Lagrangian Solid Modeling

Matthew David Marko

Abstract

The author demonstrates a stable Lagrangian solid modeling method, tracking the interactions of solid mass particles, rather than using a meshed grid. This numerical method avoids the problem of tensile instability often seen with Smooth Particle Applied Mechanics by having the solid particles apply stresses expected with Hooke's law, as opposed to using a smoothing function for neighboring solid particles. This method has been tested successfully with a bar in tension, compression, and shear, as well as a disk compressed into a flat plate, and the numerical model consistently matched the analytical Hooke's law as well as Hertz contact theory for all examples. The solid modeling numerical method was then built into a 2-D model of a pressure vessel, which was tested with liquid water particles under pressure and simulated with Smoothed Particle Hydrodynamics. This simulation was stable, and demonstrated the feasibility of Lagrangian specification modeling for Fluid Solid Interactions.

1. Introduction

Computational solid modeling is an incredibly valuable tool for todays engineers [1–4], thankfully due to the powerful computers available at low costs. Finite Element Analysis (FEA) is just one of many meshed solid modeling techniques used in countless industries to study mechanical stresses in numerous different components today. Computational Fluid Mechanics (CFD) is constantly evolving and is an important tool in engineering design. These numerical techniques enable a detailed and robust study of complicated geometries and nonlinear behavior with far less need for costly and time-consuming experimental studies.

The vast majority of numerical methods in engineering, including Finite Element, are meshed, analyzing stresses and mass flows in a fixed region of space. This approach to solving continuum mechanics is considered the Eulerian specification. This has the advantage of being simple to implement, and avoids the need for complex link-listing, as the neighboring particles or elements are fixed in space throughout the study. The disadvantage of this method is that the entire domain needs to be modeled, and if there are large voids and empty spaces, there is a waste in computational effort as empty domains are studied repeatedly at each time step.

Another approach to avoid this wasted computational effort is to use meshless numerical methods, studying the stresses and forces in the Lagrangian specification [5–8]. The Reynolds Transport Theorem is most often used to convert a continuity equation from Eularian to the Lagrangian domain,

$$\frac{D\mathbf{F}}{Dt} = \frac{\partial}{\partial t}\int, \tag{1}$$

where $\partial/\partial t$ is the partial derivative, and D/Dt is the total derivative

$$\frac{D\mathbf{F}}{Dt} = \frac{\partial \mathbf{F}}{\partial t} + \mathbf{v}\cdot\frac{\partial \mathbf{F}}{\partial t}, \tag{2}$$

When characterizing continuum mechanics in the Lagrangian specification, rather than studying the mass that travels in and out of a specific discrete meshed domain, the mass itself is simulated as a set of discrete particles. Each particle has its own unique location, velocity, and stresses. At every time step, every particle is affected by all neighboring particles; because of this it is necessary to calculate the changes in relative distances between individual particles. A big challenge of meshless methods is the need to constantly determine the relative distances between all of the neighboring particles, a task that grows exponentially with increasing particle quantity. This can be mitigated with link-listing [9] and other optimizing techniques. Meshless methods, however, have the advantage of not requiring a grid space for empty regions of space. This can be advantageous for simulations such as large deformations and explosion studies, the study of planetary motion, or extremely small nanoparticles floating through a nanofluid.

While meshless methods are a minority of numerical methods in practical applications, a few have been investigated. One popular method is Smoothed Particle Hydrodynamics (SPH) [10–13]. SPH utilizes a host of different smoothing functions in order to determine the magnitude of the force impacts from each neighboring particles, to discretely solve the

Lagrangian Navier Stokes Equations [5–7, 14]

$$\begin{aligned}\rho\frac{Dv_i}{Dt} &= -\frac{\partial P}{\partial x_i} + \mu(\frac{\partial^2 v_i}{\partial {x_j}^2}) + (\rho B_i), \\ &= \rho(\frac{\partial v_i}{\partial t} + v_j\frac{\partial v_i}{\partial x_j}),\end{aligned} \tag{3}$$

where i and j represent the Einstein notation for the dimensional direction, v_i (m/s) is the velocity, B_i (Newtons) is the body force (such as gravity), P (Pa) is the pressure, and μ is the dynamic viscosity.

At every time-step, it is necessary to calculate the separation distance and smoothing function for each neighboring pair of particles, and thus the computational resources grow exponentially with particle quantity; link-listing is often used to mitigate this. SPH also only models incompressible fluids, using a modified Lennard-Jones (LJ) potential force to represent a fixed solid boundary [10, 11, 13, 15].

Attempts have previously been made to branch off SPH to apply to solid modeling; this has been referred to as Smoothed Particle Applied Mechanics (SPAM) [16–19]. SPAM has its origins as an effort to model planetary interaction in space, as well as statistical mechanics [20]. The Lagrangian based method is quite practical when dealing with relatively small particles (such as planets and stars) in a large domain filled with empty space; it is computationally wasteful to model vast sums of empty space with no activity in it. At smaller scales, however, SPAM and SPH suffers from tensile instability [21–25], as particles under tensile stress eventually become unstable regardless of the size of time-integration steps. Efforts to use artificial viscosity approaches have only had limited success [16, 19]. If these limitations could be overcome, SPH and SPAM could be used together for fluid-solid interaction (FSI) simulations, a capability that most commercial FEA and CFD software packages lack.

This effort is to investigate meshless modeling of solid mechanics, with the goals of eventually evolving into a practical SPAM-like tool for modeling solid mechanics. The eventual goal is to have a tool that can interact with SPH fluid particles, and perhaps become a useful FSI tool for fluid flows over a large domain. With an accurate model consisting of particles of liquids and solids interacting, an engineer could investigate eventual material failures and crack propagation in real time for highly dynamic fluid flow within a moving solid boundary.

2. Mechanics

In a Lagrangian solid modeling algorithm such as SPAM, each neighboring particle would be characterized by a smoothing function, such as

$$\begin{aligned} W(\lambda) = &\quad (10/7\pi)\cdot(1-3\lambda^2/2+3\lambda^3/4), && \lambda < 1 \\ = &\quad (10/7\pi)\cdot(2-\lambda)^3/4, && 1 < \lambda < 2 \\ = &\quad 0, && \lambda > 2 \end{aligned} \tag{4}$$

where λ is the dimensionless ratio of the absolute distance between two specific particles (m) and the smoothing length h (m),

$$\lambda_{ab} = |x_a - x_b|/h. \tag{5}$$

The density is calculated as

$$\rho_a = \Sigma_b m_b \cdot W(\lambda_{ab}), \tag{6}$$

where ρ_a (kg/m^3) is the density of particle a, and m_b (kg) is the mass of neighboring particle b.

The Lennard-Jones potential [10, 15, 16] is calculated as

$$\begin{aligned} F = &\quad D\cdot\{(\tfrac{r_0}{r_{ab}})^M - (\tfrac{r_0}{r_{ab}})^N\}\cdot(\tfrac{x_{ab}}{r_{ab}})^2, && r_{ab} < r_0, \\ = &\quad 0, && r_{ab} > r_0, \end{aligned} \tag{7}$$

where D (Newtons) is a constant of force proportional to the particle velocity squared, r_0 (m) is the specified width of a solid particle, r_{ab} (m) is the total distance between particle a and b, and x_{ab} (m) is the directional distance between particle a and b

$$r_{ab}^2 = x_{i,ab}^2.$$

The values of M and N are arbitrary coefficients; M=12 and N=4 often has the best results in practical applications of SPH.

The acceleration of a particle is thus

$$v_a = -m\cdot\Sigma_b\{(P_a/\rho_a) + (P_b/\rho_b)\}\cdot\nabla W(\lambda_{ab}), \tag{8}$$

where P_a (Pa) is the pressure of particle a, and can be calculated by the stress vector

$$P = -\sigma_{ii}, \tag{9}$$

where ii represents Einstein notation

$$i = \Sigma_{i=1}^{3}.$$

One of the biggest challenge of Lagrangian solid modeling is overcoming the tensile instability [10, 16, 19]. If the fluid or solid is under pressure ($P > 0$), these Lagrangian specification methods work well. If the solid is under tension, however, where ($P < 0$) and the particles of mass are attracted to each other, there is a tendency for all of the mass particles to clump together due to the fact that the derivative of most smoothing functions grow exponentially as the particles become closer together. This is a challenge to Lagrangian modeling of solid mechanics that must be overcome.

3. Algorithm

In previous studies [16, 19], the solid particles were treated similarly to liquid particles with SPH algorithms, with various techniques to avoid the tensile instability. Rather than use the traditional smoothing algorithms seen in SPAM, this model works by applying different steps for liquid-liquid, solid-solid, and liquid-solid particle interactions. All of the particles move freely (unless specified as fixed) within the domain, but accelerations and stress calculations are specific to the different classes of particles. The liquid-liquid particle interactions were all studied using the established Lagrangian CFD method of SPH [10–12].

The solid-solid particle interactions, however, used a much different approach from traditional SPH. The solid particles are given a specific cubic shape (that undergoes elastic strain), and particles of mass linked in tension are linked together in a specific contact matrix. Only particles linked together in this matrix can experience tension stress with a displacement apart from each other. Non-linked particles exert no stress on each other when they are proximate to each other unless they are close enough to be within the particles shaped boundary; in this circumstance they are under compressive stress. While this bears similarities to a meshed approach, it is not Eulerian as the contact matrix merely relates to each mass particle which can travel freely within the domain.

This approach avoids the concerns of the tensile instability entirely. Solid particles that have not always been fused together but comes into contact (such as during an impact) do not experience any attractive forces; only a repulsive force that only exists when the particles are within the cubic boundary. When outside of the boundary, no repulsive force is possible. For particles pre-defined as in contact and fused together, they only experience a tensile force when pulled apart; this force reverses itself entirely when the particles are close enough that they cross each other's solid boundaries. By using this approach, the issue of tensile instability, where the attractive forces of particles in tension grow exponentially and result in solid particle clumping, is avoided entirely.

When there is liquid-solid particle interaction, the particles exert a repulsive force on each other not dissimilar to Lennard Jones with some unique differences. The biggest difference in this approach is that the force is proportional to what is needed to stop the particle from crossing the boundary and stop it from further travel. The traditional LJ approach (Eq. 7) was originally developed to describe the interactions of molecules; at times using this approach for macroscopic fluid solid interactions results in liquid particles passing through a boundary of solid particles, and at other times the exponential nature of the equation results in unrealistic repulsive accelerations. By using the combination of these approaches, a stable Lagrangian simulation of solid mechanics and fluid solid interactions can be achieved.

4. Study

4.1. Tension and Compression

A series of studies was conducted to verify this Lagrangian algorithm as a valid means of studying solid mechanics. First, an extremely simply 3-D bar was pulled in tension, to determine if the tensile stress would match Hooke's Law [8, 26]

$$\sigma \quad = \quad E_Y \cdot \epsilon, \tag{10}$$

where σ (Pa) is the tensile stress, E_Y (Pa) is Young's modulus, and ϵ is the dimensionless tensile strain

$$\epsilon \quad = \quad \frac{\delta L}{L}. \tag{11}$$

In addition, the simulation aimed to verify that the *necking* that occured would properly match the *Poisson's* ratio ν,

$$\delta d \quad = \quad -d \cdot \{1 - (1 + \frac{\delta L}{L})^{-\nu}\}, \tag{12}$$

where L (m) and d (m) are dimensions of the solid under stress.

For this case study, the material parameters of steel will be used. For steel, the Young's modulus is $E_Y = 207$ GPa, and the Poisson's Ratio is $\nu = 0.3$. The 3-D steel block was

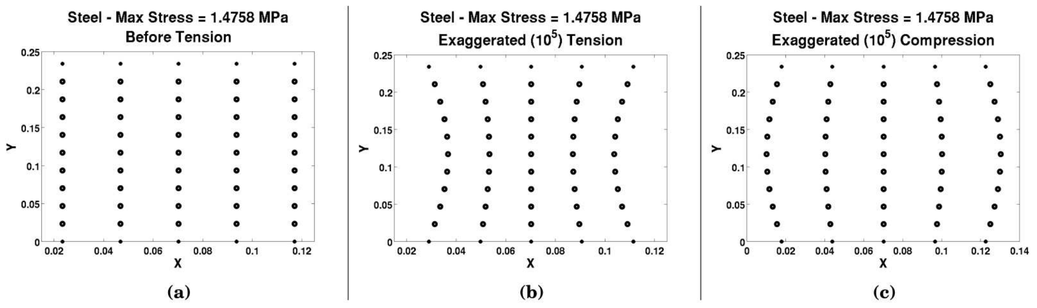


Figure 1: The Steel Bar (a) with no stress, (b) in tension, and in (c) compression, with 10^5 exaggerated deflection

represented by a series of 23.4 mm^3 cubic particles, with the particle dimensions of 5·11·5, pulled 0.8566 μm in tension along the axial direction. All of the particles were in tensile contact with their nearest neighbor. The peak tensile stress of 1.4758 MPa was observed at the center of the bar, matching near identically to the analytical stress predicted with Hooke's Law. In addition, the width in the X and Z direction decreased at a distance of 0.1329 μm for a Y increase of 0.8566 μm, yielding an equivalent Poisson's Ratio of 0.34125; within 13% of the analytical Poisson's Ratio of 0.3.

This study was then reversed for the model, but in compression rather than tension. The 5·11·5 block with a Young's Modulus of 207 GPa and a Poisson's Ratio of 0.3 was compressed to have 0.8566 μm of deflection, and as expected, the magnitude of the stress was identical to the compression case, with 1.4758 MPa of compression stress. In addition, the width in the X and Z direction increased the exact same distance of 0.1329 μm for a Y increase of 0.8566 μm; the only difference was the direction. As is observable in Fig. 1, the tensile pulling of the bar resulted necking in the bar in the X and Z direction, whereas compression results in a bulging in the X and Z direction.

4.2. Shear

The next step in the validation of this numerical model would be to test it in shear. This model would also be in steel, with a 11·3·3 block of 23.4 mm^3 cubic particles. With the Young's Modulus E_Y of 207 GPa and a Poisson's ratio of 0.3, the Shear Modulus G_Y (Pa) can be found simply as

$$\begin{aligned} G_Y &= \frac{E_Y}{2\cdot(1+\nu)}, \\ &= \frac{207}{2\cdot(1+0.3)}, \end{aligned} \tag{13}$$

which ultimately results in a shear modulus of $G_Y = 79.6154$ GPa. The shear modulus can be used to find the shear stress as a linear function of shear strain,

$$\tau \quad = \quad G_Y{\cdot}\gamma, \tag{14}$$

where τ (Pa) is the shear stress, and γ is the dimensionless shear strain

$$\gamma \quad = \quad \frac{\delta L}{H}, \tag{15}$$

where δL (m) is the tangential deflection, and H is the height 90° of the object tangent to the deflection.

The model used was subjected to a shear deflection of 18.3429 μm in the X direction. The dimensionless shear strain γ is found by taking the deflection over the height (9.3619 cm) of the bar (Eq. 15)

$$\gamma = \frac{18.3429{\cdot}10^{-6}}{9.3619{\cdot}10^{-2}} = 1.9593{\cdot}10^{-4},$$

and the shear strain can be used in Eq. 14 to find the shear stress τ

$$\tau = (79.6154{\cdot}10^{9}){\cdot}(1.9593{\cdot}10^{-4}) = 15.5992{\cdot}10^{6}.$$

The numerical maximum shear stress was observed to be 15.8993 MPa, an error of less than 2%. This close match further validates this Lagrangian numerical method as a reasonable approach to solving simple solid mechanics.

4.3. Hertz Contact Simulation

Now that this Lagrangian solid modeling effort was demonstrated effective in tension, compression, and shear of a simple 3-D steel bar, it will be further validated by simulations of Hertz contact [27–30] between a large disk and a flat elastic plate. The 2-D model comprises of an 81 by 10 flat plate of steel, with a particle dimension of 25 cm. The 2-D disk is represented as a series of 25 particles of identical dimensions assembled to give a one-particle disk with a radius of 2 meters (Fig. 2). This disk will experience no elastic deflection due to having an infinite Young's modulus; the disk would be forced down up to 49 μm into the elastic plate. The elastic plate particles are free to move, except for the final bottom row (opposite side of the Hertz contact); these particles are fixed. The model will be validated by comparing the deflection and stresses in this elastic plate, and comparing the numerical results to analytical Hertz predictions.

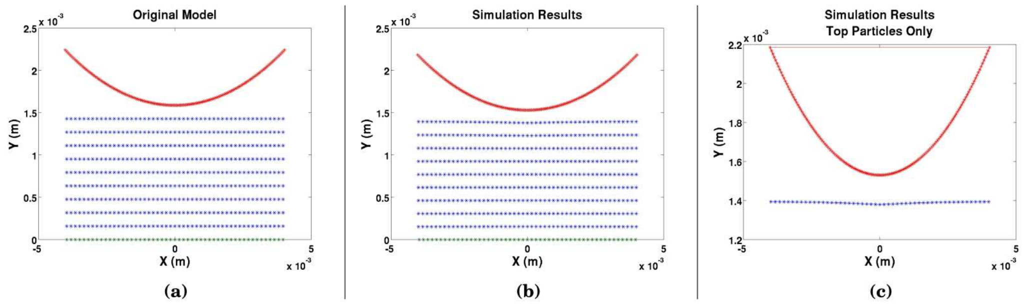


Figure 2: The disk-flat model.

What is the clear control parameter in this simulation is the actual deflection down at the center of the point of contact δ (m); this deflection can be used within Hertz contact model to determine the maximum stress. The first step is to determine the reduced Young's Modulus E'_Y (Pa) and reduced radius *R'*. As the disk does not deflect, it is treated as an infinitely stiff material $E_Y = \infty$, and thus

$$\frac{1}{E'_Y} = \frac{1-\nu^2_{flat}}{E_{Y,flat}} + \frac{1-\nu^2_{disk}}{E_{Y,disk}}, \tag{16}$$

where E_Y (Pa) is the Young's Modulus, and ν is the dimensionless Poisson's Ratio. As the disk is infinitely stiff, $E_{Y,disk} = \infty$, and thus the reduced Young's Modulus (in MPa) is

$$E'_Y = \frac{E_{Y,flat}}{1-\nu^2_{flat}} = \frac{207}{1-0.3^2} = 227.4725. \tag{17}$$

The reduced radius is easily found as

$$\frac{1}{R'} = \frac{1}{R_{flat}} + \frac{1}{R_{disk}} = \frac{1}{\infty} + \frac{1}{R_{disk}} = \frac{1}{R_{disk}},$$
$$R' = R_{disk}.$$

Because the disk is of infinite stiffness and does not deflect elastically, the width a (m) of the contact region can be found with simple trigonometry

$$a = R_{disk} \cdot sin(cos^{-1}\{\frac{R_{disk}-\delta}{R_{disk}}\}). \tag{18}$$

Hertz theory would therefore predict that the maximum stress at the point of contact would be

$$P_{max} = \frac{a \cdot E'}{2 \cdot R'}. \tag{19}$$

The model described was run for five simulations of forced deflections, ranging from 26 to 49 μm. According to Hertz contact mechanics equation the analytical load to accomplish

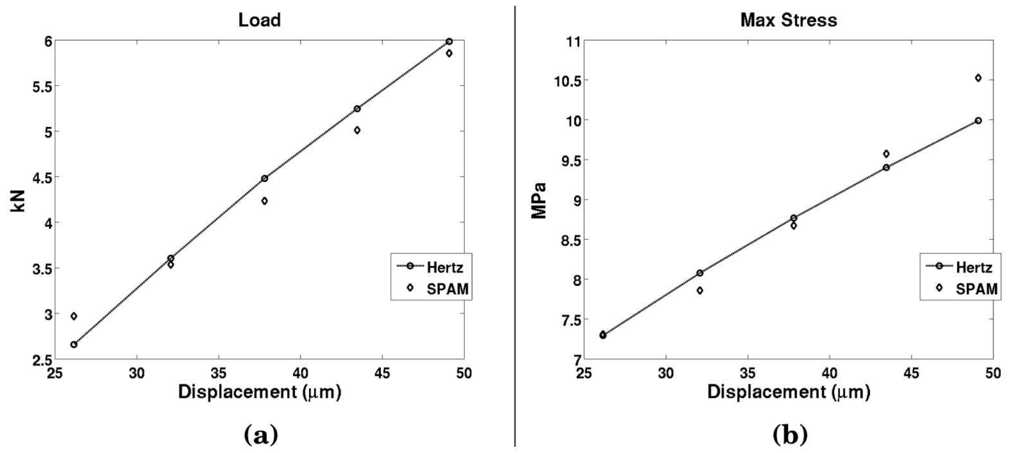


Figure 3: Comparison of Hertz and numerical solid modeling, for both (a) the numerically integrated total load, and (b) the maximum stress, calculated as a function for a given displacement δ.

this would be 2.66 to 5.98 kN, with the peak stress ranging from 7.3 to 10 GPa (Eq. 19). As observed in Fig. 3, the load and peak stress matched remarkably with the analytical Hertz predicted stresses and loads, and the displacement (Fig. 4) and velocity (Fig. 5) all settled into place after a period of time. The error percentages for the load varied from 2% to 10.4%; the error percentages for the peak stress were even lower, ranging from 0.2% to 5.4%. This close match was repeated for models of identical dimensions, with small disk radii ranging from 2-5 inches as well as 20 to 50 meter, and in all cases, the predicted load and maximum stress always matched the Hertz predicted values remarkably. This Hertz study strongly demonstrates the feasibility of this Lagrangian numerical model to predict the stresses and strains in a solid model.

4.4. Pressure Vessel

The last step in this effort is to join the Lagrangian specification solid modeling efforts with Smoothed Particle Hydrodynamics; this was demonstrated with a 2-D pressure vessel. A model of a 2-D circular pressure vessel was built; the solid pressure vessel was five particles thick, whereas the liquid was comprised of a 2-D circular region with a radius of twenty particles (Fig. 6). Each particle, both fluid and solid, had a particle length of 23.4 mm. The solid particles were steel, with the same parameters as the earlier studies; the Young's modulus is E_Y = 207 GPa, the Poisson's Ratio is ν = 0.3, and the default density ρ =7800 kg/m^3. The liquid water has a default density of ρ =1000 kg/m^3, and a bulk modulus of K_{bulk} = 2.15 GPa. The water is initially set in the pressure vessel at a pressure of 1

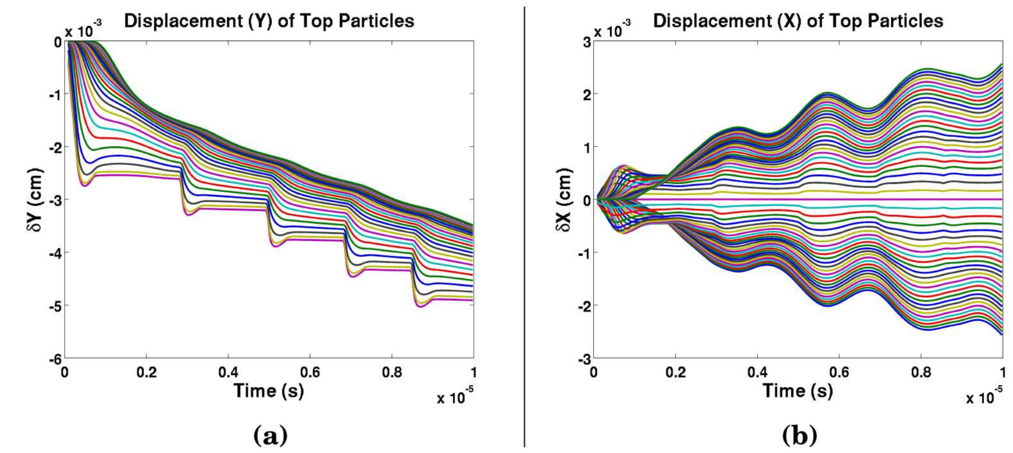


Figure 4: The displacement.

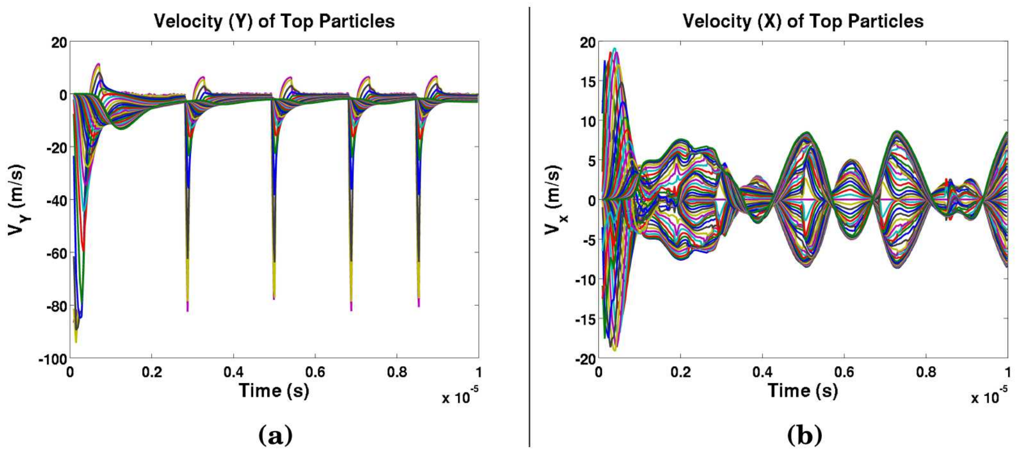


Figure 5: The velocity change.

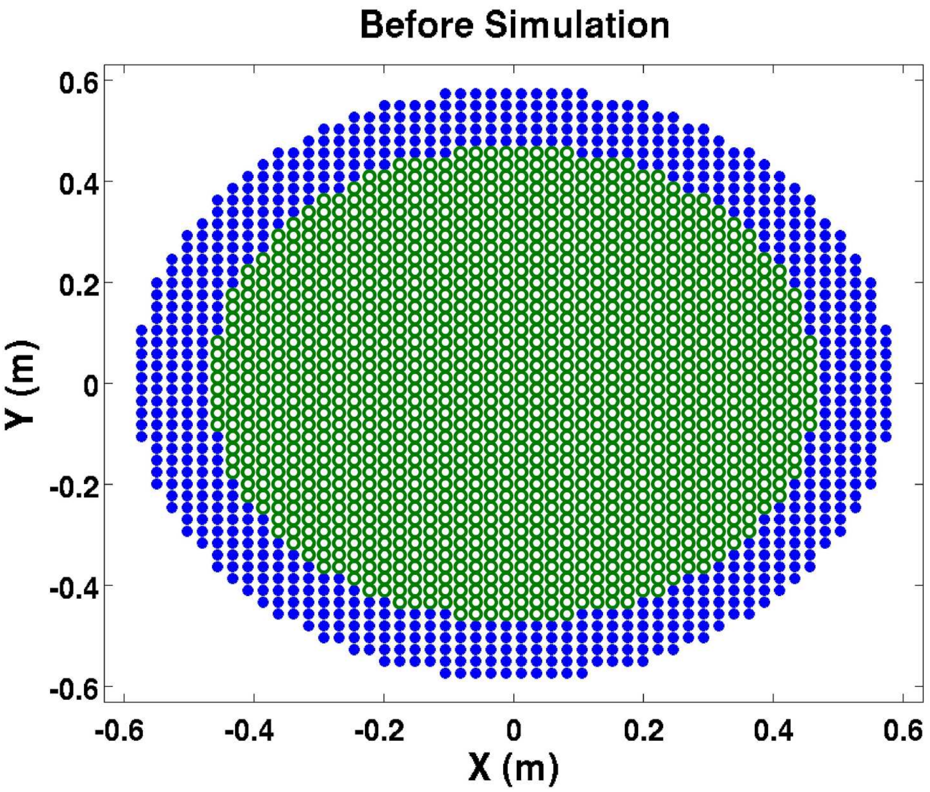


Figure 6: The pressure vessel, at the start of the simulation. Green circles represent water particles, and blue dots represent steel particles.

atmosphere (101,135 Pa).

The simulation was ran for 1000 time steps, averaging 146.8 nanoseconds in duration. The model was stable, with little dramatic shifts in particle position; this is expected as in the pressure vessel, only elastic expansions are expected as the particles settle into place. It was observed that the steel particles all pushed outwards (Fig. 7-a). The liquid particles fluctuated, as they were trapped within the pressure vessel, evenly shifting up and down radially as the liquid settled in the pressure vessel (Fig. 7-b). This model demonstrated the feasibility of merging the Lagrangian liquid numerical method of SPH with Lagrangian solid modeling, with applications in the study of Fluid Solid Interactions.

5. Conclusion

This effort demonstrated a stable method to numerically model solid mechanics with a Lagrangian specification. Rather than using Eulerian mechanics which utilizes a meshed

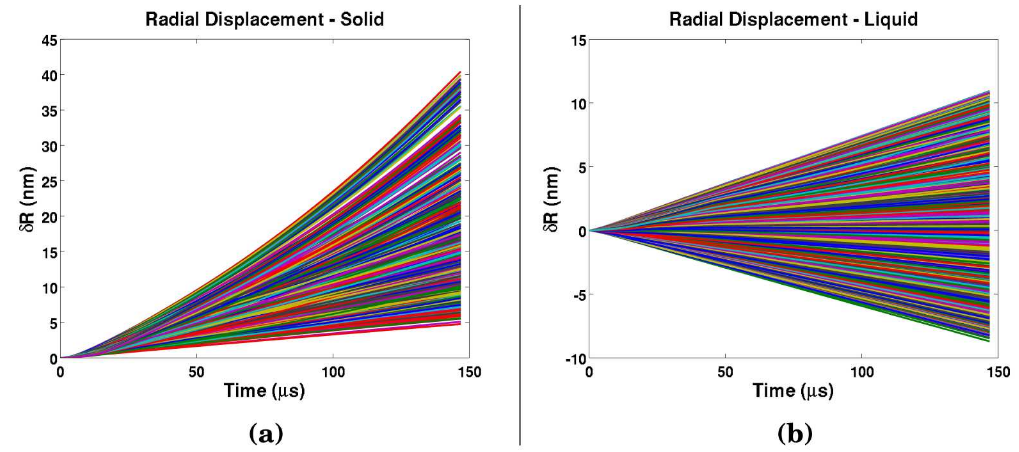


Figure 7: The pressure vessel particle radial movement as a function of time, for the (a) solid steel particles as well as (b) the liquid water particles.

grid, this model used a Lagrangian approach that tracked individual particles of the mass, and how these particles interacted with each other. This approach has the advantage of not being confined to a fixed domain, as well as reduced computational expense for models with large regions of open space. A solid bar in compression, tension, and shear was simulated, and it matched the stresses and strains remarkably with the analytical results expected with Hooke's Law. A much more detailed simulation of a rigid disk being applied to a flat plate was then studied, and the model matched the analytical loads, strains, and stresses expected with Hertz contact theory; the Hertz model matched the numerical model for a large host of loads, particle dimensions, and disk sizes. Finally, this Lagrangian solid model was implemented with the Lagrangian computational fluid dynamics method of Smooth Particle Hydrodynamics to build a stable model of water under pressure in a 2-D pressure vessel. This demonstrated the ability of using a Lagrangian solid mechanics method to study fluid solid interactions simultaneously with the modeling of the fluid and the solid, which often is modeled separately. By using this model, a host of solid mechanics applications can be better modeled, resulting in overall better engineering design.

Acknowledgement

Sources of funding for this effort include the Navy Air Systems Command (NAVAIR)-4.0T Chief Technology Officer Organization as an Independent Laboratory In-House Research (ILIR) Basic Research Project (Smooth Particle Applied Mechanics); and the Science

Mathematics And Research for Transformation (SMART) fellowship. The author thanks Elon Terrell, Jon Kyle, Yuanyuan Wang, Tirupati Chandrupa, Aleksander Navratil, Michael Singer, and Jenny Ardelean for fruitful discussions.

References

[1] A. Garcia, *Numerical Methods for Physics 2nd Edition.* Boston: Addison-Wesley, 1999.

[2] G. B. Arfken and H. J. Weber, *Mathematical Methods for Physicists, Sixth Edition.* 30 Corporate Drive, Suite 400, Burlington MA 01803: Elsevier, 2005.

[3] D. G. Zill and M. R. Cullen, *Advanced Engineering Mathematics, Second Edition.* Sudbury MA: Jones and Bartlett Publishers, 2000.

[4] G. Strang, *Linear Algebra and its Applications, 3*rd *edition.* 1 Progress Dr, Horsham, PA 19044: Thomas Learning Inc, 1988.

[5] I. G. Currie, *Fundamental Mechanics of Fluids, 3rd Edition.* 270 Madison Avenue, New York NY 10016: Marcel Dekker Inc, 2003.

[6] W. Lai, D. Rubin, and E. Krempl, *Introduction to Continuum Mechanics, 4*th *Edition.* 30 Corporate Drive, Suite 400, Burlington MA 01803: Butterworth-Heinemann of Elsevier, 2010.

[7] S. Timoshenko and J. Goodier, *Theory of Elasticity, 3*rd *Edition.* 1221 Avenue of the Americas, New York NY 10020: McGraw Hill, 1970.

[8] W. F. Riley, L. D. Sturges, and D. H. Morris, *Statics and Mechanics of Solids, 2*nd *Edition.* 111 River Street, Hoboken NJ 07030: John Wiley and Sons, 2002.

[9] B. Stroustrup, *The C++ Programming Language, 3rd Edition.* One Jacob Way, Reading, Massachusetts 01867: Addison-Wesley Professional, 2000.

[10] G. R. Liu and M. B. Liu, *Smoothed Particle Hydrodynamics, A Meshfree Partical Method.* 27 Warren Street, Suite 401-402, Hackensack, NJ 07601: World Scientific Publishing Co, 2003.

[11] J. P. Kyle and E. J. Terrell, “Application of smoothed particle hydrodynamics to full-film lubrication,” *Journal of Tribology*, vol. 135, p. 041705, 2013.

[12] J. J. Monaghan, “Why particle methods work,” *Siam Journal of Science Statistical Computation*, vol. 3, no. 4, pp. 422–433, 1982.

[13] L. D. Libersky, “High strain lagrangian hydrodynamics, a three-dimensional SPH code for dynamic material response,” *Journal of Computational Physics*, vol. 109, pp. 67–75, 1993.

[14] F. White, *Fluid Mechanics Fifth Edition.* Boston, MA: McGraw-Hill, 2003.

[15] J. E. Lennard-Jones, “On the determination of molecular fields,” *Proceedings of the Royal Society of London A*, vol. 106, pp. 463–477, 1924.

[16] W. G. Hoover, *Smooth Particle Applied Mechanics, the State of the Art.* 27 Warren Street, Suite 401-402, Hackensack, NJ 07601: World Scientific Publishing Co, 2006.

[17] W. G. Hoover, T. G. Pierce, C. G. Hoover, J. . Shugart, C. M. Stein, and A. L. Edwards, “Molecular dynamics, smoothed-particle applied mechanics, and irreversibility,” *Computers and Math Applications*, vol. 28, no. 10-12, pp. 155–174, 1994.

[18] R. C. Batra and G. M. Zhang, “Modified smoothed particle hydrodynamics (msph) basis functions for meshless methods, and their application to axisymmetric taylor impact test,” *Journal of Computational Physics*, vol. 227, pp. 1962–1981, 2008.

[19] C. Antoci, M. Gallati, and S. Sibilla, “Numerical simulation of fluid–structure interaction by SPH,” *Computers and Structures*, vol. 85, pp. 879–890, 2007.

[20] R. K. Pathria, *Statistical Mechanics, 2^{nd} Edition.* 30 Corporate Drive, Suite 400, Burlington, MA 01803 USA: Butterworth-Heinemann, 1972.

[21] D. S. Balsara, “Von neumann stability analysis of smoothed particle hydrodynamics-suggestions for optimal algorithms,” *Journal of Computational Physics*, vol. 121, pp. 357–372, 1995.

[22] C. T. Dyka and R. P. Ingel, “An approach for tension instability in smoothed particle hydrodynamics (SPH),” *Computers and Structures*, vol. 57, pp. 573–580, 1995.

[23] C. T. Dyka, R. W. Randles, and R. P. Ingel, "Stress points for tension instability in smoothed particle hydrodynamics," *International Journal for Numerical Methods in Engineering*, vol. 40, pp. 2325–2341, 1997.

[24] J. W. Swegle and S. W. Attaway, "On the feasibility of using smoothed particle hydrodynamics for underwater explosion calculations," *Computational Mechanics*, vol. 17, pp. 151–168, 1995.

[25] J. W. Swegle, D. L. Hicks, and S. W. Attaway, "Smoothed particle hydrodynamics stability analysis," *Journal of Computational Phyisics*, vol. 116, no. 1, pp. 123–134, 2002.

[26] W. D. Callister, *Materials Science and Engineering An Introduction, 6th Edition.* 111 River Street, Hoboken NJ 07030: John Wiley and Sons, 2003.

[27] S. Hiermaier, D. Konke, A. J. Stilp, and K. Thomas, "Computational simulation of the hypervelocity impact of al-sphere on thin plates of different materials," *International Journal of Impact Engineering*, vol. 20, no. 1-5, pp. 363–374, 1997.

[28] K. Johnson, *Contact Mechanics.* 32 Avenue of the Americas, New York NY 10013: Cambridge University Press, 1987.

[29] R. Gohar, *Elastohydrodynamics, Second Edition.* 1060 Main Street, Suite 1B, River Edge NJ 07661: World Scientific Publishing Co, 2001.

[30] G. Stachowiak and A. Batchelor, *Engineering Tribology 4th Edition.* Oxford, UK: Butterworth-Heinemann, 2005.

[31] R. K. Nagel, E. B. Saff, and A. D. Snider, *Fundamentals of Differential Equations, 5th Edition.* 75 Arlington Street, Suite 300 Boston, MA 02116: Addison Wesley, 1999.

[32] R. Haberman, *Applied Partial Differential Equations With Fourier Series and Boundary Value Problems, 4th Edition.* Upper Saddle River, New Jersey: Prentice Hall, 2003.

Supplement

Included is a sample of all of the Lagrangian solid modeling code used within this study. The core of this code, which is written for a Fortran 90 compiler, is included along with several function files: a bar in tension, a bar in compression, a disk compressed into an elastic steel bar, and the pressure vessel simulation. The code is written so that the core file *spam.f* can be compiled along with the model-building function of choice, and the simulation will run accordingly. The files are:

- **spam.f**: this is the core of the code, and is entirely self contained except for the model function file, which defines the model and specifies the material and simulation properties.
- **tension_steel.f**: the model function for the bar in tension.
- **compress_steel.f**: the model function for the bar in compression. It is identical to the tension function except the top and bottom *FixXY* values are reversed so the direction is reversed.
- **ModelSmFixDisk.f**: The model function for a rigid 2D disk compressing into an elastic flat plat.
- **PressVessel.f**: The model function for the 2D pressure vessel, with both steel solid particles and liquid particles under pressure, to demonstrate Lagrangian Fluid Solid Interactions.

In addition, there are several MatLab files used to post-process the data:

- **Analyze_Data.m**: This file is first run, which reads all of the ASCII data files, and saves it as a single, clean binary MatLab data file *Data.mat*.
- **PlotTension.m**: The file processes the tension plot. It will prompt the model before and after the simulation (exaggerated deflection), as well as calculating the analytical tension stress and transverse deflections, and compares it to the numerical results.

- **PlotComp.m**: Effectively the same as the *PlotTension.m* script, but with small modifications for compression simulations rather than tensile.
- **Plot_Hertz.m**: The plotting function for the Hertz disk-flat simulation. Various exaggerated deflection plots are generated, as well as calculation of the Hertz analytical stresses to compare to the analytical results.
- **MakeFigs_PresVes.m**: Plots the 2D pressure vessel model, as well as the relative radial deflections.

To run the simulation, first the user compiles the *spam.f* function with the model function of interest. The machine-language program of the simulation is run, and the code will output the results as various ASCII text files of the simulation results. The user can then go into MatLab and run the *Analyze_Data.m* script, which reads all of the ASCII data files and outputs a single compressed binary MatLab file (*Data.mat*) of the simulation results. The user can then select the relevant MatLab script to load the MatLab data file and plot and analyze the results of the simulation.

The *Analyze_Data.m* script will consistently save the results as a binary *Data.mat* file, regardless of the study performed. The saved results are renamed, and the associated MatLab plotting scripts read these different file-names. The scripts are as follows:

- **Tension_steel.mat**
- **compress_steel.mat**
- **Hertz.mat**
- **PressVess.mat**

FORTRAN SOURCE CODE

spam.f

```
      program spam

c     --------------------------------------------------------------------
      implicit none

      integer ii,jj,kk,jj0,uu,vv,ctbar(3),ctZ,ctZmod
      integer ct,ct2,xx,yy,N,Nsphere,ts,fooint,StudyCt,CenterPt(2)
      integer Nts,LoopCT,LoopCT2,stop,start2,stop2,ctCyl,StopWeight
      integer xxx,yyy,uv(2),break,breakct,abreak,split,StartStop
      integer BSx,cubecyl,ctx(2)
      complex i
      double precision pi,dx3(3),third,Xloc,Yloc,Zloc,StartDefl,NewDef
      double precision dx00, dxE, dTfactor,dTdxfactor,dTdxfactor2,TTxx
      double precision masX,rho_solid,foo3,Xr0,Yr0,Vydt,dt0x,dx0x
      double precision deflect, deflectWeight, Rred, Ered, bWeight,mas
      double precision h, c02, K_bulk, Vy0,foo,r,dwdx(3),t1,t2
      double precision g(3), foo2, foo3vv, dxJ, Arange, dxEj
      double precision dt,dt0,Dij(3,3),OMGij(3,3),Sij3(3,3)
      double precision dSdt(6),RijAB(3,3),Wij,rho_ij,Radius,RadiusFact
      double precision Weight0,Weight,Pweight(3),Vtest(3),Tfract,Efrac
      double precision dx,dxd,dE,deltX,deltX2,dxi,a,angleFrac,angle
      double precision lambda,mu,Ey,poisson,TT,Time,Bulk_water
      double precision Csound,rho0min,dV,gamma,dVdx0
      double precision X1(3),X2(3),V1(3),V2(3)
      integer, allocatable, dimension(:) :: Mat, FixXY, IsSolid
      integer, allocatable, dimension(:) :: WeightXY
      integer, allocatable, dimension(:,:) :: Contact,ContactDir
      integer, allocatable, dimension(:,:) :: ContactDirCT
      integer, allocatable, dimension(:,:) :: ContactX,ContactDirX
      integer, allocatable, dimension(:,:) :: ContactDirCTX
      integer, allocatable, dimension(:,:) :: Links
      integer, allocatable, dimension(:) :: BreakContact, RadiusCrap
      double precision, allocatable, dimension(:,:) :: X,X0,X00
      double precision, allocatable, dimension(:,:) :: V,V0,dVdx
      double precision, allocatable, dimension(:,:) :: dVdxFct,dVdyFct
      double precision, allocatable, dimension(:,:) :: dVdzFct
      double precision, allocatable, dimension(:,:) :: V00
      double precision, allocatable, dimension(:,:) :: TcomboOut
      double precision, allocatable, dimension(:,:,:) :: DSDtN,DSDtN0
      double precision, allocatable, dimension(:,:,:) :: Tij,Eij,Eij0
      double precision, allocatable, dimension(:,:,:) :: TTij,Tij0
      double precision, allocatable, dimension(:,:,:) :: TijCombo
      double precision, allocatable, dimension(:) :: rho,rho0,P,P0
      double precision, allocatable, dimension(:) :: printVar,Tvm0
      double precision, allocatable, dimension(:) :: TimeFct
      double precision, allocatable, dimension(:) :: massFct
      double precision, allocatable, dimension(:,:) :: D0,Omg0
      double precision, allocatable, dimension(:,:) :: VonMiss
      double precision, allocatable, dimension(:,:) :: Xout,Yout,Zout
      double precision, allocatable, dimension(:,:) :: VoutX,VoutY,Vou
      double precision, allocatable, dimension(:,:) :: dVdy,Tvm
      double precision, allocatable, dimension(:,:) :: Pout,Rout
      double precision, allocatable, dimension(:,:) :: DPDT,DPDT0
      double precision, allocatable, dimension(:,:) :: T22o
      double precision, allocatable, dimension(:,:) :: T11,T12,T13
      double precision, allocatable, dimension(:,:) :: T21,T22,T23
      double precision, allocatable, dimension(:,:) :: T31,T32,T33
      double precision, allocatable, dimension(:,:) :: E22,E11
      double precision, allocatable, dimension(:) :: dx0
      double precision, allocatable, dimension(:) :: zOffset


c     ------------------------------------------------------------------
c     These are the universal constants
c     ------------------------------------------------------------------
      pi = 3.141592653589793 ! set the value of pi
      i = (0, 1) ! set the imaginary number i=sqrt(-1)
      g = (/ 0.0, 0.0, 0.0 /)
      third=1.0/3.0

c     ------------------------------------------------------------------
c     Declare array sizes
c     ------------------------------------------------------------------

      call ModelBlock(N)

      open (unit=1,file="SimSpec.dat",STATUS='OLD',ACTION='READ')
        read (1,*),Ey
        read (1,*),poisson
        read (1,*),rho_solid
        read (1,*),Vtest(1)
        read (1,*),Vtest(2)
        read (1,*),Vtest(3)
        read (1,*),gamma
        read (1,*),Nts
        read (1,*),LoopCT
        read (1,*),StudyCt
        read (1,*),StartDefl
        read (1,*),NewDefl
        read (1,*),dTfactor
        read (1,*),dTdxfactor
        read (1,*),stop
        read (1,*),Bulk_water
      close (1)

      Vy0 = Vtest(2)
      K_bulk = Ey/(3*(1-(2*poisson))) ! bulk modulus of iron
      mu=Ey/(2*(1+poisson))
      lambda=K_bulk-(2*mu/3)
      Ered=2/((1-(poisson**2))/Ey)

      Nts=Nts*StudyCt

      ALLOCATE (X(N,3))
      ALLOCATE (X0(N,3))
      ALLOCATE (X00(N,3))
      ALLOCATE (V(N,3))
      ALLOCATE (V0(N,3))
      ALLOCATE (V00(N,3))
      ALLOCATE (dx0(N))
      ALLOCATE (dVdx(N,3))
      ALLOCATE (dVdxFct(N,Nts))
      ALLOCATE (dVdyFct(N,Nts))
      ALLOCATE (dVdzFct(N,Nts))
      ALLOCATE (Mat(N))
      ALLOCATE (FixXY(N))
      ALLOCATE (IsSolid(N))
      ALLOCATE (rho(N))
      ALLOCATE (rho0(N))
      ALLOCATE (massFct(N))
      ALLOCATE (P(N))
      ALLOCATE (P0(N))
      ALLOCATE (Tij(N,3,3))
      ALLOCATE (TTij(N,3,3))
      ALLOCATE (Tij0(N,3,3))
      ALLOCATE (TijCombo(N,3,3))
      ALLOCATE (Eij(N,3,3))
      ALLOCATE (Eij0(N,3,3))
      ALLOCATE (DSDtN(N,3,3))
      ALLOCATE (DSDtN0(N,3,3))
      ALLOCATE (DPDT(N,3))
      ALLOCATE (DPDT0(N,3))
      ALLOCATE (D0(N,6))
      ALLOCATE (Omg0(N,6))
      ALLOCATE (Links(N,N+1))
      ALLOCATE (Xout(N,Nts))
      ALLOCATE (Yout(N,Nts))
      ALLOCATE (Zout(N,Nts))
      ALLOCATE (VoutX(N,Nts))
      ALLOCATE (VoutY(N,Nts))
      ALLOCATE (VoutZ(N,Nts))
      ALLOCATE (dVdy(N,Nts))
      ALLOCATE (Pout(N,Nts))
      ALLOCATE (Rout(N,Nts))
      ALLOCATE (TimeFct(Nts))
      ALLOCATE (Tvm0(N))
      ALLOCATE (Tvm(N,Nts))
      ALLOCATE (TcomboOut(N,Nts))
      ALLOCATE (T11(N,Nts))
      ALLOCATE (T12(N,Nts))
      ALLOCATE (T13(N,Nts))
      ALLOCATE (T21(N,Nts))
      ALLOCATE (T22(N,Nts))
      ALLOCATE (T23(N,Nts))
      ALLOCATE (T31(N,Nts))
      ALLOCATE (T32(N,Nts))
      ALLOCATE (T33(N,Nts))
      ALLOCATE (T22o(N,Nts))
      ALLOCATE (E22(N,Nts))
      ALLOCATE (E11(N,Nts))
      ALLOCATE (VonMiss(N,Nts))
      ALLOCATE (Contact(N,(N+1)))
      ALLOCATE (ContactDir(N,(N+1)))
      ALLOCATE (ContactDirCT(N,3))
      ALLOCATE (ContactX(N,(N+1)))
      ALLOCATE (ContactDirX(N,(N+1)))
      ALLOCATE (ContactDirCTX(N,3))
      ALLOCATE (BreakContact(N))

      ALLOCATE (printVar(N))

      ALLOCATE (RadiusCrap(N))

c     ------------------------------------------------------------------
c     Declare size and velocity of particles
c     ------------------------------------------------------------------

      open (unit=1,file="Fixed.dat",STATUS='OLD',ACTION='READ')
      do ii=1,N
        read (1,*),FixXY(ii)
      enddo
      close (1)

      open (unit=1,file="Contact.dat",STATUS='OLD',ACTION='READ')
      do ii=1,N
        read (1,*),Contact(ii,:)
      enddo
```

```
close (1)

open (unit=1,file="ContactDir.dat",STATUS='OLD',ACTION='READ')
do ii=1,N
  read (1,*),ContactDir(ii,:)
enddo
close (1)

open (unit=1,file="ContactDirCT.dat",STATUS='OLD',ACTION='READ')
do ii=1,N
  read (1,*),ContactDirCT(ii,:)
enddo
close (1)

open (unit=1,file="ContactX.dat",STATUS='OLD',ACTION='READ')
do ii=1,N
  read (1,*),ContactX(ii,:)
enddo
close (1)

open (unit=1,file="ContactDirX.dat",STATUS='OLD',ACTION='READ')
do ii=1,N
  read (1,*),ContactDirX(ii,:)
enddo
close (1)

open (unit=1,file="ContactDirCTX.dat",STATUS='OLD',ACTION='READ'
do ii=1,N
  read (1,*),ContactDirCTX(ii,:)
enddo
close (1)

open (unit=1,file="Mass.dat",STATUS='OLD',ACTION='READ')
do ii=1,N
  read (1,*),massFct(ii)
enddo
close (1)

open (unit=1,file="dX.dat",STATUS='OLD',ACTION='READ')
do ii=1,N
```

```
  read (1,*),dx0(ii)
enddo
close (1)

open (unit=1,file="X0.dat",STATUS='OLD',ACTION='READ')
do ii=1,N
  read (1,*),X(ii,:)
enddo
close (1)

open (unit=1,file="V0.dat",STATUS='OLD',ACTION='READ')
do ii=1,N
  read (1,*),V(ii,:)
enddo
close (1)

open (unit=1,file="dVdX.dat",STATUS='OLD',ACTION='READ')
do ii=1,N
  read (1,*),dVdx(ii,:)
enddo
close (1)

open (unit=1,file="rho0.dat",STATUS='OLD',ACTION='READ')
do jj=1,N
  read (1,*),rho0(jj)
enddo
close (1)

open (unit=1,file="rho_init.dat",STATUS='OLD',ACTION='READ')
do jj=1,N
  read (1,*),rho(jj)
enddo
close (1)

open (unit=1,file="IsSolid.dat",STATUS='OLD',ACTION='READ')
do jj=1,N
  read (1,*),IsSolid(jj)
enddo
close (1)
```

```
c ----------------------------------------------------------------
c ----------------------------------------------------------------

      call SpeedSound(Ey,poisson,rho_solid,Csound)
      dt0=dTfactor*0.5*(0.25*(2*(MINVAL(dx0)))/Csound)

      X00=X
      open (unit = 1, file = "Xoriginal.dat")
        do ii=1,N
          write (1,*),X00(ii,:)
        enddo
      close (1)
      Time=0

      do ii=1,N
        do jj=1,3
          do kk=1,3
            Tij(ii,jj,kk)=0
            TTij(ii,jj,kk)=0
            Eij(ii,jj,kk)=0
          enddo
          if (Vtest(jj)==0) then
            Tij0(:,jj,jj)=0
          else
            Tij0(:,jj,jj)=Vtest(jj)/(abs(Vtest(jj)))
          endif
        enddo
      enddo
      Tij0=Tij0*(1e-9)
      deflect=0

      call cpu_time ( t1 )

      do ts=1,Nts
        call cpu_time ( t2 )
        print *,ts,'/',Nts,', Elapsed CPU time = ', (t2 - t1),' seconds

        xxx=((ts-1)*StudyCt/Nts)
        if (xxx==0) then
```

```
  LoopCT2=3*LoopCT
else
  LoopCT2=LoopCT
endif
deflectWeight=MINVAL(dx0)*(StartDefl+(xxx*NewDefl/StudyCt))

do yyy=1,LoopCT2

dt=dTdxfactor*(MINVAL(dx0))/(MAXVAL(abs(V))+(1e-10))
if (abs(deflect)<deflectWeight) then
  dt0x=abs(dTdxfactor*(MINVAL(dx0))/Vtest(2))
else
  dt0x=dt0
endif
if (dt0x<dt) then
  dt=dt0x
endif
if (dt0<dt) then
  dt=dt0
endif
Time=Time+dt

if (ts<=stop) then
  if (abs(deflect)<deflectWeight) then
    deflect=deflect+(Vtest(2)*dt)
  endif
else
  deflect=deflect
endif


call LinkList(N,X,MAXVAL(dx0),Links)
call ContactStress(N,Tij,Contact,ContactDir,Tij0)

Contact=ContactX
ContactDir=ContactDirX
ContactDirCT=ContactDirCTX

do jj=1,N
  if (IsSolid(jj)==1) then
```

```
            ct=ContactX(jj,1)
            do jj0=1,Links(jj,1)
              ii=Links(jj,jj0+1)

              if (ii/=jj) then
                call kernel(X(ii,:),X(jj,:),2*dx0(jj),Wij,dwdx,r)
                do kk=1,3
                  dx3(kk)=abs(X(ii,kk)-X(jj,kk))
                enddo
                fooint=MAXLOC(dx3,1)
                dxE=dx0(jj)*(1+Eij(jj,fooint,fooint))
                if (dxE<(dx0(jj)*1.05)) then
                  dxE=(dx0(jj)*1.05)
                endif

                if (r<dxE) then
                  kk=1
                  do uu=2,(ContactX(jj,1)+1)
                    vv=ContactX(jj,uu)
                    if (ii==vv) then
                      kk=0
                    endif
                  enddo
                  if (kk==1) then
                    ct=ct+1
                    Contact(jj,ct+1)=ii
                    ContactDir(jj,ct+1)=fooint
                    ContactDirCT(jj,fooint)=ContactDirCT(jj,fooint)+1
                    Tij0(jj,fooint,fooint)=-1
                  endif
                endif
              endif
            enddo
            Contact(jj,1)=ct
            ContactDir(jj,1)=ct
          endif
        enddo

c ____________________________________________________________
```

```
c ____________________________________________

c_______Calculate the new velocity. __________

        X0=X
        V0=V
        do xx=1,3
          do ii=1,N
            dxE=dx0(ii)*(1+Eij(ii,xx,xx))
            foo = g(xx)
            mass=massFct(ii)
            if (IsSolid(ii)==1) then

            if (Contact(ii,1)>0) then
            do uu=2,((Contact(ii,1))+1)
              jj=Contact(ii,uu)
              if (ContactDir(ii,uu)==xx) then
                if (uu>(1+ContactX(ii,1))) then
                  call Compression(xx,ii,jj,N,X,Eij,Ey,dx0,mass,foo2,a
                else
                  call Tension(xx,ii,jj,N,X,Eij,Ey,dx0,mass,foo,foo2,T
                endif
                foo=foo+foo2
              else
                yy=ContactDir(ii,uu)
                call Shear(xx,yy,ii,jj,N,X,Eij,mu,dx0,mass,foo2,TT)
                foo=foo+foo2
              endif
              enddo
            endif
            endif

            if (IsSolid(ii)==1) then
             do jj=1,N
               if (IsSolid(jj)==0) then
                 X1=X(ii,:)
                 X2=X(jj,:)
                 call LJfctSolid(xx,X1,X2,dx0(ii),P(ii),a)
                 foo=foo+(a/mass)
          endif
        enddo
      else
        do jj=1,N
          if (IsSolid(jj)==1) then

            X1=X(ii,:)
            X2=X(jj,:)
            V1=V(ii,:)
            V2=V(jj,:)
            call LJfct(xx,X1,X2,V1,V2,dx0(ii),dt,a)

            foo=foo+a
          endif
        enddo
      endif


      ct=2
      do jj0=1,Links(ii,1)
        jj=Links(ii,jj0+1)
        call kernel(X(ii,:),X(jj,:),2*dx0(ii),Wij,dwdx,r)
        if (IsSolid(jj)==0) then
          foo2=(P(jj)-P(ii))*(dx0(ii)**2)/mass
          foo2=-foo2*((X(ii,xx)-X(jj,xx))/r)
          foo=foo2
        endif
      enddo


      dVdx0=dVdx(ii,xx)
      dVdx(ii,xx) = foo
      V(ii,xx)=V(ii,xx)+(dt*(dVdx0+dVdx(ii,xx))/2)
    enddo
  enddo

  X0=X
  V00=V
  do xx=1,3
    do ii=1,N
```

```
            if (IsSolid(ii)==1) then
              if ((Contact(ii,1))>0) then
                foo=0
                do uu=2,((Contact(ii,1))+1)
                  jj=Contact(ii,uu)
                  foo=foo+V00(jj,xx)
                enddo
                foo=foo/(Contact(ii,1))
                foo=(foo+(V00(ii,xx)))/2
                V(ii,xx)=foo
              endif
            endif
          enddo
        enddo


c_______Definition of FixXY___________________

c       FixXY(ii)=0 --> Free Particle
c       FixXY(ii)=1 --> Fixed in space
c       FixXY(ii)=2 --> Fixed in X/1-direction
c       FixXY(ii)=3 --> Fixed in Y/2-direction
c       FixXY(ii)=4 --> Fixed in Z/3-direction
c       FixXY(ii)=5 --> Free in X/1-direction only
c       FixXY(ii)=6 --> Free in Y/2-direction only
c       FixXY(ii)=7 --> Free in Z/3-direction only
c       FixXY(ii)=8 --> Follows V_test
c       FixXY(ii)=9 --> Follows -V_test
c       FixXY(ii)=10 --> Follows V_test in the X/1-direction
c       FixXY(ii)=11 --> Follows -V_test in the X/1-direction
c       FixXY(ii)=12 --> Follows V_test in the Y/2-direction
c       FixXY(ii)=13 --> Follows -V_test in the Y/2-direction
c       FixXY(ii)=14 --> Follows V_test in the Z/3-direction
c       FixXY(ii)=15 --> Follows -V_test in the Z/3-direction

c_______End Definition of FixXY_______________


        foo2=0
c_______Calculate the new location. __________
```

```
do uu=1,3
  do ii=1,N
    if (IsSolid(ii)==1) then
    dV=V(ii,uu)+V0(ii,uu)
    if (dV>(0.1*(dx0(ii))/dt)) then
      dV=0
      V(ii,uu)=0
    elseif (abs(dV)<(1e-6)) then
      dV=0
      V(ii,uu)=0
    endif

    if (FixXY(ii)==1) then
      X(ii,uu)=X00(ii,uu)
    elseif (FixXY(ii)==2) then
      if (uu==1) then
        X(ii,uu)=X00(ii,uu)
      else
        X(ii,uu)=X(ii,uu)+(dt*dV/2)
      endif
    elseif (FixXY(ii)==3) then
      if (uu==2) then
        X(ii,uu)=X00(ii,uu)
      else
        X(ii,uu)=X(ii,uu)+(dt*dV/2)
      endif
    elseif (FixXY(ii)==4) then
      if (uu==3) then
        X(ii,uu)=X00(ii,uu)
      else
        X(ii,uu)=X(ii,uu)+(dt*dV/2)
      endif
    elseif (FixXY(ii)==5) then
      if (uu==1) then
        X(ii,uu)=X(ii,uu)+(dt*dV/2)
      else
        X(ii,uu)=X00(ii,uu)
      endif
    elseif (FixXY(ii)==6) then
      if (uu==2) then
      X(ii,uu)=X(ii,uu)+(dt*dV/2)
    else
      X(ii,uu)=X00(ii,uu)
    endif
  elseif (FixXY(ii)==7) then
    if (uu==3) then
      X(ii,uu)=X(ii,uu)+(dt*dV/2)
    else
      X(ii,uu)=X00(ii,uu)
    endif
  elseif (FixXY(ii)==8) then
    if (uu==2) then
      X(ii,uu)=X00(ii,uu)+deflect
    else
      X(ii,uu)=X00(ii,uu)
    endif
  elseif (FixXY(ii)==9) then
    if (uu==2) then
      X(ii,uu)=X00(ii,uu)-deflect
    else
      X(ii,uu)=X00(ii,uu)
    endif
  elseif (FixXY(ii)==10) then
    if (uu==1) then
      X(ii,uu)=X00(ii,uu)+deflect
    else
      X(ii,uu)=X(ii,uu)+(dt*dV/2)
    endif
  elseif (FixXY(ii)==11) then
    if (uu==1) then
      X(ii,uu)=X00(ii,uu)-deflect
    else
      X(ii,uu)=X(ii,uu)+(dt*dV/2)
    endif
  elseif (FixXY(ii)==12) then
    if (uu==2) then
      X(ii,uu)=X00(ii,uu)+deflect
    else
      X(ii,uu)=X(ii,uu)+(dt*dV/2)
    endif
```

```
              elseif (FixXY(ii)==13) then
                if (uu==2) then
                  X(ii,uu)=X00(ii,uu)-deflect
                else
                  X(ii,uu)=X(ii,uu)+(dt*dV/2)
                endif
              elseif (FixXY(ii)==14) then
                if (uu==3) then
                  X(ii,uu)=X00(ii,uu)+deflect
                else
                  X(ii,uu)=X(ii,uu)+(dt*dV/2)
                endif
              elseif (FixXY(ii)==15) then
                if (uu==3) then
                  X(ii,uu)=X00(ii,uu)-deflect
                else
                  X(ii,uu)=X(ii,uu)+(dt*dV/2)
                endif
              else
                X(ii,uu)=X(ii,uu)+(dt*dV/2)
              endif
              else
                X(ii,uu)=X(ii,uu)+(dt*dV/2)
              endif
            enddo
          enddo


c________Get new Stress. ______________________
          call GetDensity(X,V,N,dx0,dt,massFct,rho,IsSolid,rho)

c Calculate the Tensial Stress
          Tij=Tij-TTij
          do xx=1,3
            do ii=1,N
              mass=massFct(ii)
              if (IsSolid(ii)==1) then

              if (Contact(ii,1)>0) then
                foo=0
              ct2=0
              do uu=2,((Contact(ii,1))+1)
                TTxx=0
                do vv=1,3
                  TTxx=TTxx+Tij0(ii,vv,vv)
                enddo

                jj=Contact(ii,uu)
                if (ContactDir(ii,uu)==xx) then
                 if (uu>(1+ContactX(ii,1))) then
                   call Compression(xx,ii,jj,N,X,Eij,Ey,dx0,mass,a,TT)
                 else
                   call Tension(xx,ii,jj,N,X,Eij,Ey,dx0,mass,TTxx,a,TT
                 endif
                 foo=foo+TT
                 ct2=ct2+1
                endif
              enddo

              if (FixXY(ii)>0) then
                foo=foo/2
              endif
              if (ct2==0) then
                TTij(ii,xx,xx)=0*TTij(ii,xx,xx)
              else
                TTij(ii,xx,xx)=foo/ct2
              endif
            endif

            else
              TTij(ii,xx,xx)=(Bulk_water/3)*((rho(ii)/rho0(ii))-1)
            endif
          enddo
        enddo



c Calculate the Shear Stress
        do vv=1,3
          call GetUV(vv,uv)
          do ii=1,N
            if (IsSolid(ii)==1) then
              foo=0
              do uu=2,((Contact(ii,1))+1)
                jj=Contact(ii,uu)
                if (ContactDir(ii,uu)==uv(2)) then
                  call Shear(uv(1),uv(2),ii,jj,N,X,Eij,mu,dx0,mass,a,T
                  foo=foo+TT
                endif
              enddo

              if (FixXY(ii)==0) then
                if (ContactDirCT(ii,uv(2))==0) then
                  foo=0
                else
                  foo=foo/ContactDirCT(ii,uv(2))
                endif
              else
                foo=foo/2
              endif

              TTij(ii,uv(2),uv(1))=foo
              TTij(ii,uv(1),uv(2))=foo
            endif
          enddo
        enddo

        Tij=Tij+TTij


c _______________Get new strain_______________

        do kk=1,N
          do ii=1,3
            Eij(kk,ii,ii)=(1/Ey)*(Tij(kk,ii,ii))
            call GetUV(ii,uv)
            foo=(poisson/Ey)*(Tij(kk,uv(1),uv(1)))
            foo=foo+(poisson/Ey)*(Tij(kk,uv(2),uv(2)))
            Eij(kk,ii,ii)=Eij(kk,ii,ii)-foo
          enddo
          do ii=1,3
            do jj=1,3
              if (jj/=ii) then
                Eij(kk,ii,jj)=Tij(kk,ii,jj)/(2*mu)
              endif
            enddo
          enddo
        enddo




c _______________Save Data____________________

        do ii=1,N
          foo=(Tij(ii,1,1)-Tij(ii,2,2))**2
          foo=foo+(Tij(ii,2,2)-Tij(ii,3,3))**2
          foo=foo+(Tij(ii,1,1)-Tij(ii,3,3))**2
          foo2=(Tij(ii,1,2)**2)+(Tij(ii,2,3)**2)+(Tij(ii,3,1)**2)
          foo=sqrt((foo+(6*foo2))/2)
          Tvm0(ii)=foo
          P(ii)=(Tij(ii,1,1)+Tij(ii,2,2)+Tij(ii,3,3))/3
        enddo

        TimeFct(ts)=Time
        Xout(:,ts)=X(:,1)
        Yout(:,ts)=X(:,2)
        Zout(:,ts)=X(:,3)
        VoutX(:,ts)=V(:,1)
        VoutY(:,ts)=V(:,2)
        VoutZ(:,ts)=V(:,3)
        Rout(:,ts)=rho
        Pout(:,ts)=P
        T11(:,ts)=Tij(:,1,1)
        T12(:,ts)=Tij(:,1,2)
        T13(:,ts)=Tij(:,1,3)
        T21(:,ts)=Tij(:,2,1)
        T22(:,ts)=Tij(:,2,2)
        T23(:,ts)=Tij(:,2,3)
        T31(:,ts)=Tij(:,3,1)
        T32(:,ts)=Tij(:,3,2)
        T33(:,ts)=Tij(:,3,3)
        Tvm(:,ts)=Tvm0
        E22(:,ts)=Eij(:,2,2)
        E11(:,ts)=Eij(:,1,1)
        dVdxFct(:,ts)=dVdx(:,1)
        dVdyFct(:,ts)=dVdx(:,2)
        dVdzFct(:,ts)=dVdx(:,3)

        enddo
      enddo

      call cpu_time ( t2 )
      print *,'Elapsed CPU time = ', (t2 - t1),' seconds'


c -------------------------------------------------------
c  Print data to dat-files
c -------------------------------------------------------

      open (unit = 1, file = "VarDat.dat")
        write (1,*),Ey
        write (1,*),mu
        write (1,*),StudyCt
      close (1)

      open (unit = 1, file = "X.dat")
      do jj=1,Nts
        printVar=Xout(:,jj)
        write (1,*),printVar
      enddo
      close(1)

      open (unit = 1, file = "Y.dat")
      do jj=1,Nts
        printVar=Yout(:,jj)
        write (1,*),printVar
      enddo
      close(1)
```

```
open (unit = 1, file = "Z.dat")
do jj=1,Nts
  printVar=Zout(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "P.dat")
do jj=1,Nts
  printVar=Pout(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "rho.dat")
do jj=1,Nts
  printVar=Rout(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "T11.dat")
do jj=1,Nts
  printVar=T11(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "T12.dat")
do jj=1,Nts
  printVar=T12(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "T13.dat")
do jj=1,Nts
  printVar=T13(:,jj)
  write (1,*),printVar
enddo
```

```
close(1)

open (unit = 1, file = "T21.dat")
do jj=1,Nts
  printVar=T21(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "T22.dat")
do jj=1,Nts
  printVar=T22(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "T23.dat")
do jj=1,Nts
  printVar=T23(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "T31.dat")
do jj=1,Nts
  printVar=T31(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "T32.dat")
do jj=1,Nts
  printVar=T32(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "T33.dat")
do jj=1,Nts
  printVar=T33(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "E22.dat")
do jj=1,Nts
  printVar=E22(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "E11.dat")
do jj=1,Nts
  printVar=E11(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "VonMises.dat")
do jj=1,Nts
  printVar=Tvm(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "Vx.dat")
do jj=1,Nts
  printVar=VoutX(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "Vy.dat")
do jj=1,Nts
  printVar=VoutY(:,jj)
  write (1,*),printVar
enddo
close(1)

open (unit = 1, file = "Vz.dat")
```

```
      do jj=1,Nts
        printVar=VoutZ(:,jj)
        write (1,*),printVar
      enddo
      close(1)

      open (unit = 1, file = "Time.dat")
      do jj=1,Nts
        printVar=TimeFct(jj)
        write (1,*),printVar
      enddo
      close(1)

c ----------------------------

      open (unit = 1, file = "Fixed.dat")
      do jj=1,N
        write (1,*),FixXY(jj)
      enddo
      close (1)

      open (unit = 1, file = "Contact.dat")
      do jj=1,N
        write (1,*),Contact(jj,:)
      enddo
      close (1)

      open (unit = 1, file = "ContactDir.dat")
      do jj=1,N
        write (1,*),ContactDir(jj,:)
      enddo
      close (1)

      open (unit = 1, file = "ContactDirCT.dat")
      do jj=1,N
        write (1,*),ContactDirCT(jj,:)
      enddo
      close (1)

      open (unit = 1, file = "ContactX.dat")
```

```
do jj=1,N
  write (1,*),ContactX(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactDirX.dat")
do jj=1,N
  write (1,*),ContactDirX(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactDirCTX.dat")
do jj=1,N
  write (1,*),ContactDirCTX(jj,:)
enddo
close (1)

open (unit = 1, file = "Links.dat")
do jj=1,N
  write (1,*),Links(jj,:)
enddo
close (1)

open (unit = 1, file = "Mass.dat")
do jj=1,N
  write (1,*),massFct(jj)
enddo
close (1)

open (unit = 1, file = "dX.dat")
do jj=1,N
  write (1,*),dx0(jj)
enddo
close (1)


open (unit = 1, file = "X0.dat")
do jj=1,N
  write (1,*),X(jj,:)
enddo
```

```
      close (1)

      open (unit = 1, file = "V0.dat")
      do jj=1,N
        write (1,*),V(jj,:)
      enddo
      close (1)

      open (unit = 1, file = "dVdX.dat")
      do jj=1,N
        write (1,*),dVdxFct(jj,:)
      enddo
      close (1)

      open (unit = 1, file = "dVdY.dat")
      do jj=1,N
        write (1,*),dVdyFct(jj,:)
      enddo
      close (1)

      open (unit = 1, file = "dVdZ.dat")
      do jj=1,N
        write (1,*),dVdzFct(jj,:)
      enddo
      close (1)


      end program



c ________________________________________________________________________

      subroutine GetUV(ii,uv)
c     -------------------------------------------------------------------
      implicit none

      integer, intent(in) :: ii
      integer, intent(out) :: uv(2)
      integer jj,ct
      ct=0
      do jj=1,3
        if (jj/=ii) then
          ct=ct+1
          uv(ct)=jj
        endif
      enddo

      END subroutine GetUV


c ______________________________________________________________________

      subroutine FindL(N,h,mu,X,V,P,Tij,DSDtN)
c     ----------------------------------------------------------------------
      implicit none

      integer, intent(in) :: N
      double precision, intent(in) :: Tij(N,3,3)
      double precision, intent(in) :: X(N,3),V(N,3),h
      double precision, intent(in) :: mu
      double precision, intent(out) :: DSDtN(N,3,3),P(N)

      integer ii,jj, kk, uu, vv
      double precision L(3,3),D(3,3),Omg(3,3),r,W,Wtotal
      double precision dV,dx,D0(3,3),Omg0(3,3),DSDt(3,3)
      double precision foo,foo1,foo2,foo3,foo4,Sij(3,3)
      double precision dwdx(3)

      do jj=1,N
        Wtotal = 0
        do vv=1,3
          do uu=1,3
            L(uu,vv)=0
          enddo
        enddo
        do ii=1,N
          call kernel(X(jj,:),X(ii,:),h,W,dwdx,r)
          do vv = 1,3
```

```
    do uu = 1,3
      dV=(V(ii,uu)-V(jj,uu))
      dx=(X(ii,vv)-X(jj,vv))
      if (dx==0) then
        L(uu,vv)=L(uu,vv)
      else
        L(uu,vv)=L(uu,vv)+(dwdx(vv)*dV/dx)
        Wtotal=Wtotal+W
      endif
    enddo
  enddo
enddo
L=L*0/Wtotal

do vv=1,3
  do uu=1,3
    D(uu,vv)=(L(uu,vv)+L(vv,uu))/2
    Omg(uu,vv)=(L(uu,vv)-L(vv,uu))/2
  enddo
enddo


do vv=1,3
  do uu=1,3
    Sij(uu,vv)=Tij(jj,uu,vv)
    if (uu==vv) then
      Sij(uu,vv)=Sij(uu,vv)-P(jj)
    endif
  enddo
enddo

do vv=1,3
  do uu=1,3
    foo1=0
    foo2=0
    do kk=1,3
      foo1=foo1+(Sij(uu,kk)*Omg(vv,kk))
      foo2=foo2+(Omg(uu,kk)*Sij(kk,vv))
    enddo
    foo3=2*mu*D(uu,vv)
```

```
            if (uu==vv) then
              foo4=(-2*mu/3)*D(uu,vv)
            else
              foo4=0
            endif
            DSDtN(jj,uu,vv)=foo1+foo2+foo3+foo4
          enddo
        enddo




      enddo

      END subroutine FindL

c ____________________________________________________________________

      subroutine kernel(x1,x2,h,w,dwdx,r)

c---------------------------------------------------------------------
c   Subroutine to calculate the smoothing kernel wij and its
c   derivatives dwdxij.

c     r    : Distance between particles i and j                    [i
c     dx   : x-, y- and z-distance between i and j                 [i
c     h : Smoothing length                                       [in]
c     w    : Kernel for all interaction pairs                     [ou
c     dwdx : Derivative of kernel with respect to x, y and z      [ou

      implicit none

      double precision, intent(in) :: x1(3),x2(3),h
      double precision, intent(out) :: w,dwdx(3),r
      integer i, j, d, skf
      double precision q, dw, factor,dx(3),pi,u

      do i=1,3
        dx(i)=abs(X1(i)-X2(i))
      enddo
      r=(dx(1)**2)+(dx(2)**2)+(dx(3)**2)
```

```
r=sqrt(r)

pi = 3.14159265358979
u=10/(7*pi)
q = r/h
w = 0.e0
do d=1,3
  dwdx(d) = 0.e0
enddo

if (r==0) then
  w=0
  dwdx(1)=0
  dwdx(2)=0
  dwdx(3)=0
else
  if (q<1) then
    w=1+(-1.5*(q**2))+(0.75*(q**3))
    do i=1,3
      dwdx(i)=((9*r/(4*h))-3)*(dx(i)/(h**2))
    enddo
  else
    if (q<2) then
      w=((2-q)**3)/4
      do i=1,3
        dwdx(i)=(-3/(4*h*r))*((2-q)**2)*dx(i)
      enddo
    else
      w=0
      dwdx(1)=0
      dwdx(2)=0
      dwdx(3)=0
    endif
  endif
endif
w=w*u
do i=1,3
  dwdx(i)=u*dwdx(i)
enddo
```

```
      END subroutine kernel

c ________________________________________________________________________

      subroutine GetDPDT(N,X,V,dx,K,massFct,rho,DPDT)
c     ------------------------------------------------------------------
      implicit none

      integer, intent(in) :: N
      double precision, intent(in) :: X(N,3),V(N,3)
      double precision, intent(in) :: dx(N),massFct(N)
      double precision, intent(in) :: K,rho(N)
      double precision, intent(out) :: DPDT(N,3)

      integer ii,jj, kk
      double precision W0, dwdx(3),foo,dV,r
      double precision h,mass

      do jj=1,N
        h=2*dx(jj)
        mass=massFct(jj)
        do ii=1,N
          call kernel(X(ii,:),X(jj,:),h,W0,dwdx,r)
          foo=0
          do kk=1,3
            dV=V(ii,kk)-V(jj,kk)
            foo=-K*mass*dV*dwdx(kk)/rho(ii)
            DPDT(jj,kk)=DPDT(jj,kk)+foo
          enddo
        enddo
      enddo

      END subroutine GetDPDT

c ________________________________________________________________________

      subroutine GetDensity0(X,N,dx,mass,rho0,IsSolid,rho)
c     ------------------------------------------------------------------
      implicit none
      integer, intent(in) :: N, IsSolid(N)
      double precision, intent(in) :: X(N,3),rho0(N)
      double precision, intent(in) :: dx(N),mass(N)
      double precision, intent(out) :: rho(N)

      integer ii,jj, kk
      double precision W0, r0, fooN, fooD, h, r, dwdx(3)
      double precision rhoIn(N)

      rhoIn=rho0
      do jj=1,N
        fooN=0
c         fooD=0
        h = 3*dx(jj)
        do ii=1,N
          if (IsSolid(ii)==IsSolid(jj)) then
            call kernel(X(ii,:),X(jj,:),h,W0,dwdx,r)
            fooN=fooN+(mass(ii)*W0)
          endif
        enddo
        rho(jj)=((3.14159*4/3)*fooN/(h**3))
      enddo

      END subroutine GetDensity0


c ______________________________________________________________________

      subroutine GetDensity(X,V,N,dx,dt,massFct,rho0,IsSolid,rho)
c     -------------------------------------------------------------------
      implicit none

      integer, intent(in) :: N, IsSolid(N)
      double precision, intent(in) :: X(N,3),V(N,3),rho0(N)
      double precision, intent(in) :: dt,dx(N),massFct(N)
      double precision, intent(out) :: rho(N)

      integer ii,jj, kk
      double precision W,r,dwdx(3),foo1,foo2
      double precision h,mass,rhoIn(N)
      rhoIn=rho0
      do jj=1,N
        h=dx(jj)
        mass=massFct(jj)
        foo1=0
        do ii=1,N
          if (IsSolid(ii)==IsSolid(jj)) then
            call kernel(X(ii,:),X(jj,:),h,W,dwdx,r)
            do kk=1,3
              foo1=foo1-((mass/rhoIn(ii))*V(ii,kk)*dwdx(kk))
            enddo
          else
            foo1=0
          endif
        enddo
        foo2=dt*foo1*rhoIn(jj)
        rho(jj)=rhoIn(jj)+foo2
      enddo


      END subroutine GetDensity

c _______________________________________________________

      subroutine SpeedSound(YM,poisson,rho0min,Csound)

      implicit none

      double precision, intent(in) :: YM,poisson,rho0min
      double precision, intent(out) :: Csound
      double precision CsoundT,CsoundS,G

      CsoundT=(YM*(1-poisson))/rho0min
      CsoundT=CsoundT/((1+poisson)*(1-(2*poisson)))
      CsoundT=sqrt(CsoundT)

      G=(3*(1-poisson)/(1+poisson))-1
      G=G*YM/(4*(1-(2*poisson)))
      CsoundS=sqrt(G/rho0min)
      if (CsoundT>CsoundS) then
        Csound=CsoundT
      else
        Csound=CsoundS
      endif

      end subroutine SpeedSound

c ______________________________________________________________________

      subroutine LJfct(p,X1,X2,V1,V2,r0,dt,a)

      implicit none

      integer, intent(in) :: p
      double precision, intent(in) :: X1(3),X2(3)
      double precision, intent(in) :: V1(3),V2(3)
      double precision, intent(in) :: r0,dt
      double precision, intent(out) :: a

      integer ii
      double precision foo,r,r00,coeff,dir,foo2

      r=0
      do ii=1,3
        r=r+((X1(ii)-X2(ii))**2)
      enddo
      r=sqrt(r)
      if ((abs(X1(p)-X2(p)))==0) then
        dir=0
      else
        dir=(X1(p)-X2(p))/abs(X1(p)-X2(p))
      endif

      if (r>r0) then
        foo=0
      else
        coeff=(((r0/r)**12)-((r0/r)**4))
        foo=(V1(p)-V2(p))*coeff*dir/dt
      endif
      a=foo

      end subroutine LJfct

c ________________________________________________________________________

c ________________________________________________________________________

      subroutine LJfctSolid(p,X1,X2,r0,P2,f)

      implicit none

      integer, intent(in) :: p
      double precision, intent(in) :: X1(3),X2(3)
      double precision, intent(in) :: P2,r0
      double precision, intent(out) :: f

      integer ii
      double precision foo,r,del,trig

      r=0
      do ii=1,3
        r=r+((X1(ii)-X2(ii))**2)
      enddo
      del=(X1(p)-X2(p))
      r=sqrt(r)
      trig=del/r


      if (r>r0) then
        foo=0
      else
        foo=trig*P2*r0*r0
      endif
      f=foo

      end subroutine LJfctSolid
```

```
c ____________________________________________________________________

      subroutine Tension(xx,ii,jj,N,X,E,Ey,dx0,mass,TTxx,a,TT)

      implicit none

      integer, intent(in) :: xx,ii,jj,N
      double precision, intent(in) :: X(N,3),E(N,3,3)
      double precision, intent(in) :: Ey,dx0(N),mass,TTxx
      double precision, intent(out) :: a,TT


      integer ct,uv(2)
      double precision foo,dx,strain,Ai,A0,dir
      double precision dxE,strainE,a2,TT1,TT2,TTxxR

      A0=(dx0(ii))**2
      dx=X(jj,xx)-X(ii,xx)
      dxE=(1+((E(ii,xx,xx)+E(jj,xx,xx))/2))*dx0(ii)

      if (abs(dx)>0) then
        dir=dx/abs(dx)
      else
        dir=0
      endif

      strain=(abs(dx)-dx0(ii))/dx0(ii)
      strainE=(abs(dx)-dxE)/dxE

      a=0
      if (ii==jj) then
        a=0
        TT1=0
      else

        call GetUV(xx,uv)
        Ai=A0*(1+E(ii,uv(1),uv(1)))
        Ai=Ai*(1+E(ii,uv(2),uv(2)))
        a=dir*Ai*Ey*strainE/mass
```

```
    if (strain>0) then
      TT1=Ey*strain
    else
      TT1=0
    endif
  endif

  call Compression(xx,ii,jj,N,X,E,Ey,dx0,mass,a2,TT2)

  TTxxR=TTxx
  if (TTxxR>0) then
    TT=TT1
  elseif (TTxxR<0) then
    TT=TT2
  else
    if (strainE<0) then
      TT=TT2
    elseif (strainE>0) then
      TT=TT1
    else
      TT=(TT1+TT2)/2
    endif
  endif


  end subroutine Tension

c ______________________________________________________________________

  subroutine Compression(xx,ii,jj,N,X,E,Ey,dx0,mass,a,TT)

  implicit none

  integer, intent(in) :: xx,ii,jj,N
  double precision, intent(in) :: X(N,3),E(N,3,3)
  double precision, intent(in) :: Ey,dx0(N),mass
  double precision, intent(out) :: a,TT

  integer ct,uv(2)
  double precision foo,dx,strain,Ai,A0,dir
double precision dxE,strainE

A0=(dx0(ii))**2
dx=X(jj,xx)-X(ii,xx)
dxE=(1+((E(ii,xx,xx)+E(jj,xx,xx))/2))*dx0(ii)

if (abs(dx)>0) then
  dir=dx/abs(dx)
else
  dir=0
endif

strain=(abs(dx)-dx0(ii))/dx0(ii)
strainE=(abs(dx)-dxE)/dxE

a=0
if (ii==jj) then
  a=0
  TT=0
else

  call GetUV(xx,uv)
  Ai=A0*(1+E(ii,uv(1),uv(1)))
  Ai=Ai*(1+E(ii,uv(2),uv(2)))
  a=dir*Ai*Ey*strainE/mass

  if (strain<0) then
    TT=Ey*strain
  else
    TT=0
  endif
endif

if (TT>0) then
  TT=0
  a=0
endif

end subroutine Compression
```

```
C  ____________________________________________________________________

      subroutine Shear(xx,yy,ii,jj,N,X,E,G,dx0,mass,a,TT)

      implicit none

      integer, intent(in) :: xx,yy,ii,jj,N
      double precision, intent(in) :: X(N,3),E(N,3,3)
      double precision, intent(in) :: G,dx0(N),mass
      double precision, intent(out) :: a,TT

      integer ct,uv(2)
      double precision delta,gamma,L
      double precision foo,Ai,A0,dir

      L=dx0(ii)
      A0=(dx0(ii))**2
      delta=(X(jj,xx)-X(ii,xx))
      if (abs(delta)>0) then
        dir=delta/abs(delta)
      else
        dir=0
      endif
      delta=abs(delta)
      gamma=delta/L


      if (ii==jj) then
        a=0
        TT=0
      else
        if (gamma>0) then
          TT=G*gamma
        else
          TT=0
        endif
```

```
          if (gamma>0) then
            call GetUV(yy,uv)
            Ai=A0*(1+E(ii,uv(1),uv(1)))
            Ai=Ai*(1+E(ii,uv(2),uv(2)))
            a=dir*Ai*G*gamma/mass
          else
            a=0
          endif

        endif


        end subroutine Shear


c ______________________________________________________________________

        subroutine ContactStress(N,TijIn,Contact,ContactDir,TijOut)

        implicit none

        integer, intent(in) :: N,Contact(N,N+1),ContactDir(N,N+1)
        double precision, intent(in) :: TijIn(N,3,3)
        double precision, intent(out) :: TijOut(N,3,3)

        integer ii,jj,xx,uu,cycle,ContactDirCTx
        double precision Tij0(N,3,3),Tij(N,3,3)
        double precision foo,Total(3),Avg(3)

        Tij0=TijIn

        do cycle=1,1000
        do ii=1,N
          do xx=1,3
            Avg(xx)=0
            ContactDirCTx=0
            do jj=2,(Contact(ii,1))
              if (ContactDir(ii,jj)==xx) then
                uu=Contact(ii,jj)
            Avg(xx)=Avg(xx)+Tij0(uu,xx,xx)
            ContactDirCTx=ContactDirCTx+1
          endif
        enddo
        if (ContactDirCTx==0) then
          Tij(ii,xx,xx)=Tij0(ii,xx,xx)
        else
          foo=Avg(xx)/ContactDirCTx
          Tij(ii,xx,xx)=(Tij0(ii,xx,xx)+foo)/2
        endif
      enddo
    enddo
    Tij0=Tij
    enddo
    TijOut=Tij


    end subroutine ContactStress


c ____________________________________________________________________

    subroutine LinkList(N,X,h,Links)

    implicit none

    integer, intent(in) :: N
    double precision, intent(in) :: X(N,3),h
    integer, intent(out) :: Links(N,(N+1))

    integer ii,jj,xx,uu,ct,fooInt,LinkCT(3),LLloc(N,3)
    double precision foo,DistCT(3),Wij,dwdx(3),r

    do ii=1,3
      DistCT(ii)=MAXVAL(X(:,ii))-MINVAL(X(:,ii))
      LinkCT(ii)=CEILING(DistCT(ii)/h)
    enddo
    Links(:,:)=0

    do ii=1,N
```

```
  do jj=1,3
    foo=(X(ii,jj)-MINVAL(X(:,jj)))/DistCT(jj)
    foo=ceiling(foo*LinkCT(jj))
    if (foo==0) then
      foo=foo+1
    endif
    LLloc(ii,jj)=foo
  enddo
enddo

do ii=1,N
  ct=1
  do jj=1,N
    xx=1
    do uu=1,3
      fooInt=abs(LLloc(ii,uu)-LLloc(jj,uu))
      if (fooInt>1) then
        xx=0
      endif
    enddo
    if (xx==1) then
      call kernel(X(ii,:),X(jj,:),h,Wij,dwdx,r)
      if (Wij>0) then
        ct=ct+1
        Links(ii,ct)=jj
      endif
    endif
  enddo
  Links(ii,1)=ct-1
enddo


end subroutine LinkList


c ____________________________________________________________
```

tension_steel.f

```
      subroutine ModelBlock(Nout)

      implicit none

      integer, intent(out) :: Nout
      integer N,ctbar(3),Nsphere,ct,ii,jj,kk,uu
      integer fooint,split
      double precision RadiusFactor,Radius,masX,dx00
      double precision angleFrac,angle,Yr0,dx3(3),third
      double precision Zloc,Yloc,Xloc,r,pi,rho_solid
      integer, allocatable, dimension(:) :: FixXY,IsSolid,BreakContact
      integer, allocatable, dimension(:,:) :: Contact,ContactX
      integer, allocatable, dimension(:,:) :: ContactDir,ContactDirX
      integer, allocatable, dimension(:,:) :: ContactDirCT,ContactDirC
      double precision, allocatable, dimension(:,:) :: X,V,dVdx
      double precision, allocatable, dimension(:) :: massFct,dx0
      double precision, allocatable, dimension(:) :: rho0,rho

      open (unit = 1, file = "SimSpec.dat")
        write (1,*),207e9        ! Young’s Modulus of Steel
        write (1,*),0.3          ! Poisson’s Ratio of Steel
        write (1,*),7800         ! Density of Steel
        write (1,*),0            ! Forced Density in X direction (Vtes
        write (1,*),1e3         ! Forced Density in Y direction (Vtest
        write (1,*),0            ! Forced Density in Z direction (Vtes
        write (1,*),0.3          ! Gamma (blend stress)
        write (1,*),250          ! Number of Recorded Time Steps (Nts)
        write (1,*),6            ! Time Steps between recorded Time St
        write (1,*),1            ! Time Steps between recorded Time St
        write (1,*),0.18         ! (StartDefl)
        write (1,*),0.05         ! (NewDefl)
        write (1,*),0.25         ! (dTfactor)
        write (1,*),0.01         ! (dTdxfactor)
        write (1,*),250          ! (stop)
        write (1,*),2.15e9       ! (Bulk_water)
      close (1)
      ctbar(1)=3      ! 3
      ctbar(2)=11     ! 11
      ctbar(3)=3      ! 3
      masX=0.1
      rho_solid=7800


      third=1.0/3.0
      dx00=(masX/rho_solid)**third
      N=(ctbar(1)*ctbar(2)*ctbar(3))


C  _____________________________________________
C                  ALLOCATION
C  _____________________________________________


      ALLOCATE (FixXY(N))
      ALLOCATE (IsSolid(N))
      ALLOCATE (BreakContact(N))
      ALLOCATE (X(N,3))
      ALLOCATE (V(N,3))
      ALLOCATE (dVdx(N,3))
      ALLOCATE (rho(N))
      ALLOCATE (rho0(N))
      ALLOCATE (massFct(N))
      ALLOCATE (dx0(N))
      ALLOCATE (Contact(N,(N+1)))
      ALLOCATE (ContactDir(N,(N+1)))
      ALLOCATE (ContactDirCT(N,3))
      ALLOCATE (ContactX(N,(N+1)))
      ALLOCATE (ContactDirX(N,(N+1)))
      ALLOCATE (ContactDirCTX(N,3))

C  _____________________________________________
```

```
c Set the parameters for the steel bar
      ct = 0
      Zloc=-dx00
      do uu=1,ctbar(3)
        Zloc=Zloc+dx00
        Yloc=-dx00
        do jj=1,ctbar(2)
          Yloc = Yloc + dx00
          Xloc = 0
          do ii=1,ctbar(1)
            ct = ct + 1
            if (jj==ctbar(2)) then
              FixXY(ct)=12
            elseif (jj==1) then
              FixXY(ct)=13
            else
              FixXY(ct)=0
            endif
            Xloc = Xloc + dx00
            X(ct,1) = Xloc
            X(ct,2) = Yloc
            X(ct,3) = Zloc
            V(ct,1) = 0
            V(ct,2) = 0
            V(ct,3) = 0
            dVdX(ct,1) = 0
            dVdX(ct,2) = 0
            dVdX(ct,3) = 0
            rho(ct) = rho_solid
            rho0(ct) = rho_solid
            dx0(ct) = dx00
            IsSolid(ct) = 1
            massFct(ct) = masX
            if (jj==(ctbar(2)/2)) then
              BreakContact(ct)=1
            elseif (jj==(1+(ctbar(2)/2))) then
              BreakContact(ct)=2
              else
                BreakContact(ct)=0
              endif
            enddo
          enddo
        enddo


  c Set Contact links
        do jj=1,N
          if (IsSolid(jj)==1) then
            ct=0
            do ii=1,N
              if (IsSolid(ii)==1) then
                if (ii/=jj) then
                  r=0
                  do kk=1,3
                    dx3(kk)=abs(X(ii,kk)-X(jj,kk))
                    r=r+((X(ii,kk)-X(jj,kk))**2)
                  enddo
                  r=sqrt(r)
                  if (r<(dx0(jj)*1.1)) then
                    split=1
                    if (BreakContact(ii)==1) then
                      if (BreakContact(jj)==2) then
                        split=0
                      endif
                    endif
                    if (BreakContact(ii)==2) then
                      if (BreakContact(jj)==1) then
                        split=0
                      endif
                    endif
                    split=1
                    if (split==1) then
                      ct=ct+1
                      Contact(jj,ct+1)=ii
                      fooint=MAXLOC(dx3,1)
                      ContactDir(jj,ct+1)=fooint
                      ContactDirCT(jj,fooint)=ContactDirCT(jj,fooint)+1
            endif
          endif
        endif
      endif
    enddo
    Contact(jj,1)=ct
    ContactDir(jj,1)=ct
  endif
enddo

ContactX=Contact
ContactDirX=ContactDir
ContactDirCTX=ContactDirCT



open (unit = 1, file = "Fixed.dat")
do jj=1,N
  write (1,*),FixXY(jj)
enddo
close (1)

open (unit = 1, file = "ContactDirX.dat")
do jj=1,N
  write (1,*),ContactDirX(jj,:)
enddo
close (1)

open (unit = 1, file = "Contact.dat")
do jj=1,N
  write (1,*),Contact(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactDir.dat")
do jj=1,N
  write (1,*),ContactDir(jj,:)
enddo
close (1)
```

```
open (unit = 1, file = "ContactDirCT.dat")
do jj=1,N
  write (1,*),ContactDirCT(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactX.dat")
do jj=1,N
  write (1,*),ContactX(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactDirCTX.dat")
do jj=1,N
  write (1,*),ContactDirCTX(jj,:)
enddo
close (1)

open (unit = 1, file = "Mass.dat")
do jj=1,N
  write (1,*),massFct(jj)
enddo
close (1)

open (unit = 1, file = "dX.dat")
do jj=1,N
  write (1,*),dx0(jj)
enddo
close (1)

open (unit = 1, file = "X0.dat")
do jj=1,N
  write (1,*),X(jj,:)
enddo
close (1)

open (unit = 1, file = "V0.dat")
do jj=1,N
  write (1,*),V(jj,:)
enddo
```

```
      close (1)

      open (unit = 1, file = "dVdX.dat")
      do jj=1,N
        write (1,*),dVdx(jj,:)
      enddo
      close (1)

      open (unit = 1, file = "rho0.dat")
      do jj=1,N
        write (1,*),rho0(jj)
      enddo
      close (1)

      open (unit = 1, file = "rho_init.dat")
      do jj=1,N
        write (1,*),rho(jj)
      enddo
      close (1)


      open (unit = 1, file = "IsSolid.dat")
      do jj=1,N
        write (1,*),IsSolid(jj)
      enddo
      close (1)


      Nout=N

      end subroutine ModelBlock

C ____________________________________________________________________
```

compress_steel.f

```
      subroutine ModelBlock(Nout)

      implicit none

      integer, intent(out) :: Nout
      integer N,ctbar(3),Nsphere,ct,ii,jj,kk,uu
      integer fooint,split
      double precision RadiusFactor,Radius,masX,dx00
      double precision angleFrac,angle,Yr0,dx3(3),third
      double precision Zloc,Yloc,Xloc,r,pi,rho_solid
      integer, allocatable, dimension(:) :: FixXY,IsSolid,BreakContact
      integer, allocatable, dimension(:,:) :: Contact,ContactX
      integer, allocatable, dimension(:,:) :: ContactDir,ContactDirX
      integer, allocatable, dimension(:,:) :: ContactDirCT,ContactDirC
      double precision, allocatable, dimension(:,:) :: X,V,dVdx
      double precision, allocatable, dimension(:) :: massFct,dx0
      double precision, allocatable, dimension(:) :: rho0,rho

      open (unit = 1, file = "SimSpec.dat")
        write (1,*),207e9        ! Young's Modulus of Steel
        write (1,*),0.3          ! Poisson's Ratio of Steel
        write (1,*),7800         ! Density of Steel
        write (1,*),0            ! Forced Density in X direction (Vtes
        write (1,*),-1e3         ! Forced Density in Y direction (Vtes
        write (1,*),0            ! Forced Density in Z direction (Vtes
        write (1,*),0.3          ! Gamma (blend stress)
        write (1,*),250          ! Number of Recorded Time Steps (Nts)
        write (1,*),6            ! Time Steps between recorded Time St
        write (1,*),1            ! Time Steps between recorded Time St
        write (1,*),0.18         ! (StartDefl)
        write (1,*),0.05         ! (NewDefl)
        write (1,*),0.25         ! (dTfactor)
        write (1,*),0.01         ! (dTdxfactor)
        write (1,*),250          ! (stop)
        write (1,*),2.15e9       ! (Bulk_water)
      close (1)
      ctbar(1)=3      ! 3
      ctbar(2)=11     ! 11
      ctbar(3)=3      ! 3
      masX=0.1
      rho_solid=7800


      third=1.0/3.0
      dx00=(masX/rho_solid)**third
      N=(ctbar(1)*ctbar(2)*ctbar(3))


c _____________________________________________
c                 ALLOCATION
c _____________________________________________


      ALLOCATE (FixXY(N))
      ALLOCATE (IsSolid(N))
      ALLOCATE (BreakContact(N))
      ALLOCATE (X(N,3))
      ALLOCATE (V(N,3))
      ALLOCATE (dVdx(N,3))
      ALLOCATE (rho(N))
      ALLOCATE (rho0(N))
      ALLOCATE (massFct(N))
      ALLOCATE (dx0(N))
      ALLOCATE (Contact(N,(N+1)))
      ALLOCATE (ContactDir(N,(N+1)))
      ALLOCATE (ContactDirCT(N,3))
      ALLOCATE (ContactX(N,(N+1)))
      ALLOCATE (ContactDirX(N,(N+1)))
      ALLOCATE (ContactDirCTX(N,3))

c _____________________________________________
```

```
c Set the parameters for the steel bar
      ct = 0
      Zloc=-dx00
      do uu=1,ctbar(3)
        Zloc=Zloc+dx00
        Yloc=-dx00
        do jj=1,ctbar(2)
          Yloc = Yloc + dx00
          Xloc = 0
          do ii=1,ctbar(1)
            ct = ct + 1
            if (jj==ctbar(2)) then
              FixXY(ct)=12
            elseif (jj==1) then
              FixXY(ct)=13
            else
              FixXY(ct)=0
            endif
            Xloc = Xloc + dx00
            X(ct,1) = Xloc
            X(ct,2) = Yloc
            X(ct,3) = Zloc
            V(ct,1) = 0
            V(ct,2) = 0
            V(ct,3) = 0
            dVdX(ct,1) = 0
            dVdX(ct,2) = 0
            dVdX(ct,3) = 0
            rho(ct) = rho_solid
            rho0(ct) = rho_solid
            dx0(ct) = dx00
            IsSolid(ct) = 1
            massFct(ct) = masX
            if (jj==(ctbar(2)/2)) then
              BreakContact(ct)=1
            elseif (jj==(1+(ctbar(2)/2))) then
              BreakContact(ct)=2
            else
              BreakContact(ct)=0
              endif
            enddo
          enddo
        enddo


c Set Contact links
        do jj=1,N
          if (IsSolid(jj)==1) then
            ct=0
            do ii=1,N
              if (IsSolid(ii)==1) then
                if (ii/=jj) then
                  r=0
                  do kk=1,3
                    dx3(kk)=abs(X(ii,kk)-X(jj,kk))
                    r=r+((X(ii,kk)-X(jj,kk))**2)
                  enddo
                  r=sqrt(r)
                  if (r<(dx0(jj)*1.1)) then
                    split=1
                    if (BreakContact(ii)==1) then
                      if (BreakContact(jj)==2) then
                        split=0
                      endif
                    endif
                    if (BreakContact(ii)==2) then
                      if (BreakContact(jj)==1) then
                        split=0
                      endif
                    endif
                    split=1
                    if (split==1) then
                      ct=ct+1
                      Contact(jj,ct+1)=ii
                      fooint=MAXLOC(dx3,1)
                      ContactDir(jj,ct+1)=fooint
                      ContactDirCT(jj,fooint)=ContactDirCT(jj,fooint)+1
                    endif
                  endif
        endif
      endif
    enddo
    Contact(jj,1)=ct
    ContactDir(jj,1)=ct
  endif
enddo

ContactX=Contact
ContactDirX=ContactDir
ContactDirCTX=ContactDirCT



open (unit = 1, file = "Fixed.dat")
do jj=1,N
  write (1,*),FixXY(jj)
enddo
close (1)

open (unit = 1, file = "ContactDirX.dat")
do jj=1,N
  write (1,*),ContactDirX(jj,:)
enddo
close (1)

open (unit = 1, file = "Contact.dat")
do jj=1,N
  write (1,*),Contact(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactDir.dat")
do jj=1,N
  write (1,*),ContactDir(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactDirCT.dat")
do jj=1,N
```

```
  write (1,*),ContactDirCT(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactX.dat")
do jj=1,N
  write (1,*),ContactX(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactDirCTX.dat")
do jj=1,N
  write (1,*),ContactDirCTX(jj,:)
enddo
close (1)

open (unit = 1, file = "Mass.dat")
do jj=1,N
  write (1,*),massFct(jj)
enddo
close (1)

open (unit = 1, file = "dX.dat")
do jj=1,N
  write (1,*),dx0(jj)
enddo
close (1)

open (unit = 1, file = "X0.dat")
do jj=1,N
  write (1,*),X(jj,:)
enddo
close (1)

open (unit = 1, file = "V0.dat")
do jj=1,N
  write (1,*),V(jj,:)
enddo
close (1)
```

```
      open (unit = 1, file = "dVdX.dat")
      do jj=1,N
        write (1,*),dVdx(jj,:)
      enddo
      close (1)

      open (unit = 1, file = "rho0.dat")
      do jj=1,N
        write (1,*),rho0(jj)
      enddo
      close (1)

      open (unit = 1, file = "rho_init.dat")
      do jj=1,N
        write (1,*),rho(jj)
      enddo
      close (1)


      open (unit = 1, file = "IsSolid.dat")
      do jj=1,N
        write (1,*),IsSolid(jj)
      enddo
      close (1)


      Nout=N

      end subroutine ModelBlock

c _______________________________________________________________
```

ModelSmFixDisk.f

```
      subroutine ModelBlock(Nout)

      implicit none

      integer, intent(out) :: Nout
      integer N,ctbar(3),Nsphere,ct,ii,jj,kk,DiskRat
      integer fooint
      double precision RadiusFactor,Radius,masX,masXdisk,dx0x,dx0xDisk
      double precision angleFrac,angle,Yr0,dx3(3)
      double precision Zloc,Zloc2,Yloc,Xloc,r,mass,pi,rho_solid
      integer, allocatable, dimension(:) :: FixXY,IsSolid
      integer, allocatable, dimension(:,:) :: Contact,ContactX
      integer, allocatable, dimension(:,:) :: ContactDir,ContactDirX
      integer, allocatable, dimension(:,:) :: ContactDirCT,ContactDirC
      double precision, allocatable, dimension(:,:) :: X,V,dVdx
      double precision, allocatable, dimension(:) :: massFct,dx0,rho0


c     Start the Specification Parameters

      open (unit = 1, file = "SimSpec.dat")
        write (1,*),207e9        ! Young's Modulus of Steel
        write (1,*),0.3          ! Poisson's Ratio of Steel
        write (1,*),7800         ! Density of Steel
        write (1,*),0.0          ! Forced Density in X direction (Vtes
        write (1,*),100.0        ! Forced Density in Y direction (Vtes
        write (1,*),0.0          ! Forced Density in Z direction (Vtes
        write (1,*),0.3          ! Gamma (blend stress)
        write (1,*),100          ! Number of Recorded Time Steps (Nts)
        write (1,*),1            ! Time Steps between recorded Time St
        write (1,*),1            ! Time Steps between recorded Time St
        write (1,*),5*2.54e-6    ! (StartDefl)
        write (1,*),5*2.54e-6    ! (NewDefl)
        write (1,*),0.05         ! (dTfactor)
        write (1,*),0.005         ! (dTdxfactor)
        write (1,*),15           ! (stop)
        write (1,*),2.15e9       ! (Bulk_water)
      close (1)



      ctbar(1)=101
      ctbar(2)=10
      ctbar(3)=1
      Radius=20.0*(2.54e-4)
      DiskRat=3
      dx0x=0.25*(Radius/20.0)
      pi=ACOS(-1.0)
      rho_solid=7800

      if ((ctbar(1)*dx0x)>(2*Radius)) then
        angleFrac=pi
      else
        angleFrac=2*ASIN((ctbar(1)*dx0x)/(2*Radius))
        angleFrac=angleFrac/2
      endif

      dx0xDisk=dx0x/DiskRat
      masX=(dx0x**3)*rho_solid
      masXdisk=(dx0xDisk**3)*rho_solid

      Nsphere=(angleFrac*Radius/dx0xDisk)
      N=((Nsphere*DiskRat)+(ctbar(1)*ctbar(2)))*ctbar(3)

c  ____________________________________________________________
c                   ALLOCATION
c  ____________________________________________________________



      ALLOCATE (FixXY(N))
      ALLOCATE (IsSolid(N))
      ALLOCATE (X(N,3))
      ALLOCATE (V(N,3))
      ALLOCATE (dVdx(N,3))
      ALLOCATE (rho0(N))
      ALLOCATE (massFct(N))
      ALLOCATE (dx0(N))
      ALLOCATE (Contact(N,(N+1)))
      ALLOCATE (ContactDir(N,(N+1)))
      ALLOCATE (ContactDirCT(N,3))
      ALLOCATE (ContactX(N,(N+1)))
      ALLOCATE (ContactDirX(N,(N+1)))
      ALLOCATE (ContactDirCTX(N,3))

c ______________________________________________


c Set the parameters for the steel bar


      Yr0=(ctbar(2)*dx0x)+Radius
      ct=0
      Zloc=-dx0x
      do kk=1,ctbar(3)
        Zloc=Zloc+dx0x
        Yloc=-dx0x
        do jj=1,ctbar(2)
          Yloc=Yloc+dx0x
          Xloc=-((dx0x*ctbar(1))/2)-(dx0x/2)
          do ii=1,ctbar(1)
            Xloc=Xloc+dx0x
            ct=ct+1
            if (jj==1) then
              FixXY(ct)=1
            else
              FixXY(ct)=0
            endif
            X(ct,1) = Xloc
            X(ct,2) = Yloc
            X(ct,3) = Zloc
            V(ct,1) = 0
            V(ct,2) = 0
            V(ct,3) = 0
            dVdX(ct,1) = 0
            dVdX(ct,2) = 0
            dVdX(ct,3) = 0
            rho0(ct) = rho_solid
            massFct(ct) = masX
            dx0(ct) = (massFct(ct)/rho_solid)**0.333333
            IsSolid(ct) = 1
          enddo
        enddo

        Zloc2=Zloc-(dx0xDisk*(DiskRat+1)/2)
        do ii=1,DiskRat
          Zloc2=Zloc2+dx0xDisk
          angle=(angleFrac/2)+(angleFrac/(2*Nsphere))
          do jj=1,Nsphere
            angle=angle-(angleFrac/Nsphere)
            Xloc=-(SIN(angle))*Radius
            Yloc=Yr0-((COS(angle))*Radius)
            ct=ct+1
            FixXY(ct)=8
            X(ct,1) = Xloc
            X(ct,2) = Yloc
            X(ct,3) = Zloc2
            V(ct,1) = 0
            V(ct,2) = 0
            V(ct,3) = 0
            dVdX(ct,1) = 0
            dVdX(ct,2) = 0
            dVdX(ct,3) = 0
            rho0(ct) = rho_solid
            massFct(ct) = masXdisk
            dx0(ct) = (massFct(ct)/rho_solid)**0.333333
            IsSolid(ct) = 1
          enddo
        enddo
      enddo
      print *,N,ct


c Set Contact links
      do jj=1,N
```

```
  if (IsSolid(jj)==1) then
    ct=0
    do ii=1,N
      if (IsSolid(ii)==1) then
        if (ii/=jj) then
          r=0
          do kk=1,3
            dx3(kk)=abs(X(ii,kk)-X(jj,kk))
            r=r+((X(ii,kk)-X(jj,kk))**2)
          enddo
          r=sqrt(r)
          if (r<(dx0(jj)*1.1)) then
            if (FixXY(jj)==FixXY(ii)) then
              ct=ct+1
              Contact(jj,ct+1)=ii
              fooint=MAXLOC(dx3,1)
              ContactDir(jj,ct+1)=fooint
              ContactDirCT(jj,fooint)=ContactDirCT(jj,fooint)+1
            endif
          endif
        endif
      endif
    enddo
    Contact(jj,1)=ct
    ContactDir(jj,1)=ct
  endif
enddo

ContactX=Contact
ContactDirX=ContactDir
ContactDirCTX=ContactDirCT


open (unit = 1, file = "Fixed.dat")
do jj=1,N
  write (1,*),FixXY(jj)
enddo
close (1)

open (unit = 1, file = "ContactDirX.dat")
```

```
do jj=1,N
  write (1,*),ContactDirX(jj,:)
enddo
close (1)

open (unit = 1, file = "Contact.dat")
do jj=1,N
  write (1,*),Contact(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactDir.dat")
do jj=1,N
  write (1,*),ContactDir(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactDirCT.dat")
do jj=1,N
  write (1,*),ContactDirCT(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactX.dat")
do jj=1,N
  write (1,*),ContactX(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactDirCTX.dat")
do jj=1,N
  write (1,*),ContactDirCTX(jj,:)
enddo
close (1)

open (unit = 1, file = "Mass.dat")
do jj=1,N
  write (1,*),massFct(jj)
enddo
close (1)
```

```
open (unit = 1, file = "dX.dat")
do jj=1,N
  write (1,*),dx0(jj)
enddo
close (1)

open (unit = 1, file = "X0.dat")
do jj=1,N
  write (1,*),X(jj,:)
enddo
close (1)

open (unit = 1, file = "V0.dat")
do jj=1,N
  write (1,*),V(jj,:)
enddo
close (1)

open (unit = 1, file = "dVdX.dat")
do jj=1,N
  write (1,*),dVdx(jj,:)
enddo
close (1)

open (unit = 1, file = "rho0.dat")
do jj=1,N
  write (1,*),rho0(jj)
enddo
close (1)

open (unit = 1, file = "rho_init.dat")
do jj=1,N
  write (1,*),rho0(jj)
enddo
close (1)

open (unit = 1, file = "IsSolid.dat")
do jj=1,N
  write (1,*),IsSolid(jj)
```

```
      enddo
      close (1)


      Nout=N

      end subroutine ModelBlock



c ____________________________________________________________________________________
```

PressVessel.f

```
subroutine ModelBlock(Nout)

implicit none

integer, intent(out) :: Nout
integer N,ctPV(3),Nsphere,ct,ii,jj,kk,uu
integer fooint,split
double precision RadiusFactor,Radius,masX,massL,dx00,Bulk_water
double precision angleFrac,angle,Yr0,dx3(3),third,RR,pi,P
double precision Zloc,Yloc,Xloc,rho_solid,rho_liquid,rho_liquidC
integer, allocatable, dimension(:) :: FixXY,IsSolid,BreakContact
integer, allocatable, dimension(:,:) :: Contact,ContactX
integer, allocatable, dimension(:,:) :: ContactDir,ContactDirX
integer, allocatable, dimension(:,:) :: ContactDirCT,ContactDirC
double precision, allocatable, dimension(:,:) :: X,V,dVdx
double precision, allocatable, dimension(:) :: dx0,massFct
double precision, allocatable, dimension(:) :: rho0,rho

open (unit = 1, file = "SimSpec.dat")
  write (1,*),207e9        ! Young's Modulus of Steel
  write (1,*),0.3          ! Poisson's Ratio of Steel
  write (1,*),7800         ! Density of Steel
  write (1,*),0.0          ! Forced Density in X direction (Vtes
  write (1,*),0.0          ! Forced Density in Y direction (Vtes
  write (1,*),0.0          ! Forced Density in Z direction (Vtes
  write (1,*),0.3          ! Gamma (blend stress)
  write (1,*),1000         ! Number of Recorded Time Steps (Nts)
  write (1,*),1            ! Time Steps between recorded Time St
  write (1,*),1            ! Time Steps between recorded Time St
  write (1,*),0.18         ! (StartDefl)
  write (1,*),0.05         ! (NewDefl)
  write (1,*),0.05         ! (dTfactor)
  write (1,*),0.01         ! (dTdxfactor)
  write (1,*),15           ! (stop)
  write (1,*),2.15e9       ! (Bulk_water)
close (1)
```

```
      ctPV(1)=25      ! 12
      ctPV(2)=20      ! 9
      ctPV(3)=1       ! 1

      masX=0.1
      P=101135*1
      rho_solid=7800
      rho_liquid=1000
      Bulk_water=2.15e9

      rho_liquidC=rho_liquid*((P/Bulk_water)+1)
      print *,rho_liquidC

      third=1.0/3.0
      dx00=((masX/rho_solid)**third)
      massL=rho_liquidC*(dx00**3)

      N=0
      Xloc=(-ctPV(1)*dx00)-(dx00/2)
      do ii=1,(2*ctPV(1))
      Xloc=Xloc+dx00
      Yloc=(-ctPV(1)*dx00)-(dx00/2)
      do jj=1,(2*ctPV(1))
        Yloc=Yloc+dx00
        RR=SQRT((Xloc**2)+(Yloc**2))
        if (RR<(ctPV(1)*dx00)) then
          N=N+1
        endif
      enddo
      enddo
      N=N*ctPV(3)
      print *,N


c ______________________________________________
c                    ALLOCATION
c ______________________________________________
```

```
      ALLOCATE (FixXY(N))
      ALLOCATE (IsSolid(N))
      ALLOCATE (BreakContact(N))
      ALLOCATE (X(N,3))
      ALLOCATE (V(N,3))
      ALLOCATE (dVdx(N,3))
      ALLOCATE (rho(N))
      ALLOCATE (rho0(N))
      ALLOCATE (massFct(N))
      ALLOCATE (dx0(N))
      ALLOCATE (Contact(N,(N+1)))
      ALLOCATE (ContactDir(N,(N+1)))
      ALLOCATE (ContactDirCT(N,3))
      ALLOCATE (ContactX(N,(N+1)))
      ALLOCATE (ContactDirX(N,(N+1)))
      ALLOCATE (ContactDirCTX(N,3))

c ______________________________________________


      print *,N

c Set the parameters for the steel bar

      ct=0
      Zloc=-dx00
      do uu=1,(ctPV(3))
        Zloc=Zloc+dx00
        Xloc=(-ctPV(1)*dx00)-(dx00/2)
        do ii=1,(2*ctPV(1))
          Xloc=Xloc+dx00
          Yloc=(-ctPV(1)*dx00)-(dx00/2)
          do jj=1,(2*ctPV(1))
            Yloc=Yloc+dx00
            RR=SQRT((Xloc**2)+(Yloc**2))
            if (RR<(ctPV(1)*dx00)) then
              ct = ct + 1
              if (RR<(ctPV(2)*dx00)) then
                IsSolid(ct) = 0
                massFct(ct) = massL
              rho0(ct)=rho_liquid
              rho(ct)=rho_liquidC
            else
              IsSolid(ct) = 1
              massFct(ct) = masX
              rho0(ct)=rho_solid
              rho(ct)=rho_solid
            endif
            FixXY(ct)=0
            X(ct,1) = Xloc
            X(ct,2) = Yloc
            X(ct,3) = Zloc

          endif
        enddo
      enddo
    enddo

    dx0 = dx0 + (dx00)


c Set Contact links
    do jj=1,N
      if (IsSolid(jj)==1) then
        ct=0
        do ii=1,N
          if (IsSolid(ii)==1) then
            if (ii/=jj) then
              RR=0
              do kk=1,3
                dx3(kk)=abs(X(ii,kk)-X(jj,kk))
                RR=RR+((X(ii,kk)-X(jj,kk))**2)
              enddo
              RR=sqrt(RR)
              if (RR<(dx0(jj)*1.1)) then
                ct=ct+1
                Contact(jj,ct+1)=ii
                fooint=MAXLOC(dx3,1)
                ContactDir(jj,ct+1)=fooint
                ContactDirCT(jj,fooint)=ContactDirCT(jj,fooint)+1
          endif
        endif
      endif
    enddo
    Contact(jj,1)=ct
    ContactDir(jj,1)=ct
  endif
enddo

ContactX=Contact
ContactDirX=ContactDir
ContactDirCTX=ContactDirCT



open (unit = 1, file = "Fixed.dat")
do jj=1,N
  write (1,*),FixXY(jj)
enddo
close (1)

open (unit = 1, file = "ContactDirX.dat")
do jj=1,N
  write (1,*),ContactDirX(jj,:)
enddo
close (1)

open (unit = 1, file = "Contact.dat")
do jj=1,N
  write (1,*),Contact(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactDir.dat")
do jj=1,N
  write (1,*),ContactDir(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactDirCT.dat")
```

```
do jj=1,N
  write (1,*),ContactDirCT(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactX.dat")
do jj=1,N
  write (1,*),ContactX(jj,:)
enddo
close (1)

open (unit = 1, file = "ContactDirCTX.dat")
do jj=1,N
  write (1,*),ContactDirCTX(jj,:)
enddo
close (1)

open (unit = 1, file = "Mass.dat")
do jj=1,N
  write (1,*),massFct(jj)
enddo
close (1)

open (unit = 1, file = "dX.dat")
do jj=1,N
  write (1,*),dx0(jj)
enddo
close (1)

open (unit = 1, file = "X0.dat")
do jj=1,N
  write (1,*),X(jj,:)
enddo
close (1)

open (unit = 1, file = "V0.dat")
do jj=1,N
  write (1,*),V(jj,:)
enddo
close (1)
```

```
      open (unit = 1, file = "dVdX.dat")
      do jj=1,N
        write (1,*),dVdx(jj,:)
      enddo
      close (1)

      open (unit = 1, file = "rho0.dat")
      do jj=1,N
        write (1,*),rho0(jj)
      enddo
      close (1)

      open (unit = 1, file = "rho_init.dat")
      do jj=1,N
        write (1,*),rho(jj)
      enddo
      close (1)

      open (unit = 1, file = "IsSolid.dat")
      do jj=1,N
        write (1,*),IsSolid(jj)
      enddo
      close (1)


      Nout=N

      end subroutine ModelBlock

c ________________________________________________________________________
```

MATLAB SOURCE CODE

Analyze_Data.m

```
clear
close all
tic

Position=[200 200 900 800];
TitleSz=24; LblSz=20; AxSz=16;
NL=sprintf('\n');

raw=load('VarDat.dat');
Ey=raw(1);
G=raw(2);
StudyCt=raw(3);

V0=0;

X0=load('X0.dat');
Xdat=load('X.dat');
Ydat=load('Y.dat');
Zdat=load('Z.dat');
Vx=load('Vx.dat');
Vy=load('Vy.dat');
dVdx=load('dVdX.dat');
dVdy=load('dVdY.dat');
dVdz=load('dVdZ.dat');
P=load('P.dat');
rho=load('rho.dat');
Fixed=load('Fixed.dat');
```

```
E11=load('E11.dat');
E22=load('E22.dat');
dx=load('dX.dat');
T11=load('T11.dat');
T21=load('T21.dat');
T31=load('T31.dat');
T12=load('T12.dat');
T22=load('T22.dat');
T32=load('T32.dat');
T13=load('T13.dat');
T23=load('T23.dat');
T33=load('T13.dat');
IsSolid=load('IsSolid.dat');
Mass=load('Mass.dat');
rho0=load('rho0.dat');
rho_init=load('rho_init.dat');
TimeFct=load('Time.dat');

Cylrng=find(Fixed==8);
R1=max(X0(Cylrng,2))-min(X0(Cylrng,2))+(mean(dx)/2);

foo=size(Xdat);
ct=foo(1); stop=ct; a=ct;
N=foo(2); clear foo
if stop>ct
    stop=ct;
end
plotCt=5; Range=(1:plotCt)*floor(ct/plotCt);
Vy(:,1)=-V0; Vy(:,N)=V0;
Poisson=(Ey/(2*G))-1;

Ered=1/((1-(Poisson^2))/Ey);

Xdat2=Xdat;
Ydat2=Ydat;
Zdat2=Zdat;
for ii=1:N
    Xdat2(:,ii)=Xdat2(:,ii)-(X0(ii,1));
    Ydat2(:,ii)=Ydat2(:,ii)-(X0(ii,2));
    Zdat2(:,ii)=Zdat2(:,ii)-(X0(ii,3));
```

```
end

Xdat3=Xdat2;
Ydat3=Ydat2;
Zdat3=Zdat2;
for ii=1:ct
    for jj=1:N
        Xdat3(ii,jj)=Xdat3(ii,jj)-mean(Xdat2(ii,:));
        Ydat3(ii,jj)=Ydat3(ii,jj)-mean(Ydat2(ii,:));
        Zdat3(ii,jj)=Zdat3(ii,jj)-mean(Zdat2(ii,:));
    end
end

NL=(['\n']);
%dtplot=load('Time.dat');

Vr=sqrt((Vx.^2)+(Vy.^2));
Xr=sqrt((Xdat.^2)+(Ydat.^2));
Xr2=Xr;
for ii=1:ct
    Xr2=Xr(ii,:)-Xr(1,:);
end

save Data

toc
```

PlotTension.m

```
clear
close all
tic

Position=[200 200 900 800];
TitleSz=24; LblSz=20; AxSz=16;
NL=sprintf('\n');

% load Data
load Tension_steel

X=Xdat(end,:);
Y=Ydat(end,:);
Z=Zdat(end,:);

Xdat2=Xdat;
Ydat2=Ydat;
Zdat2=Zdat;
for ii=1:N
    Xdat2(:,ii)=Xdat2(:,ii)-((Xdat2(1,ii)));
    Ydat2(:,ii)=Ydat2(:,ii)-((Ydat2(1,ii)));
    Zdat2(:,ii)=Zdat2(:,ii)-((Zdat2(1,ii)));
end

Poisson=(Ey/(2*G))-1;

exagY=1;
exag=2e1;
exagstr='(20) ';
matstr='Steel';

Xe=Xdat(1,:)+(Xdat2(end,:)*exag);
Ye=Ydat(1,:)+(Ydat2(end,:)*exagY);
Ze=Zdat(1,:)+(Zdat2(end,:)*exag);

dtplot=(TimeFct(:,1)); dt=max(diff(TimeFct)); dx=median(dx);
height=max(X0(:,2))-min(X0(:,2))+dx;
```

```
width=max(X0(:,1))-min(X0(:,1))+dx;

ff=find(X0(:,2)==max(X0(:,2)));
Tcalc=Ey*max(Ydat2(:,:)')/height;
Tavg=max(abs(T22(:,ff)'));


YY=zeros(1,N);
for ii=2:(N-1)
    YY(ii)=(abs(Y(ii)-Y(ii-1))-dx)+(abs(Y(ii)-Y(ii+1))-dx);
    YY(ii)=YY(ii)*Ey/dx;
end
ratio=max(T22').*((min(T22').^-1)); ratio=ratio-1;



PoissonError=100*abs((Poisson/((max(abs(Xdat2(ct,:)))/width)/(max(abs(Y
TensionError = 100*abs((Tcalc(ct)/Tavg(ct))-1);

MaxStress=abs(Tavg(ct));

dxmat=(max(X0(:,2))-min(X0(:,2)))/20;
axismat=[(min(Xe)-dxmat) (max(Xe)+dxmat) (min(Ye)-dxmat) (max(Ye)+dxmat
TCstr='Tension';
MaxStressStr=[num2str(MaxStress*(1e-6)) ' MPa'];
TitleStr=[matstr ' - Max Stress = ' MaxStressStr 10];

figure(1)
set(gcf,'Position',Position)
set(0,'DefaultAxesFontSize',AxSz,'DefaultAxesFontWeight','b')
hold off
for ii=1:N
    if Fixed(ii)==0
        plot(Xe(ii),Ye(ii),'ko','LineWidth',4)
        hold on
    else
        plot(Xe(ii),Ye(ii),'kx','LineWidth',4)
        hold on

    end
```

```
end
axis(axismat)
title([TitleStr 'Exaggerated ' exagstr TCstr],'fontsize',TitleSz,'fontw
xlabel('X','fontsize',LblSz,'fontweight','b');
ylabel('Y','fontsize',LblSz,'fontweight','b');

figure(2)
set(gcf,'Position',Position)
set(0,'DefaultAxesFontSize',AxSz,'DefaultAxesFontWeight','b')
hold off
for ii=1:N
    if Fixed(ii)==0
        plot(Xdat(1,ii),Ydat(1,ii),'ko','LineWidth',4)
        hold on
    else
        plot(Xdat(1,ii),Ydat(1,ii),'kx','LineWidth',4)
        hold on

    end
end
axis(axismat)
title([TitleStr 'Before ' TCstr],'fontsize',TitleSz,'fontweight','b');
xlabel('X','fontsize',LblSz,'fontweight','b');
ylabel('Y','fontsize',LblSz,'fontweight','b');

display(' ');
display(['Poisson Error = ' num2str(PoissonError) '%']);
display(['Tension Error = ' num2str(TensionError) '%']);
display(' ');

toc
```

PlotComp.m

```
clear
close all
tic

Position=[200 200 900 800];
TitleSz=24; LblSz=20; AxSz=16;
NL=sprintf('\n');

% load Data
load compress_steel

X=Xdat(end,:);
Y=Ydat(end,:);
Z=Zdat(end,:);

Xdat2=Xdat;
Ydat2=Ydat;
Zdat2=Zdat;
for ii=1:N
    Xdat2(:,ii)=Xdat2(:,ii)-((Xdat2(1,ii)));
    Ydat2(:,ii)=Ydat2(:,ii)-((Ydat2(1,ii)));
    Zdat2(:,ii)=Zdat2(:,ii)-((Zdat2(1,ii)));
end

Poisson=(Ey/(2*G))-1;

exagY=1;
exag=2e1;
exagstr='(20) ';
matstr='Steel';

Xe=Xdat(1,:)+(Xdat2(end,:)*exag);
Ye=Ydat(1,:)+(Ydat2(end,:)*exagY);
Ze=Zdat(1,:)+(Zdat2(end,:)*exag);

dtplot=(TimeFct(:,1)); dt=max(diff(TimeFct)); dx=median(dx);
height=max(X0(:,2))-min(X0(:,2))+dx;
```

```
width=max(X0(:,1))-min(X0(:,1))+dx;

ff=find(X0(:,2)==max(X0(:,2)));
Tcalc=Ey*max(Ydat2(:,:)')/height;
Tavg=max(abs(T22(:,ff)'));


YY=zeros(1,N);
for ii=2:(N-1)
    YY(ii)=(abs(Y(ii)-Y(ii-1))-dx)+(abs(Y(ii)-Y(ii+1))-dx);
    YY(ii)=YY(ii)*Ey/dx;
end
ratio=max(T22').*((min(T22').^-1)); ratio=ratio-1;



PoissonError=100*abs((Poisson/((max(abs(Xdat2(ct,:)))/width)/(max(abs(Y
TensionError = 100*abs((Tcalc(ct)/Tavg(ct))-1);

MaxStress=abs(Tavg(ct));

dxmat=(max(X0(:,2))-min(X0(:,2)))/20;
axismat=[(min(Xe)-dxmat) (max(Xe)+dxmat) (min(Ye)-dxmat) (max(Ye)+dxmat

TCstr='Compression';
MaxStressStr=[num2str(MaxStress*(1e-6)) ' MPa'];

TitleStr=[matstr ' - Max Stress = ' MaxStressStr 10];

figure(1)
set(gcf,'Position',Position)
set(0,'DefaultAxesFontSize',AxSz,'DefaultAxesFontWeight','b')
hold off
for ii=1:N
    if Fixed(ii)==0
        plot(Xe(ii),Ye(ii),'ko','LineWidth',4)
        hold on
    else
        plot(Xe(ii),Ye(ii),'kx','LineWidth',4)
        hold on
        end
    end
    axis(axismat)
    title([TitleStr 'Exaggerated ' exagstr TCstr],'fontsize',TitleSz,'fontw
    xlabel('X','fontsize',LblSz,'fontweight','b');
    ylabel('Y','fontsize',LblSz,'fontweight','b');

    figure(2)
    set(gcf,'Position',Position)
    set(0,'DefaultAxesFontSize',AxSz,'DefaultAxesFontWeight','b')
    hold off
    for ii=1:N
        if Fixed(ii)==0
            plot(Xdat(1,ii),Ydat(1,ii),'ko','LineWidth',4)
            hold on
        else
            plot(Xdat(1,ii),Ydat(1,ii),'kx','LineWidth',4)
            hold on

        end
    end
    axis(axismat)
    title([TitleStr 'Before ' TCstr],'fontsize',TitleSz,'fontweight','b');
    xlabel('X','fontsize',LblSz,'fontweight','b');
    ylabel('Y','fontsize',LblSz,'fontweight','b');

    display(' ');
    display(['Poisson Error = ' num2str(PoissonError) '%']);
    display(['Tension Error = ' num2str(TensionError) '%']);
    display(' ');

    toc
```

Plot_Hertz.m

```
clear

load Hertz

X=Xdat; Y=Ydat; Z=Zdat;
[ct N]=size(X);

rng=(1:101)+(101*9);

for ii=[1 5:5:ct]
    figure(1)
    plot(X(ii,rng),Y(ii,rng),'*')
    title([num2str(ii) '/' num2str(ct)]);
    pause(0.1)
end

figure(2)
plot(Xdat(1,:),Ydat(1,:),'*')
```

MakeFigs_PresVes.m

```
clear all
close all

load PressVess

Position=[200 200 900 600];
TitleSz=24; LblSz=20; AxSz=16;
MkFig=0; % Set to 1 to save JPEG figures
Res='-r600';
NL=sprintf('\n');

aa=find(IsSolid==1); bb=find(IsSolid==0);
TimeFct=mean(TimeFct');

del=1.10;
axismat=[(del*min(X0(:,1))) (del*max(X0(:,1))) (del*min(X0(:,2))) (del

ha=figure(1);
set(gcf,'Position',Position)
set(0,'DefaultAxesFontSize',AxSz,'DefaultAxesFontWeight','b')
plot(X0(aa,1),X0(aa,2),'*',X0(bb,1),X0(bb,2),'o','Linewidth',2)
axis(axismat);
%legend('Hertz','SPAM','Location','Best');
title('Before Simulation','fontsize',LblSz,'fontweight','b');
ylabel('Y (m)','fontsize',LblSz,'fontweight','b')
xlabel('X (m)','fontsize',LblSz,'fontweight','b');
if MkFig==1
    print(ha,'-djpeg','Start.jpeg',Res)
    close all
end

ha=figure(2);
set(gcf,'Position',Position)
set(0,'DefaultAxesFontSize',AxSz,'DefaultAxesFontWeight','b')
plot(Xdat(end,aa),Ydat(end,aa),'*',Xdat(end,bb),Ydat(end,bb),'o','Line
axis(axismat);
%legend('Hertz','SPAM','Location','Best');
```

```
title('After Simulation','fontsize',LblSz,'fontweight','b');
ylabel('Y (m)','fontsize',LblSz,'fontweight','b')
xlabel('X (m)','fontsize',LblSz,'fontweight','b');
if MkFig==1
    print(ha,'-djpeg','Final.jpeg',Res)
    close all
end

Xr2=Xr;
for ii=1:length(Xr2)
    Xr2(:,ii)=Xr(:,ii)-Xr(1,ii);
end

ha=figure(3);
set(gcf,'Position',Position)
set(0,'DefaultAxesFontSize',AxSz,'DefaultAxesFontWeight','b')
plot(TimeFct*(1e6),-Xr2(:,bb)*(1e9),'Linewidth',2)
title('Radial Displacement - Liquid','fontsize',LblSz,'fontweight','b'
ylabel(['\delta'  'R (nm)'],'fontsize',LblSz,'fontweight','b')
xlabel(['Time (' '{\mu}' 's)'],'fontsize',LblSz,'fontweight','b');
if MkFig==1
    print(ha,'-djpeg','Rfct_Liquid.jpeg',Res)
    close all
end

ha=figure(4);
set(gcf,'Position',Position)
set(0,'DefaultAxesFontSize',AxSz,'DefaultAxesFontWeight','b')
plot(TimeFct*(1e6),-Xr2(:,aa)*(1e9),'Linewidth',2)
title('Radial Displacement - Solid','fontsize',LblSz,'fontweight','b')
ylabel(['\delta'  'R (nm)'],'fontsize',LblSz,'fontweight','b')
xlabel(['Time (' '{\mu}' 's)'],'fontsize',LblSz,'fontweight','b');
if MkFig==1
    print(ha,'-djpeg','Rfct_Solid.jpeg',Res)
    close all
end
```

425

Hertz Study Results

This report discusses a detailed description of all of the simulation results when studying the Hertz Contact Stress of a Disk and Flat plat in compressive contact.

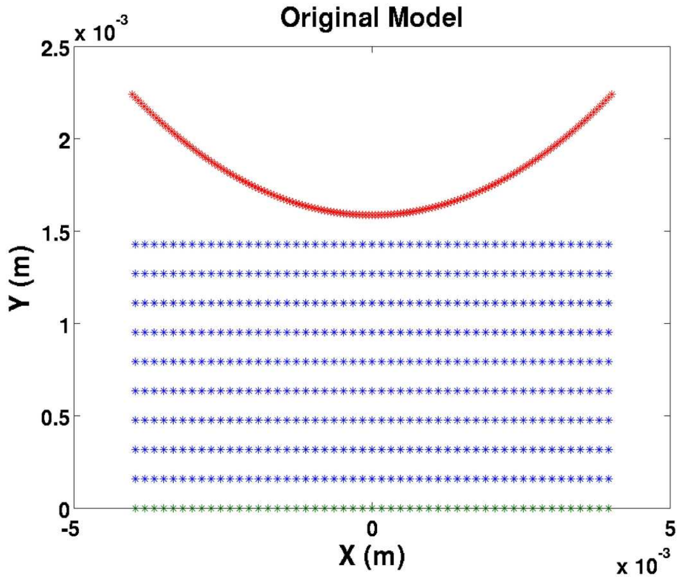
About the Study:

- The purpose of this study is to better verify and validate the Smoothed Particle Applied Mechanics (SPAM) model as it applies to Hertzian contact-mechanics.
- While the simulation is capable of 3D studies, only a 2D layer of particles are studied.
- The model will be represented by an inelastic disk being in contact with a elastic flat plate.
- The fixed 2D disk will be comprised of the same Lagrangian particles as the flat plate.
- The disk will be forced down at a user-specified velocity and then stay in place for a specified number of time steps.
- The plate will rest on a boundary of fixed solid particles beneath it.
- This effort will ensure that the deflection length is less than one tenth the disk radius.

Hertzian Equations for Comparison of SPAM:

- $P_{max} = |T_{22}|$ for the Top Center Particle
- $\delta = |Y(t) - Y(0)|$ for the Top Center Particle
- $a = R\sin(\cos^{-1}(\frac{R-\delta}{R}))$
  - R = Radius of Disk
  - a = half length of (theoretical) contact area
- Reduced Modulus:
  - $\frac{1}{E} = \frac{1-v_1^2}{E_{y,1}} + \frac{1-v_2^2}{E_{y,2}}$
    - Ey = Young's Modulus of Elasticity (Pa)
    - v = Poisson's Ration
    - 1 and 2 represent the parameters of the disk and plate respectively
  - The disk is assumed to be rigid and inelastic, and thus is assumed to have a Young's Modulus of infinity. Based on the assumptions taken for the disk radius, though it is safe to assume the disk is rigid, and thus the Young's Modulus is infinite, therefore:
    - $E = \frac{E_y}{1-v^2}$
- $Weight_N(N/m) = \frac{a^2 \pi E}{4R}$
  - This is the normalized weight, or the weight per unit length of the disk
- The calculated maximum stress is found via:
  - $Max\,Stress_{calculated} = \frac{2\,Weight_N}{\pi a}$
- Simulated Weight
  - $Weight = \Sigma_N (T_{22} * dx^2)$
  - Taken for all the fixed particles at the bottom of the flat disk
- The simulated weight is compared to a calculated total weight based on the simulated (with SPAM) maximum stress at the center of the top of the flat.
  - $Max\,Stress_{SPAM} = \frac{Weight}{\pi a\,dx} \quad \rightarrow \quad Weight = \pi a\,dx(Max\,Stress_{SPAM})$

Model:

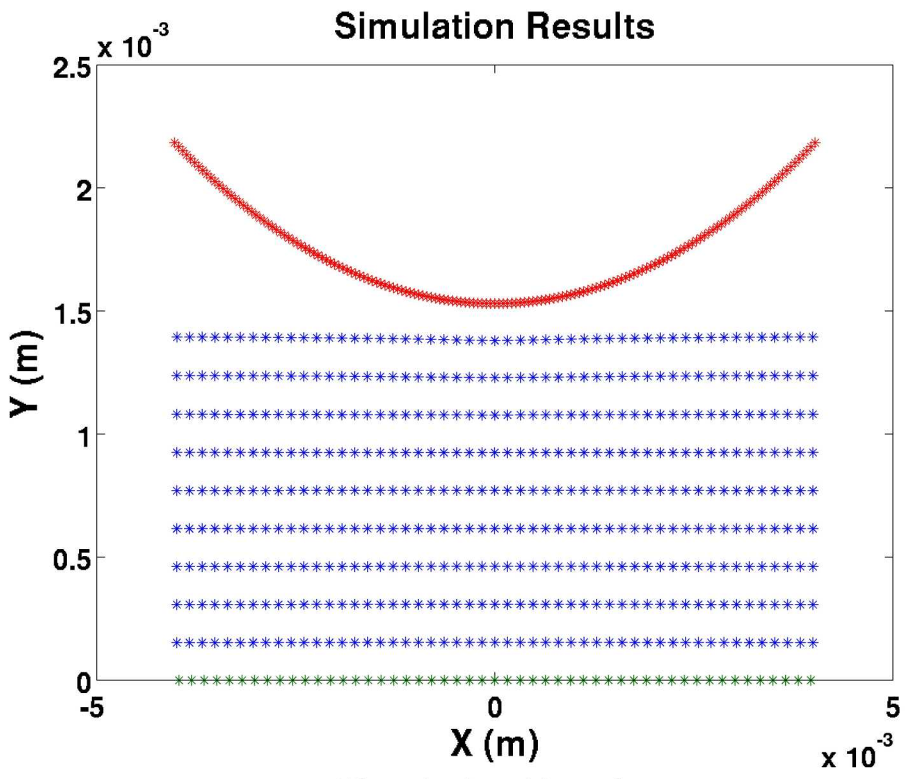
- Steel: Young's Modulus at 207 GPa, Poisson's Ratio at 0.3
- Color Code:
  - Red: Rigid Disk
  - Blue: elastic solid
  - Green = Fixed boundary
- 

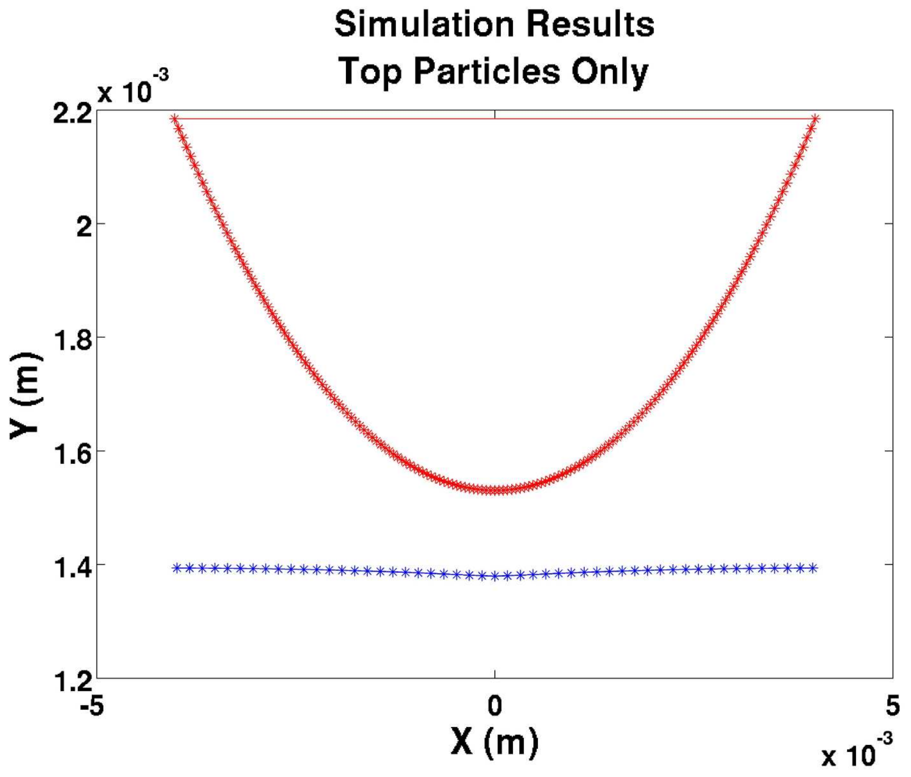
Results of Simulation:

- Calculated Contact Area Half-Length (a) = 1.6501 meters
  - a / R = 8.78%
- Simulated Deflection: -0.0125 inch
- Stress (MPa) Tensor of Top Center Particle (Tij):

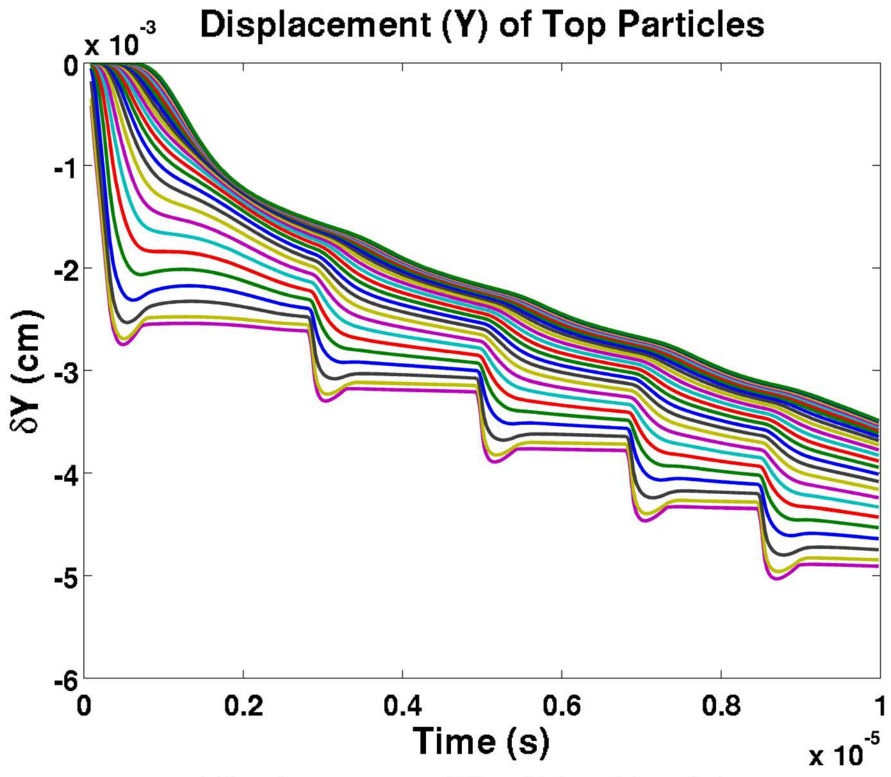
$$\begin{matrix} 0 & 6.4147 & 0 \\ 6.4147 & -4.0477 & 0 \\ 0 & 0 & 0 \end{matrix}$$

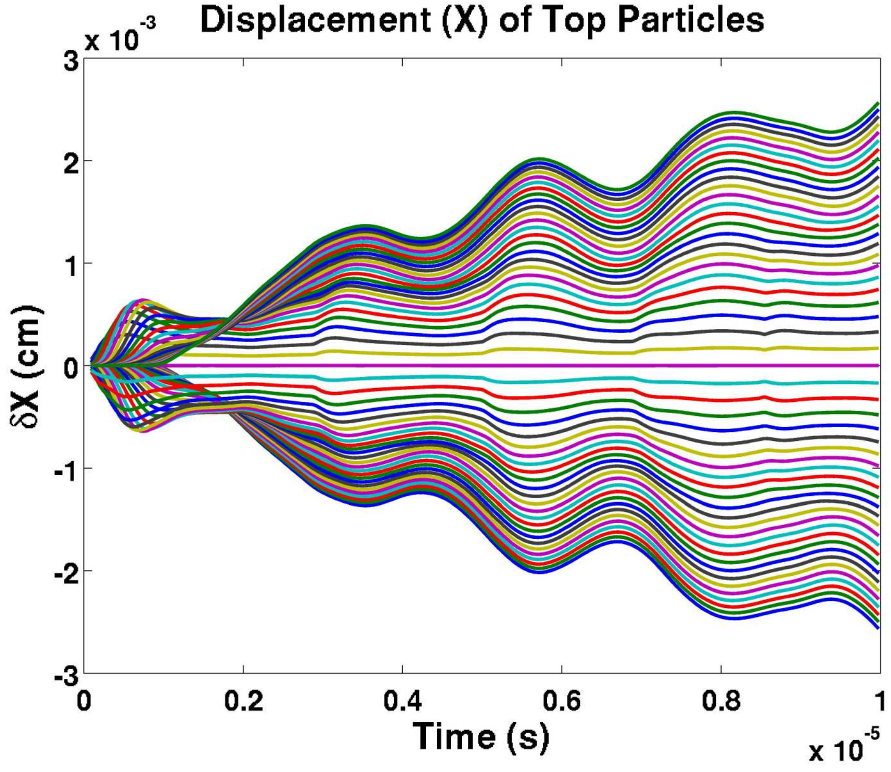
- Pressure – Error = 5.359%
  - Simulated (SPAM) Max Pressure, at Top Center Particle = 10.0525 GPa
  - Calculated (Hertz) Max Pressure, at Top Center Particle = 9.9896 GPa
- Weight – Error = 2.2053%
  - Simulated (SPAM) Max Pressure, at Top Center Particle = 5.9842 kN
  - Calculated (Hertz) Max Pressure, at Top Center Particle = 5.8552 kN

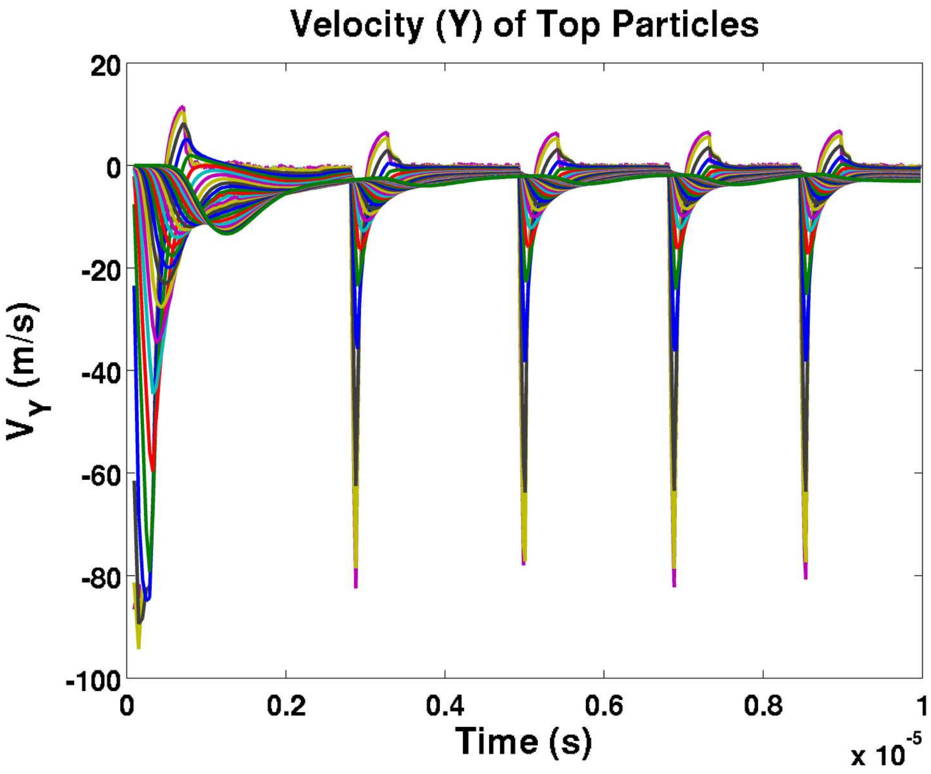

Simulation Results
x 10^-3
2.5
2
1.5
1
0.5
0
Y (m)
-5
0
5
X (m)
x 10^-3

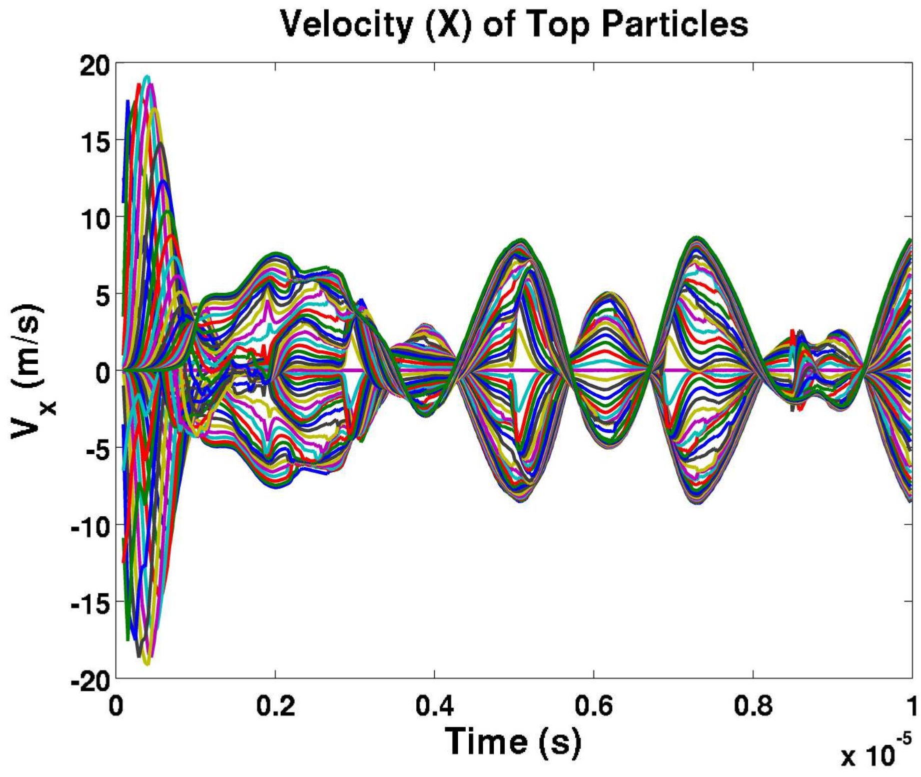

Simulation Results
Top Particles Only
x 10^-3
2.2
2
1.8
1.6
1.4
1.2
Y (m)
-5
0
5
X (m)
x 10^-3

430


Displacement (Y) of Top Particles
x 10^-3
0
-1
-2
-3
-4
-5
-6
δY (cm)
0
0.2
0.4
0.6
0.8
1
Time (s)
x 10^-5


Displacement (X) of Top Particles
x 10^-3
3
2
1
0
-1
-2
-3
δX (cm)
0
0.2
0.4
0.6
0.8
1
Time (s)
x 10^-5


Velocity (Y) of Top Particles
20
0
-20
-40
-60
-80
-100
0
0.2
0.4
0.6
0.8
1
Time (s)
x 10^-5
V_Y (m/s)


Velocity (X) of Top Particles
20
15
10
5
0
-5
-10
-15
-20
0
0.2
0.4
0.6
0.8
1
Time (s)
x 10^-5
V_X (m/s)

R = 20 meters, L = 12.25 m, H = 2.5 m, dX = 0.25 m 51 * 10 Particles

Disk Deflection (m)	Contact Length (m)	Weight – SPAM (GN)	Weight – Hertz (GN)	Max T22 – SPAM (GPa)	Max T22 – Hertz (GPa)
0.0412	1.2828	6.5983	7.3621	7.3071	7.2952
0.0505	1.4206	8.9462	8.7679	7.8587	8.0784
0.0595	1.5420	11.1197	10.5022	8.6718	8.7690
0.0684	1.6532	13.0201	12.4286	9.5720	9.4015
0.0773	1.7566	14.8473	14.5197	10.5241	9.9897

Disk Deflection (m)	% Error (Weight)	% Error (Max T22)
0.0412	10.3750	0.1624
0.0505	2.0330	2.7202
0.0595	5.8792	1.1079
0.0684	4.7594	1.8128
0.0773	2.2565	5.3490

R = 30 meters, L = 18.375 m, H = 3.75 m, dX = 0.375 m 51 * 10 Particles

Disk Deflection (m)	Contact Length (m)	Weight – SPAM (GN)	Weight – Hertz (GN)	Max T22 – SPAM (GPa)	Max T22 – Hertz (GPa)
0.0618	1.9242	14.8477	16.5667	7.3080	7.2952
0.0758	2.1308	20.1331	19.7297	7.8595	8.0783
0.0893	2.3130	25.0249	23.6305	8.6721	8.7689
0.1027	2.4798	29.3003	27.9638	9.5721	9.4013
0.1159	2.6349	33.4118	32.6699	10.5244	9.9895

Disk Deflection (m)	% Error (Weight)	% Error (Max T22)
0.0618	10.3760	0.1758
0.0758	2.0448	2.7087
0.0893	5.9011	1.1036
0.1027	4.7793	1.8172
0.1159	2.2708	5.3543

R = 40 meters, L = 24.5 m, H = 5.0 m, dX = 0.50 m 51 * 10 Particles

Disk Deflection (m)	**Contact Length (m)**	**Weight – SPAM (GN)**	**Weight – Hertz (GN)**	**Max T22 – SPAM (GPa)**	**Max T22 – Hertz (GPa)**
0.0824	2.5657	26.3945	29.4497	7.3074	7.2952
0.1010	2.8411	35.7889	35.0722	7.8588	8.0784
0.1191	3.0840	44.4844	42.0097	8.6720	8.7689
0.1369	3.3063	52.0851	49.7116	9.5717	9.4013
0.1546	3.5132	59.3943	58.0780	10.5241	9.9896

Disk Deflection (m)	**% Error (Weight)**	**% Error (Max T22)**
0.0824	10.3741	0.1670
0.1010	2.0437	2.7179
0.1191	5.8907	1.1050
0.1369	4.7745	1.8127
0.1546	2.2665	5.3505

R = 50 meters, L = 30.625 m, H = 6.25 m, dX = 0.625 m 51 * 10 Particles

Disk Deflection (m)	**Contact Length (m)**	**Weight – SPAM (GN)**	**Weight – Hertz (GN)**	**Max T22 – SPAM (GPa)**	**Max T22 – Hertz (GPa)**
0.1030	3.2070	41.2442	46.0171	7.3078	7.2951
0.1263	3.5513	55.9236	54.8013	7.8590	8.0783
0.1488	3.8549	69.5117	65.6398	8.6720	8.7689
0.1711	4.1329	81.3883	77.6770	9.5720	9.4013
0.1932	4.3916	92.8097	90.7467	10.5240	9.9896

Disk Deflection (m)	**% Error (Weight)**	**% Error (Max T22)**
0.1030	10.3718	0.1730
0.1263	2.0480	2.7142
0.1488	5.8988	1.1050
0.1711	4.7779	1.8153
0.1932	2.2735	5.3501

R = 0.2 inches, L = 0.1275 inches, H = 0.025 inches, dX = 0.0025 inches 51 * 10 Particles

Disk Deflection (mm)	**Contact Length (mm)**	**Weight – SPAM (N)**	**Weight – Hertz (N)**	**Max T22 – SPAM (GPa)**	**Max T22 – Hertz (GPa)**
0.0105	0.3258	425.3947	475.1323	7.3094	7.2953
0.0128	0.3608	576.8719	565.7163	7.8591	8.0785
0.0151	0.3917	716.9652	677.5850	8.6720	8.7690
0.0174	0.4199	839.5070	801.8216	9.5718	9.4014
0.0196	0.4462	957.3682	936.7987	10.5245	9.9897

Disk Deflection (mm)	**% Error (Weight)**	**% Error (Max T22)**
0.0105	10.4682	0.1937
0.0128	1.9719	2.7160
0.0151	5.8118	1.1066
0.0174	4.7000	1.8124
0.0196	2.1957	5.3537

R = 0.3 inches, L = 0.1913 inches, H = 0.375 inches, dX = 0.0038 inches 51 * 10 Particles

Disk Deflection (mm)	**Contact Length (mm)**	**Weight – SPAM (kN)**	**Weight – Hertz (kN)**	**Max T22 – SPAM (GPa)**	**Max T22 – Hertz (GPa)**
0.0157	0.4888	0.9572	1.0689	7.3087	7.2952
0.0192	0.5412	1.2980	1.2728	7.8590	8.0785
0.0227	0.5875	1.6132	1.5246	8.6721	8.7691
0.0261	0.6299	1.8889	1.8042	9.5721	9.4014
0.0294	0.6693	2.1541	2.1079	10.5250	9.9898

Disk Deflection (mm)	**% Error (Weight)**	**% Error (Max T22)**
0.0157	10.4565	0.1853
0.0192	1.9760	2.7177
0.0227	5.8130	1.1058
0.0261	4.6973	1.8153
0.0294	2.1928	5.3577

R = 0.4 inches, L = 0.2550 inches, H = 0.5 inches, dX = 0.005 inches 51 * 10 Particles

Disk Deflection (mm)	**Contact Length (mm)**	**Weight – SPAM (kN)**	**Weight – Hertz (kN)**	**Max T22 – SPAM (GPa)**	**Max T22 – Hertz (GPa)**
0.0209	0.6517	1.7066	1.9001	7.3076	7.2955
0.0257	0.7216	2.3128	2.2632	7.8605	8.0784
0.0302	0.7833	2.8727	2.7115	8.6760	8.7687
0.0348	0.8398	3.3629	3.2089	9.5768	9.4012
0.0393	0.8923	3.8344	3.7489	10.5296	9.9894

Disk Deflection (mm)	**% Error (Weight)**	**% Error (Max T22)**
0.0209	10.1859	0.1663
0.0257	2.1896	2.6967
0.0302	5.9464	1.0570
0.0348	4.7990	1.8678
0.0393	2.2794	5.4081

R = 0.5 inches, L = 0.3188 inches, H = 0.625 inches, dX = 0.0063 inches 51 * 10 Particles

Disk Deflection (mm)	**Contact Length (mm)**	**Weight – SPAM (kN)**	**Weight – Hertz (kN)**	**Max T22 – SPAM (GPa)**	**Max T22 – Hertz (GPa)**
0.0262	0.8146	2.6590	2.9695	7.3092	7.2952
0.0321	0.9021	3.6060	3.5358	7.8593	8.0785
0.0378	0.9792	4.4818	4.2352	8.6726	8.7690
0.0435	1.0498	5.2477	5.0117	9.5723	9.4015
0.0491	1.1155	5.9843	5.8552	10.5250	9.9896

Disk Deflection (mm)	**% Error (Weight)**	**% Error (Max T22)**
0.0262	10.4552	0.1921
0.0321	1.9856	2.7127
0.0378	5.8221	1.1000
0.0435	4.7098	1.8169
0.0491	2.2053	5.3590

R = 0.2 inches, L = 0.25 inches, H = 0.025 inches, dX = 0.0025 inches 101 * 10 Particles

Disk Deflection (mm)	**Contact Length (mm)**	**Weight – SPAM (kN)**	**Weight – Hertz (kN)**	**Max T22 – SPAM (GPa)**	**Max T22 – Hertz (GPa)**
0.0102	0.3224	0.4040	0.5156	8.0164	7.2189
0.0124	0.3551	0.6047	0.6508	9.1878	7.9494
0.0146	0.3852	0.7897	0.7912	10.2975	8.6234
0.0168	0.4129	0.9484	0.9431	11.4494	9.2449
0.0190	0.4385	1.0611	1.1126	12.7192	9.8172

Disk Deflection (mm)	**% Error (Weight)**	**% Error (Max T22)**
0.0102	21.6538	11.0477
0.0124	7.0836	15.5788
0.0146	0.1923	19.4141
0.0168	0.5628	23.8462
0.0190	4.6256	29.5609

R = 0.3 inches, L = 0.375 inches, H = 0.0375 inches, dX = 0.00375 inches 101 * 10 Particles

Disk Deflection (mm)	**Contact Length (mm)**	**Weight – SPAM (kN)**	**Weight – Hertz (kN)**	**Max T22 – SPAM (GPa)**	**Max T22 – Hertz (GPa)**
0.0154	0.4836	0.9090	1.1601	8.0157	7.2188
0.0186	0.5326	1.3602	1.4642	9.1877	7.9493
0.0219	0.5777	1.7765	1.7801	10.2968	8.6233
0.0252	0.6194	2.1337	2.1220	11.4491	9.2449
0.0284	0.6577	2.3872	2.5033	12.7189	9.8172

Disk Deflection (mm)	**% Error (Weight)**	**% Error (Max T22)**
0.0154	21.6425	11.0386
0.0186	7.1023	15.5783
0.0219	0.2067	19.4061
0.0252	0.5482	23.8431
0.0284	4.6363	29.5575

R = 0.4 inches, L = 0.5 inches, H = 0.05 inches, dX = 0.005 inches 101 * 10 Particles

Disk Deflection (mm)	**Contact Length (mm)**	**Weight – SPAM (kN)**	**Weight – Hertz (kN)**	**Max T22 – SPAM (GPa)**	**Max T22 – Hertz (GPa)**
0.0205	0.6449	1.6161	2.0623	8.0156	7.2188
0.0248	0.7101	2.4182	2.6031	9.1875	7.9494
0.0292	0.7703	3.1581	3.1648	10.2971	8.6234
0.0336	0.8258	3.7930	3.7726	11.4494	9.2449
0.0379	0.8770	4.2438	4.4502	12.7185	9.8172

Disk Deflection (mm)	**% Error (Weight)**	**% Error (Max T22)**
0.0205	21.6366	11.0375
0.0248	7.0994	15.5758
0.0292	0.2121	19.4090
0.0336	0.5425	23.8448
0.0379	4.6367	29.5541

R = 0.5 inches, L = 0.625 inches, H = 0.0625 inches, dX = 0.00625 inches 101 * 10 Particles

Disk Deflection (mm)	**Contact Length (mm)**	**Weight – SPAM (kN)**	**Weight – Hertz (kN)**	**Max T22 – SPAM (GPa)**	**Max T22 – Hertz (GPa)**
0.0256	0.8061	2.5255	3.2234	8.0182	7.2187
0.0311	0.8877	3.8447	4.0651	9.1820	7.9499
0.0366	0.9629	4.9896	4.9451	10.2974	8.6234
0.0420	1.0322	5.9783	5.8977	11.4560	9.2443
0.0474	1.0961	6.6832	6.9584	12.7286	9.8165

Disk Deflection (mm)	**% Error (Weight)**	**% Error (Max T22)**
0.0256	21.6513	11.0749
0.0311	5.4199	15.4984
0.0366	0.8983	19.4129
0.0420	1.3672	23.9251
0.0474	3.9553	29.6661