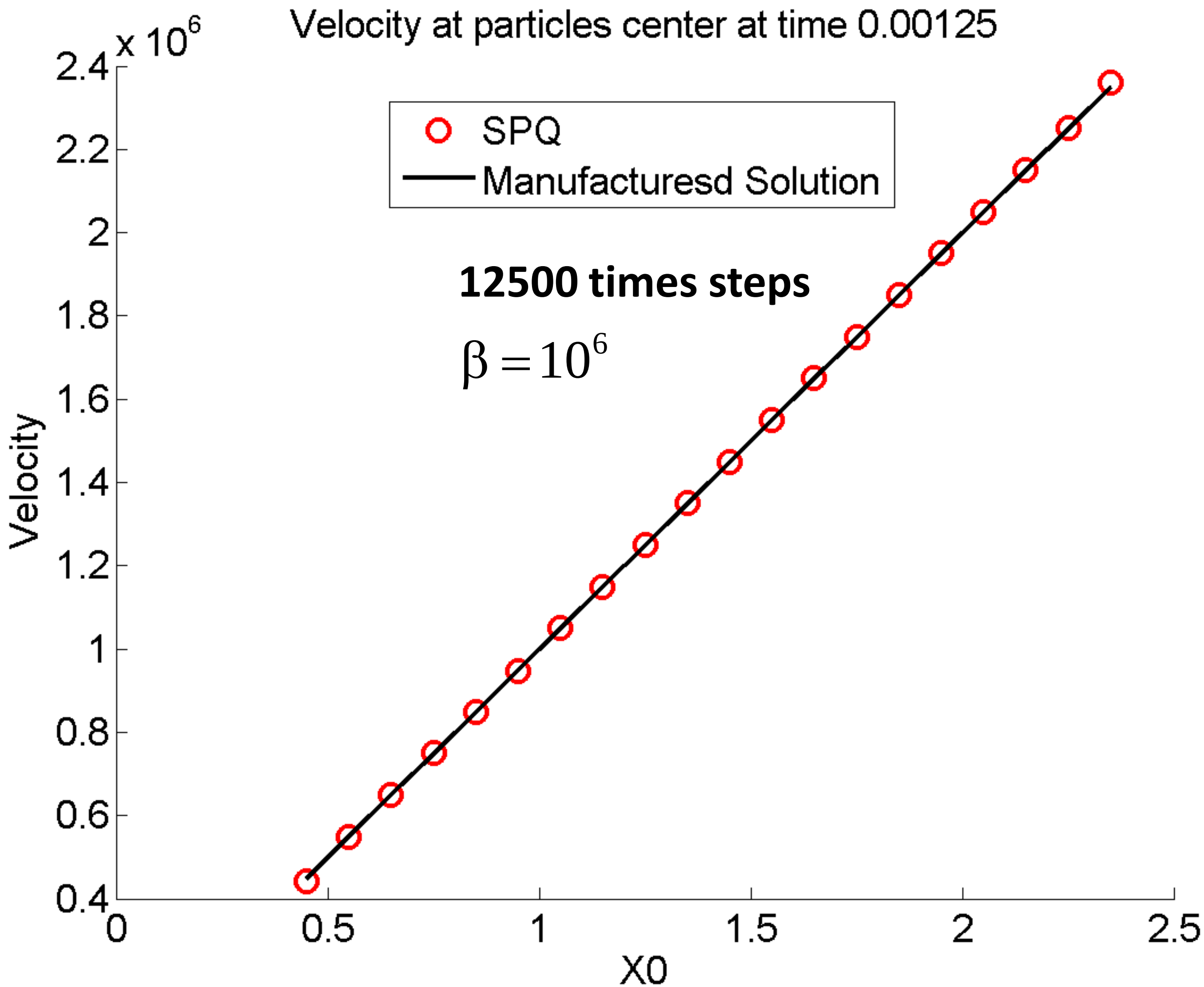
$$a_i^n = \frac{f_{ext_i}^n + f_{int_i}^n}{m_i^n} \qquad f_{int_i}^n = -\sum_p \nabla \phi_{ip} \sigma_p^n V_p$$

$$F_p^{n+1} = (1 + \nabla v_p^{n+1} \Delta t) F_p^n = (1 + \nabla v_p^{n+1} \Delta t)(1 + \nabla v_p^n \Delta t) \ldots (1 + \nabla v_p^1 \Delta t) F_p^0$$

Effects of increasing the velocity gradient



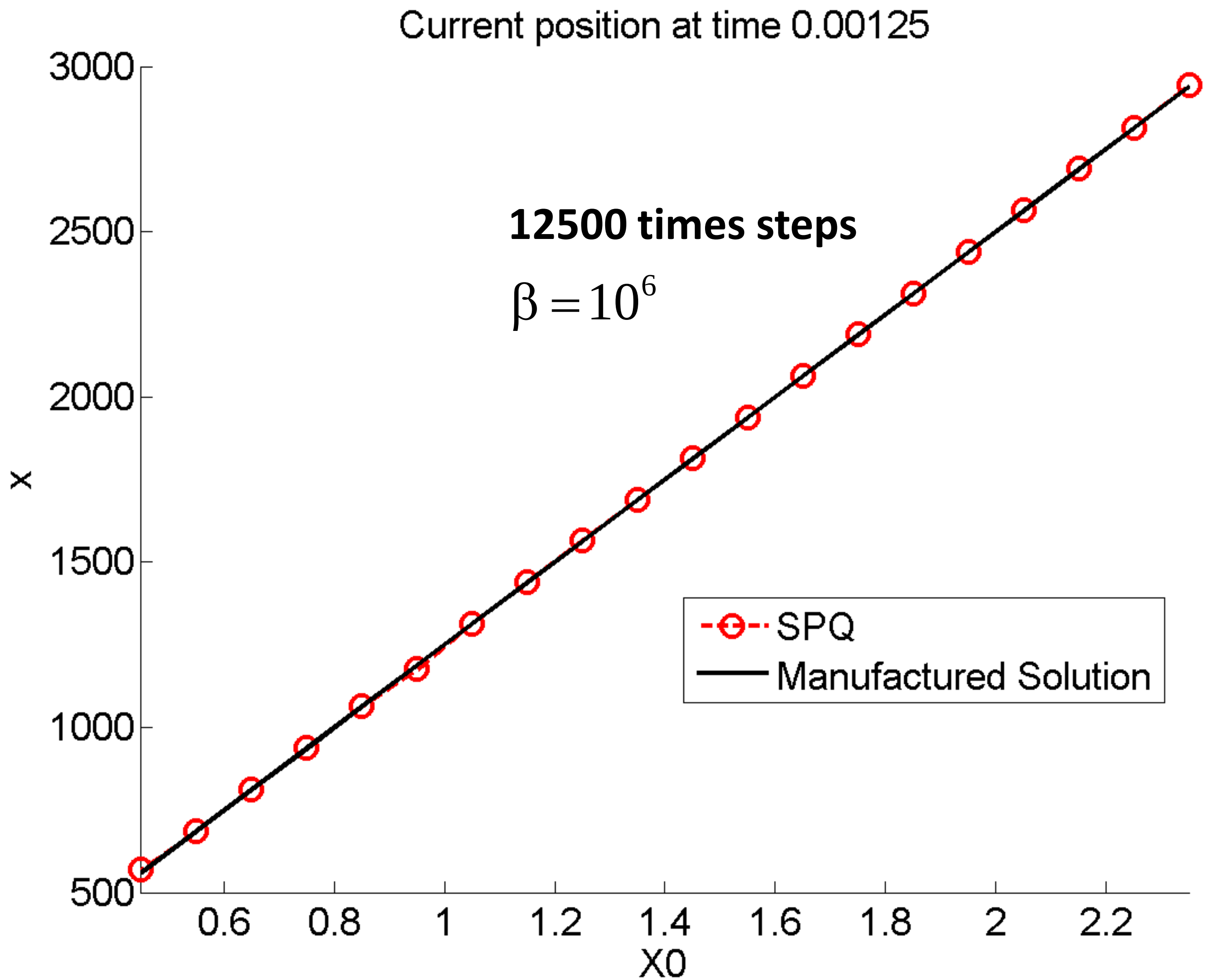
Effects of increasing the velocity gradient



12500 times steps

$\beta = 10^6$

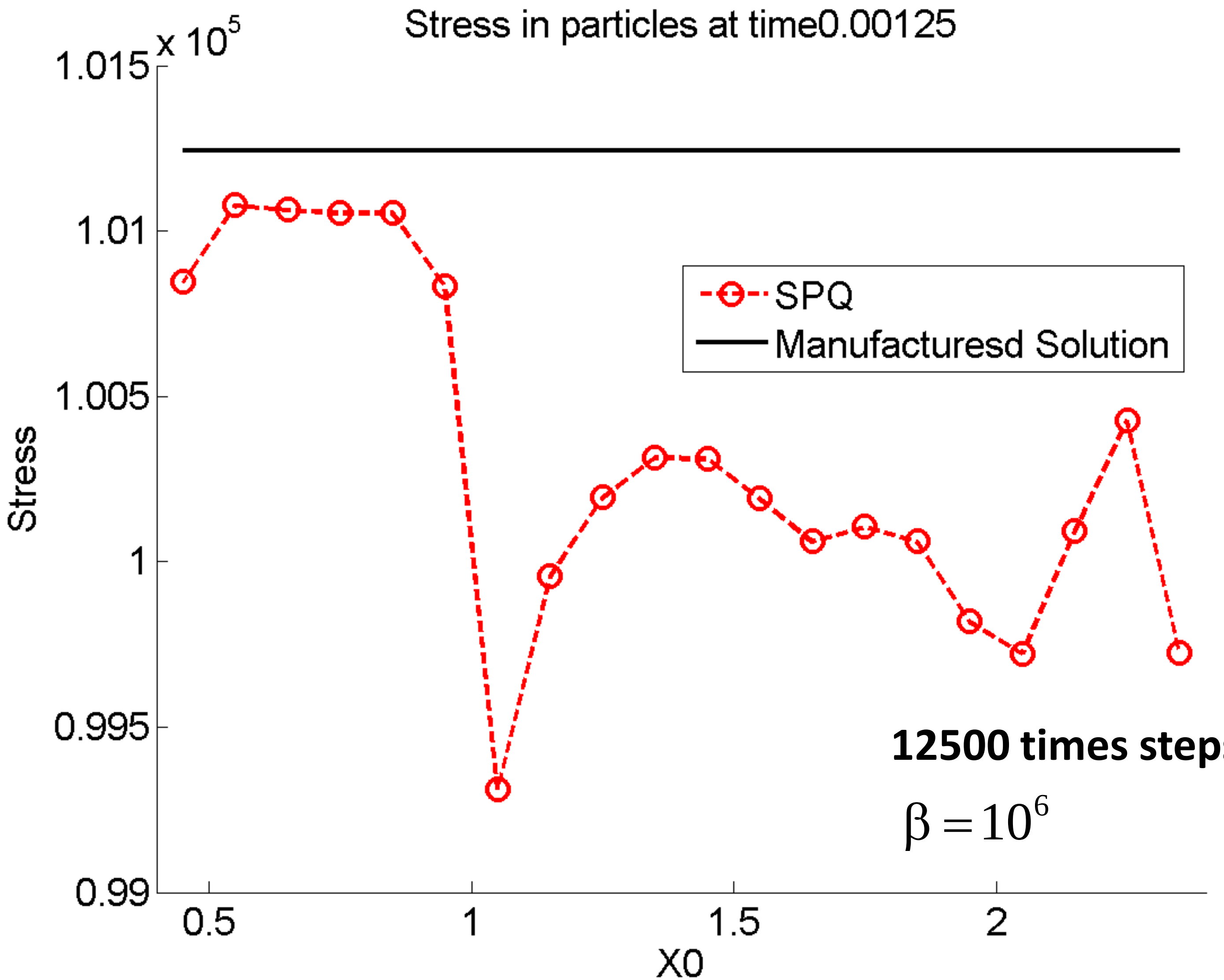
Effects of increasing the velocity gradient



12500 times steps

$\beta = 10^6$

Effects of increasing the velocity gradient



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

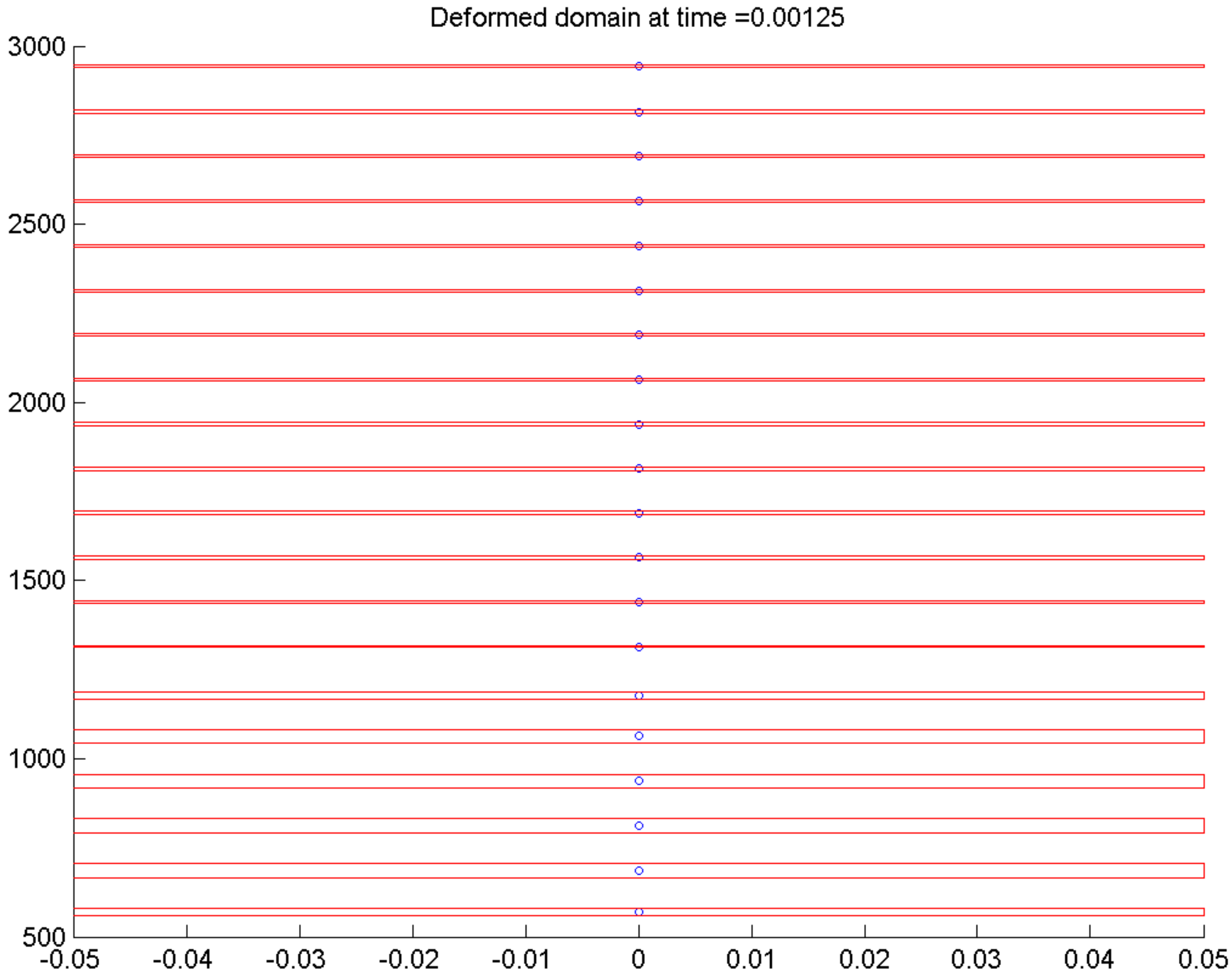
- At large velocity gradients, domains of particles start separating from each other?

$$x_{p+1}^{n} - x_{p}^{n} \neq \left(F_{p+1}^{n} + F_{p}^{n}\right) r_{0}$$

$$\left(x_{p+1}^{n} - x_{p}^{n}\right)_{\text{true}} + \delta_{x\ \text{error}} = \left(F_{p+1}^{n} + F_{p}^{n}\right)_{\text{true}} r_{0} + \delta_{F\ \text{error}}$$

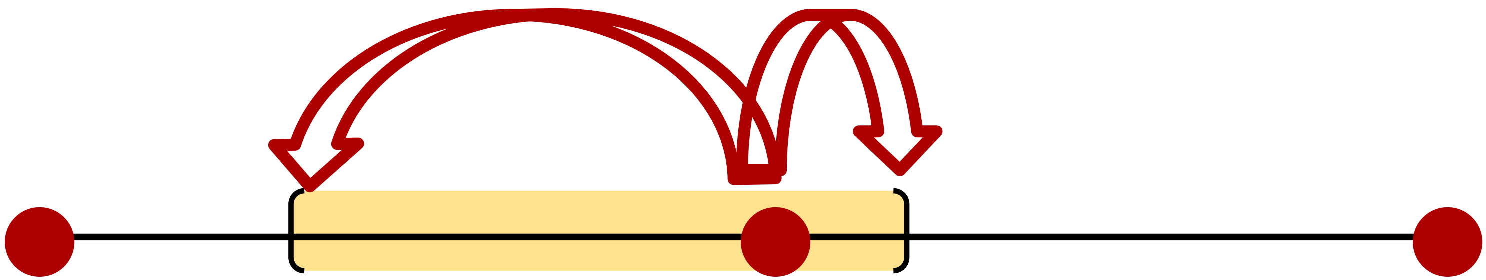
$$\delta_{x\ \text{error}} \stackrel{?}{=} \delta_{F\ \text{error}}$$

Effects of increasing the velocity gradient



Multi Point Query Method (MPQ)

Interpolate position and velocity from nodes to particle's corners



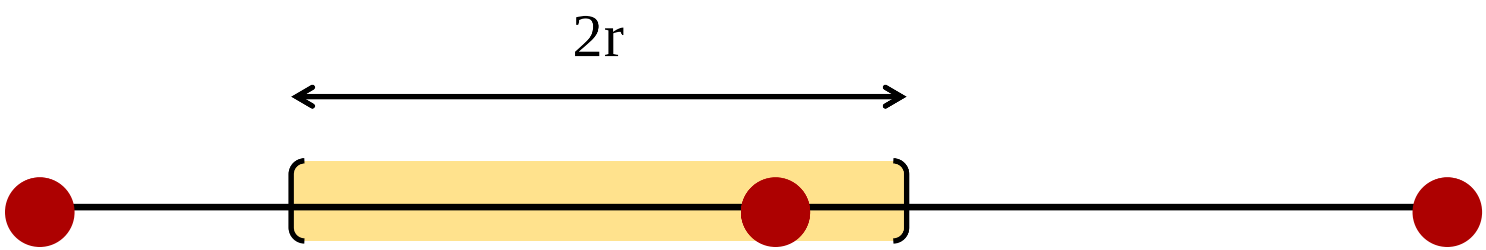
$$v_{pc}^{n+1} = \sum_i \phi_i v_i^{n+1}$$

$$x_{pc}^{n+1} = x_{pc}^{n} + v_{pc}^{n+1} \Delta t$$

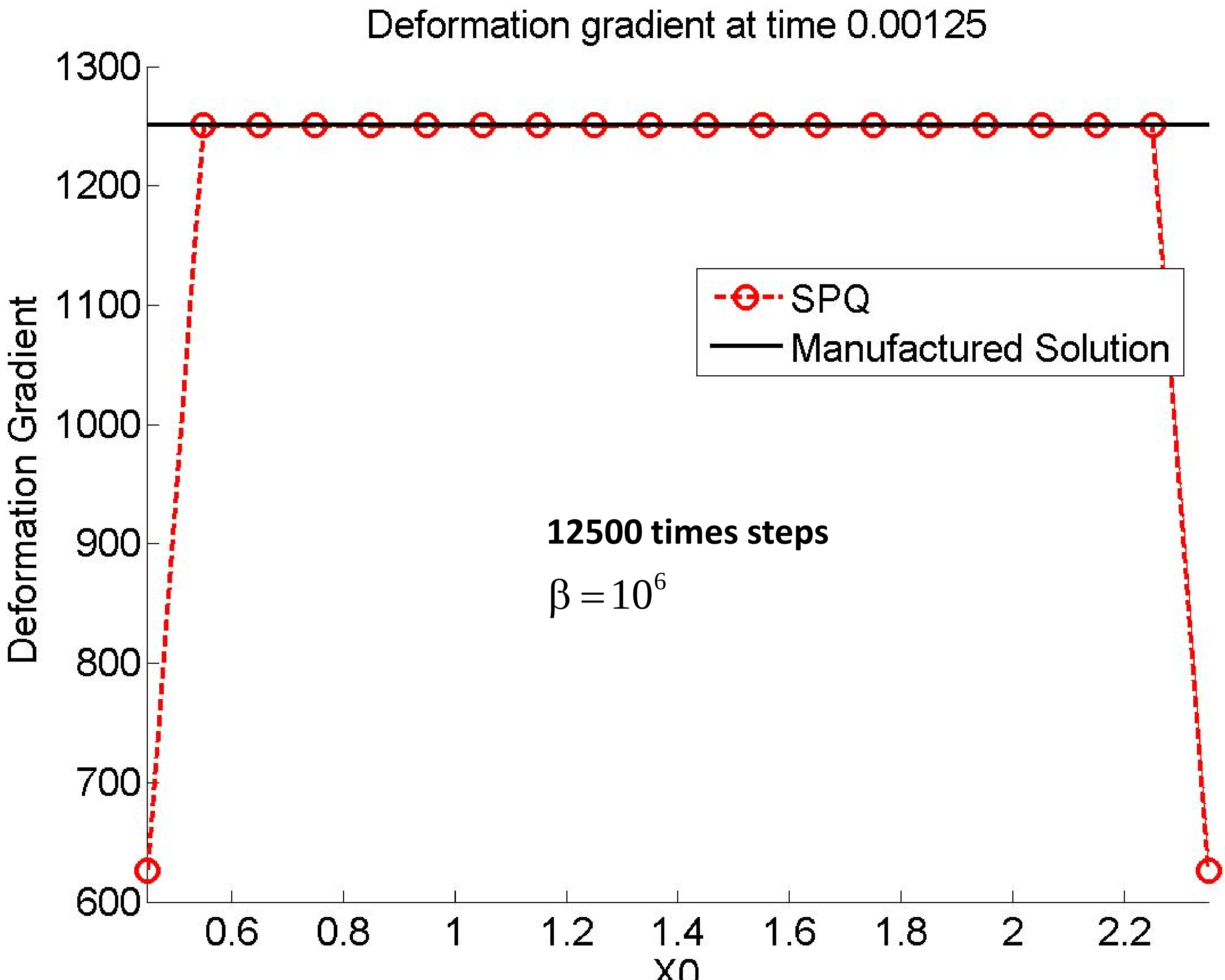
Algorithm of Multi Point Query (MPQ)

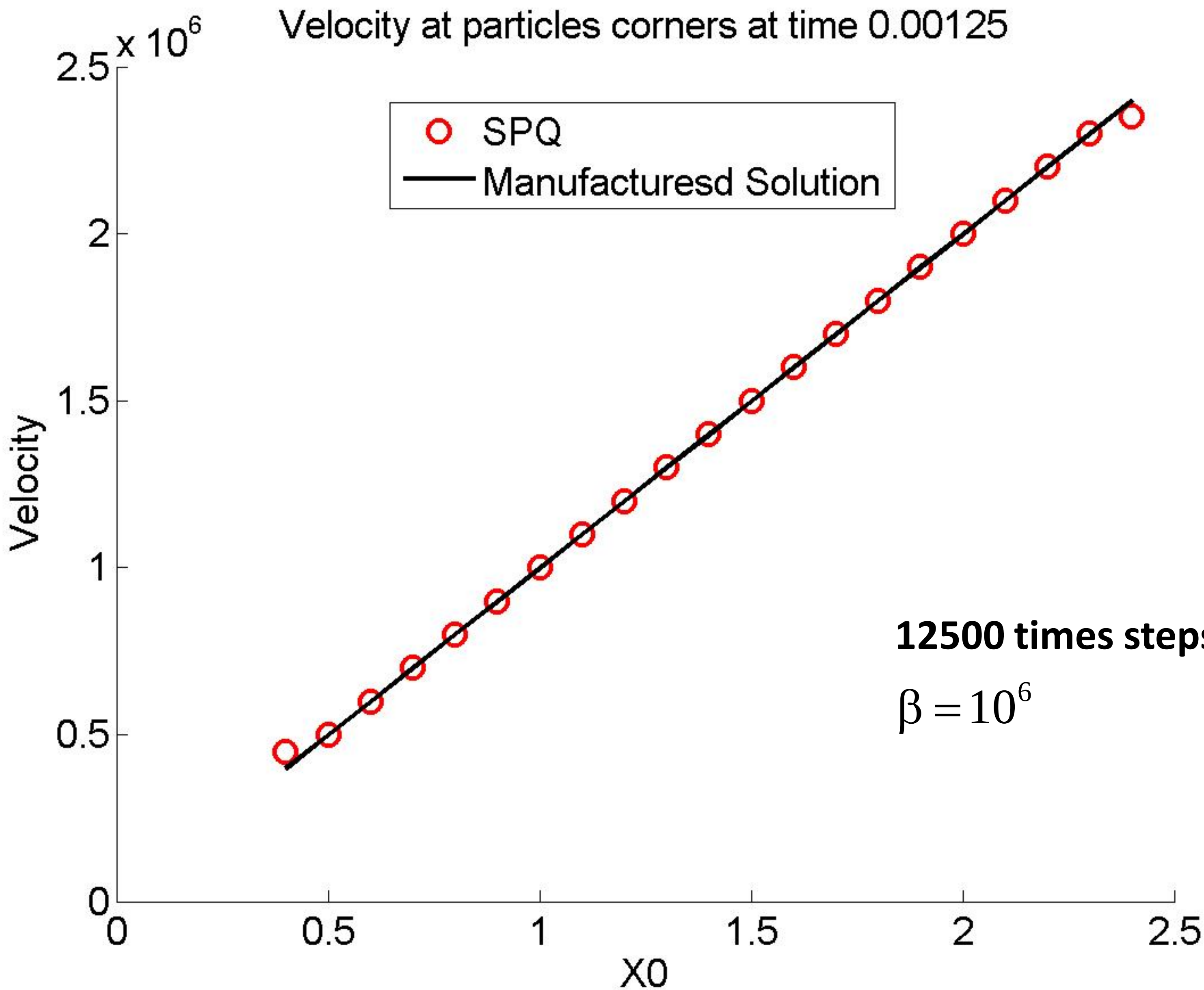
Update deformation gradient

$$F_p^{n+1} = \frac{2r^{n+1}}{2r_0}$$



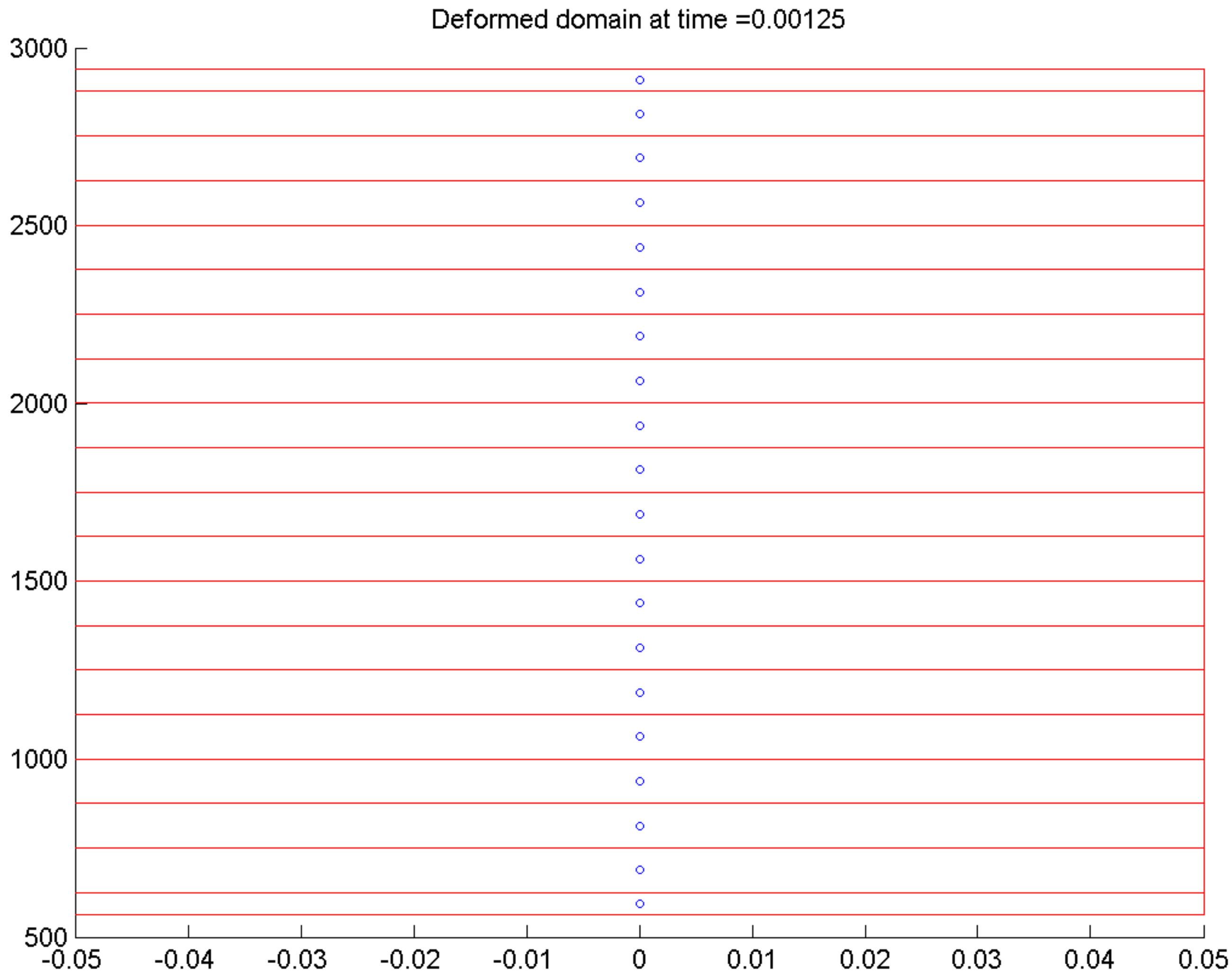
$2r_0$ Initial length of particle's domain


Deformation gradient at time 0.00125
1300
1200
1100
1000
900
800
700
600
Deformation Gradient
0.6
0.8
1
1.2
1.4
1.6
1.8
2
2.2
X0
SPQ
Manufactured Solution
12500 times steps
$\beta = 10^6$



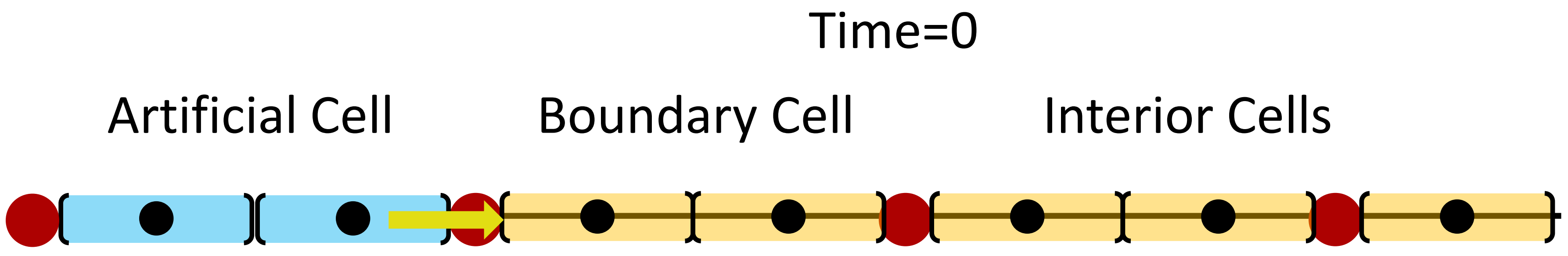
12500 times steps

$\beta = 10^6$


Deformed domain at time =0.00125
3000
2500
2000
1500
1000
500
-0.05
-0.04
-0.03
-0.02
-0.01
0
0.01
0.02
0.03
0.04
0.05

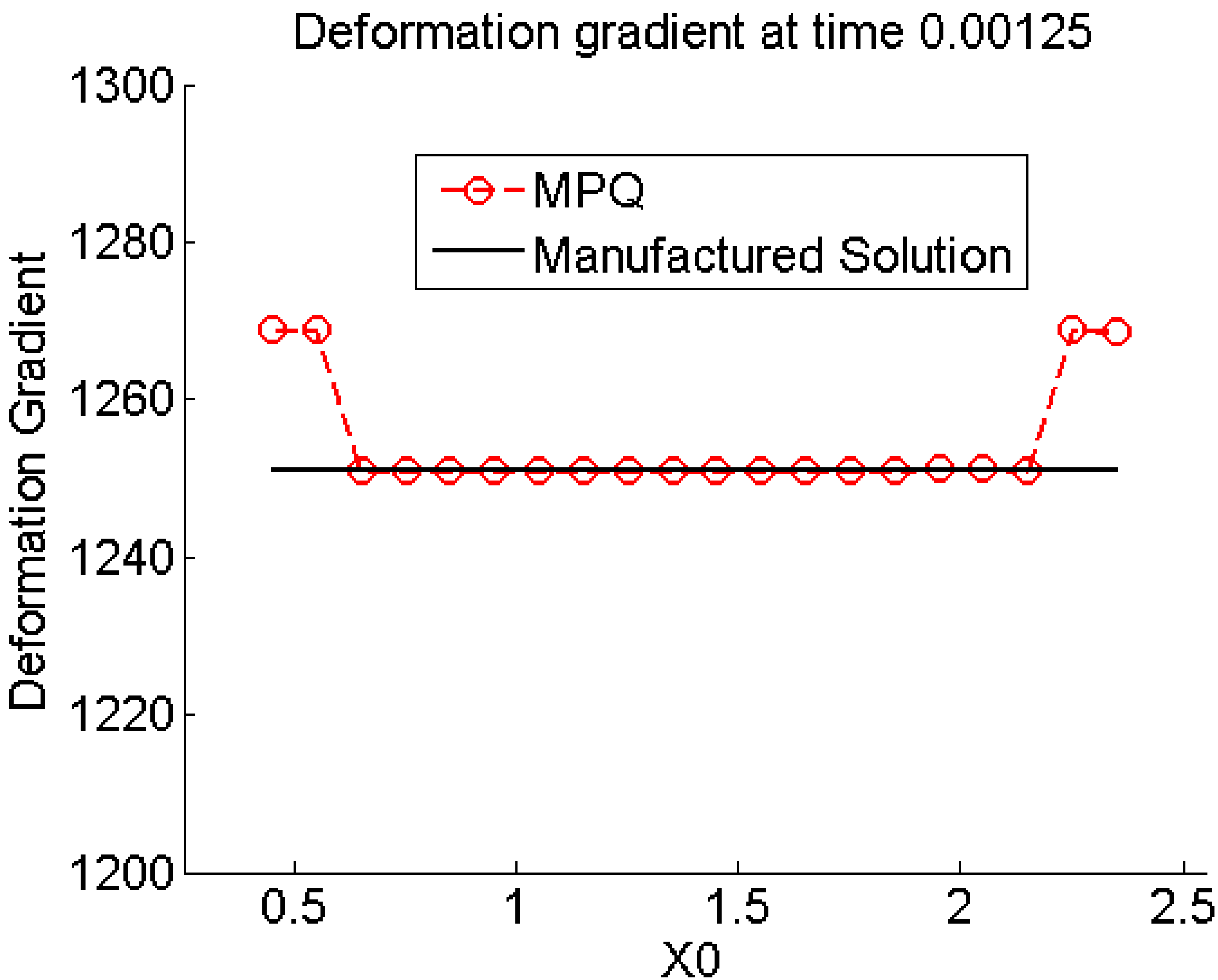
Implementation of artificial cells

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

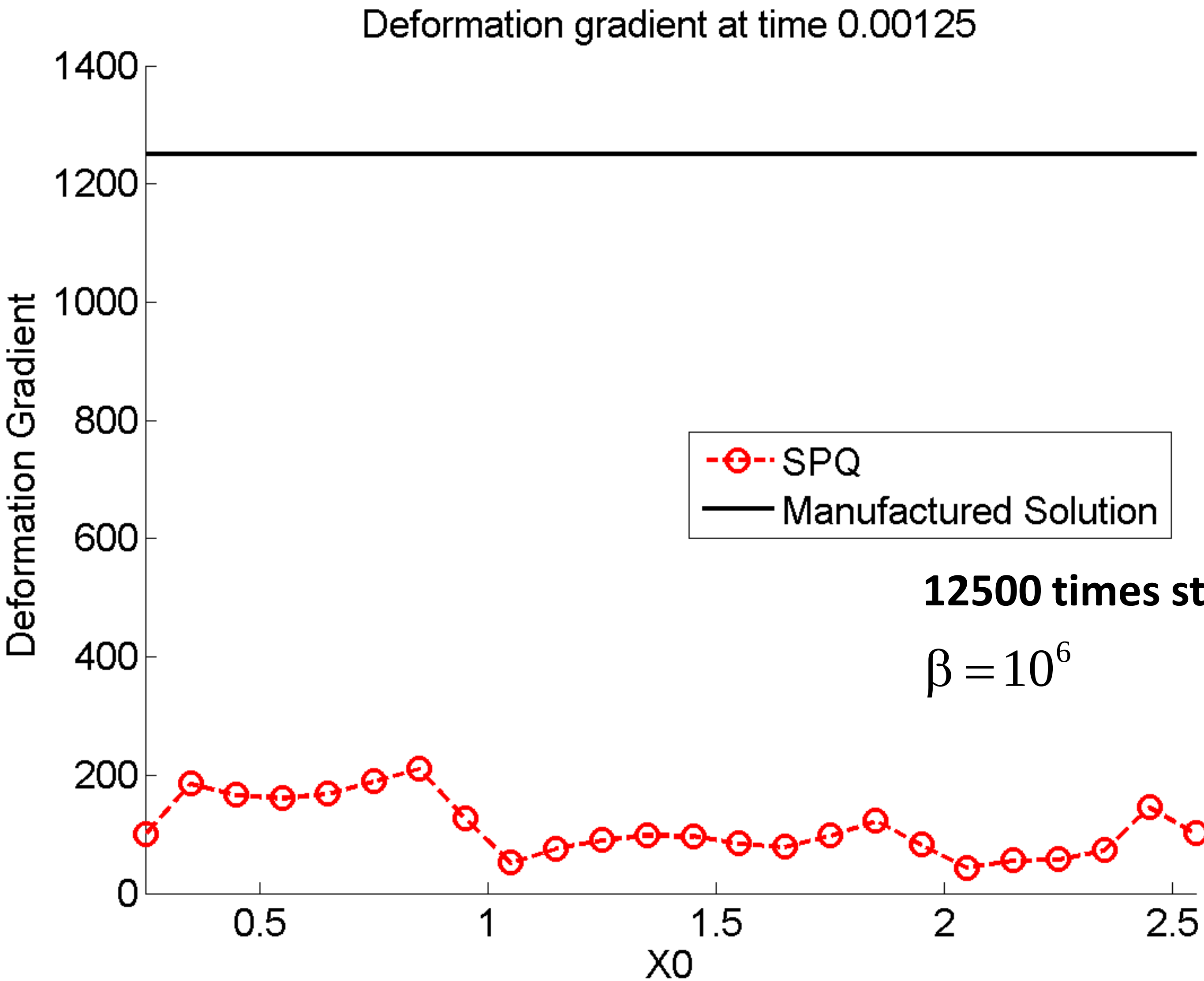


- Velocity of particles in the artificial cell are extrapolated from particles in the boundary cell at time 0

MPQ: Implemented Artificial Cells



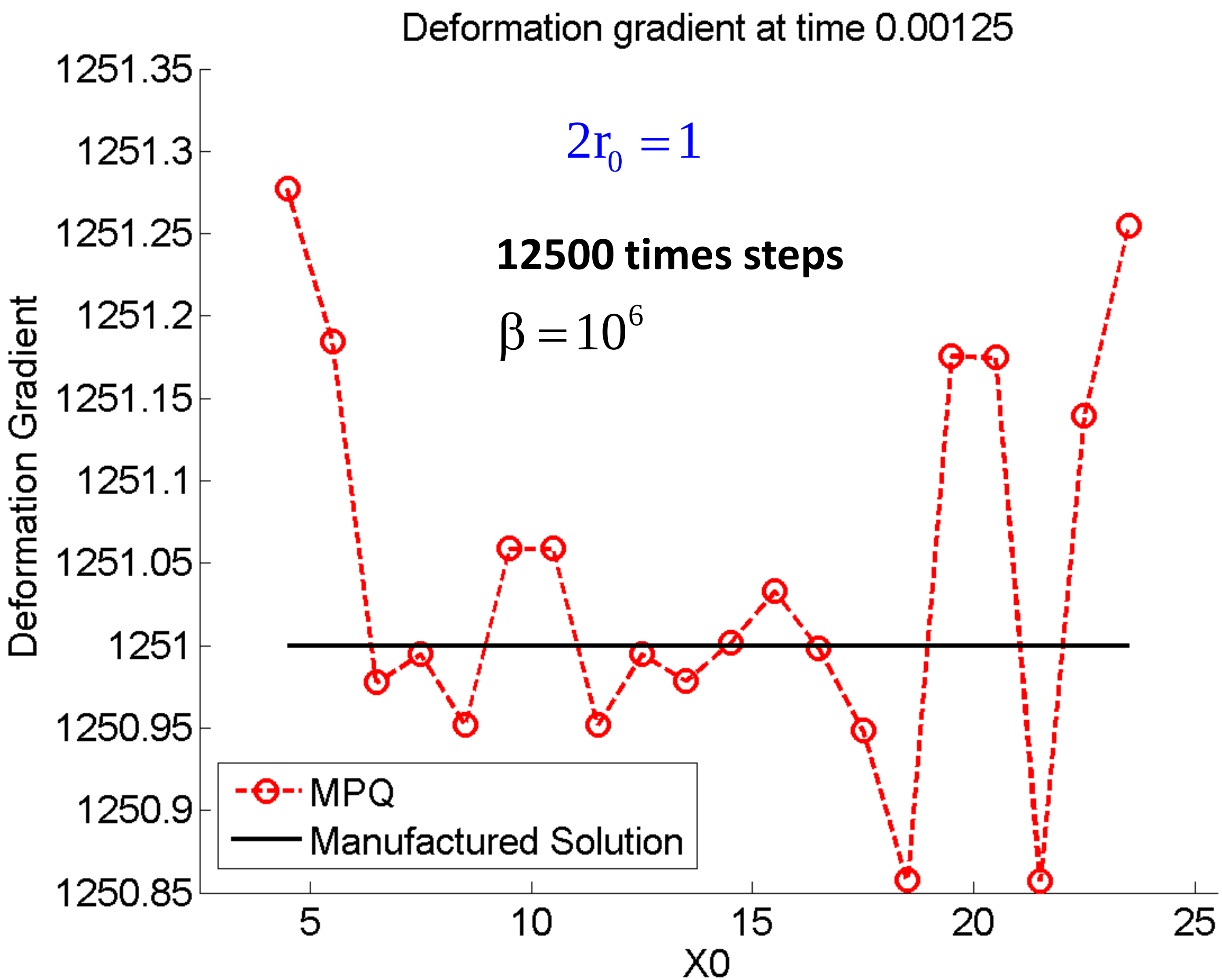
SPQ: Artificial cells implemented



12500 times steps

$$\beta = 10^6$$

MPQ: Artificial cells implemented



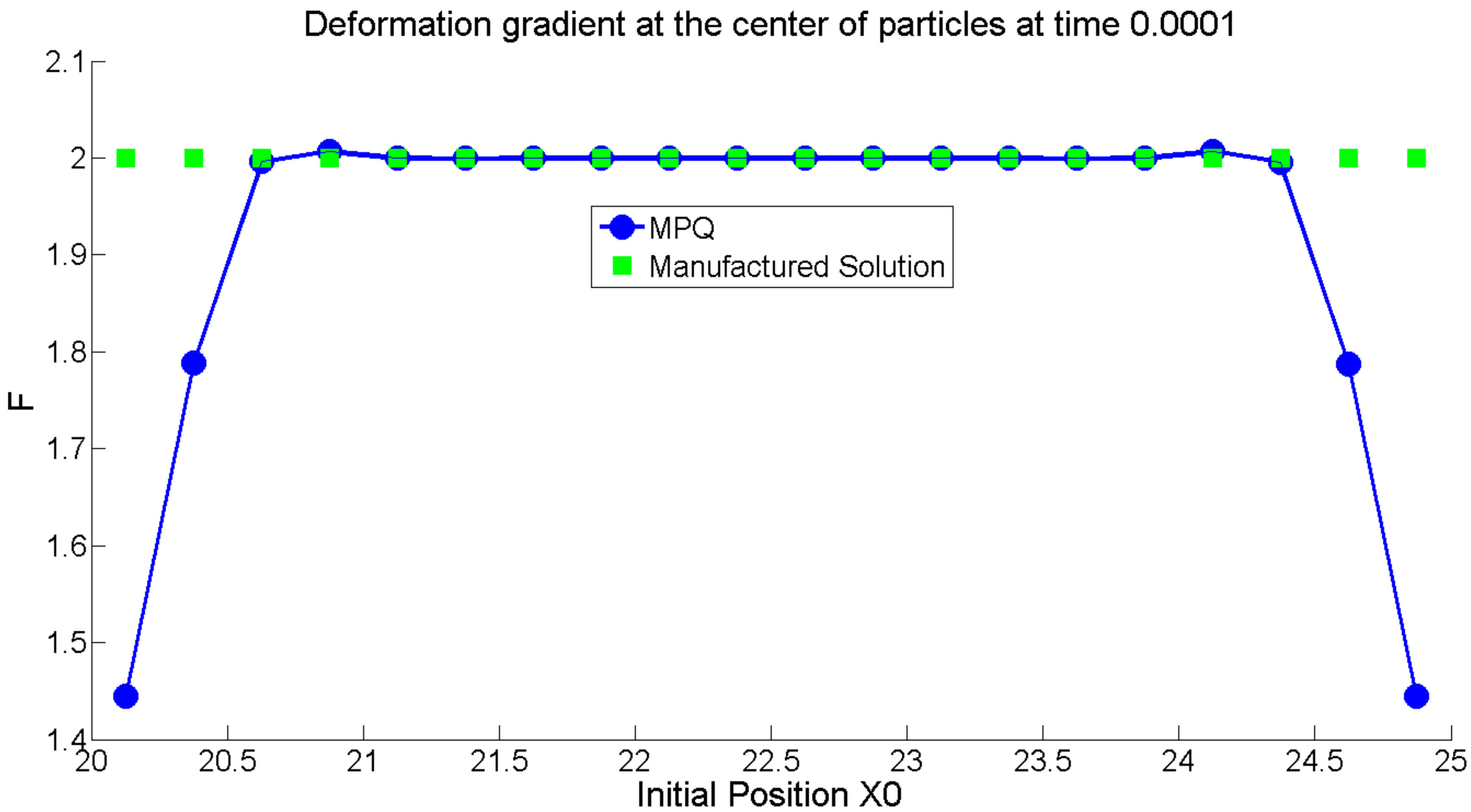
Kinematics: Conclusions

- 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

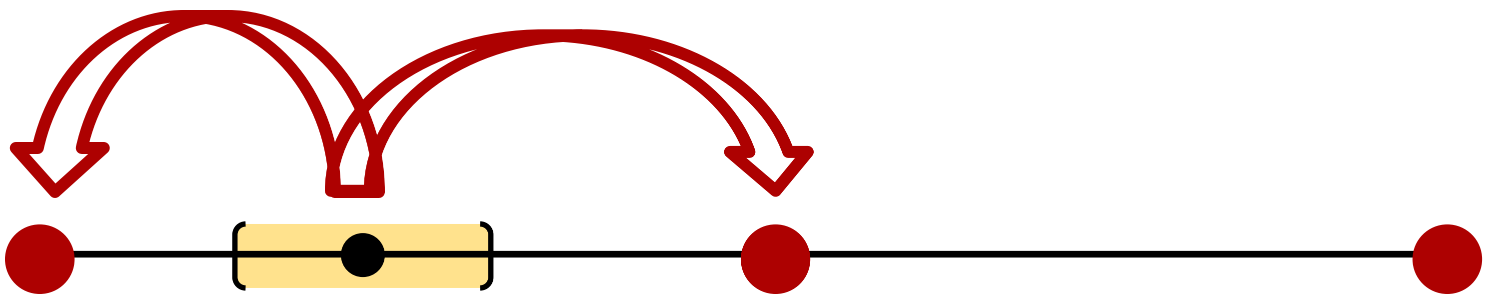
Simulations: Deformation Gradient



$$F^1_{\text{Manufactured Solution}} = 1 + \beta t \qquad F^1_{\text{Boundary Particles}} = 1 + \frac{5}{8}\beta t$$

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



$$m_i^n = \sum_p \phi_{ip} m_p$$

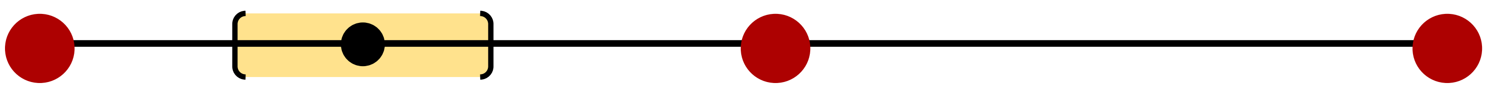
$$v_i^n = \frac{\sum_p \phi_{ip} m_p v_p^n}{m_i^n}$$

Algorithm of Multi Point Query (MPQ)

Solve for acceleration of nodes and update velocity of nodes

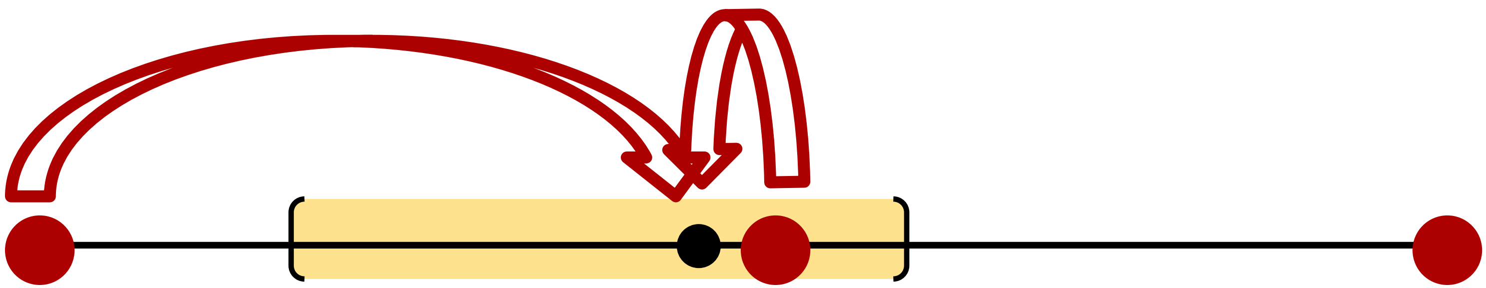
$$a_i^n = \frac{f_\mathrm{i}^{\mathrm{int}} + f_\mathrm{i}^{\mathrm{ext}}}{m_i}$$

$$v_i^{n+1} = v_i^n + a_i^n \Delta t$$



Algorithm of Multi Point Query (MPQ)

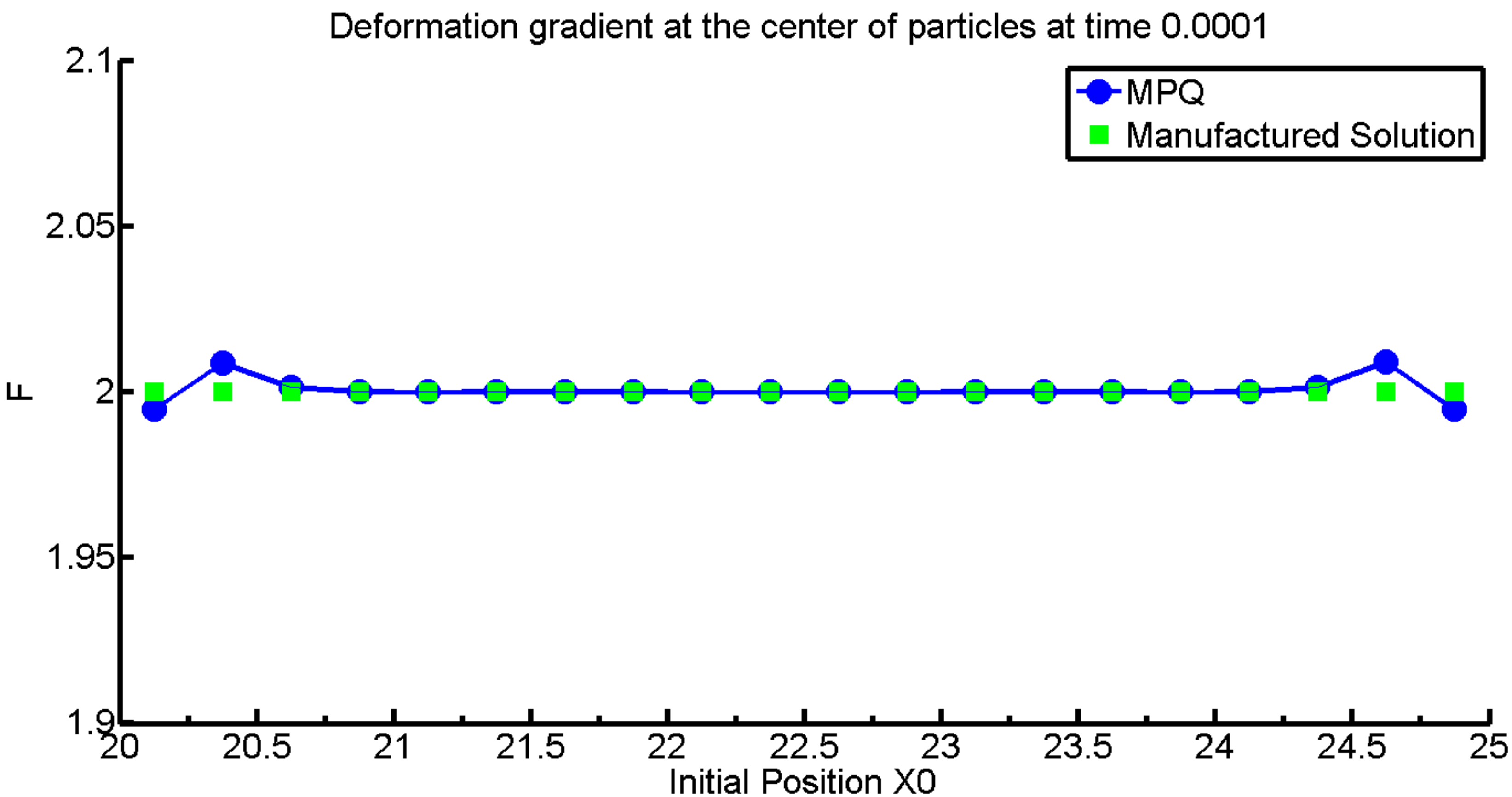
Update position and velocity of particle center (same as SPQ)
Update stress using constitutive model



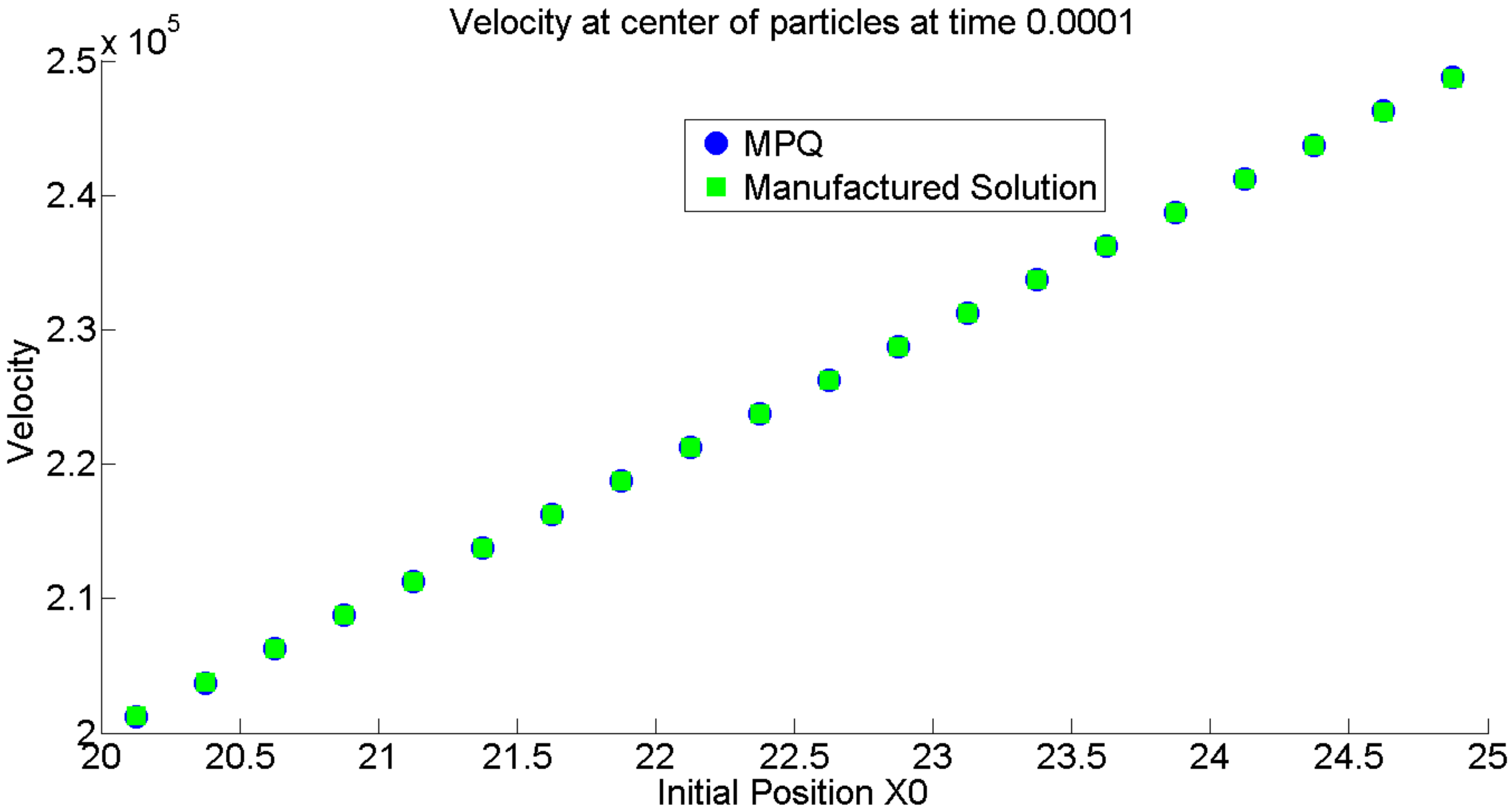
$$v_p^{n+1} = v_p^n + \sum_i \phi_{ip} a_i^n \Delta t$$

$$x_p^{n+1} = x_p^n + \sum_i \phi_{ip} v_i^{n+1} \Delta t$$

Simulations: Deformation Gradient



Simulations: Velocity at the center of particles



Simulations: Position at the center of particles