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DESIGN OPTIMIZATION FOR 2-D GRANULAR MEDIA WITH DISSIPATION

BY

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THESIS

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Abstract

We propose an optimization scheme for the tailored dynamic response through a two-dimensional packing of spherical beads. Our goal is to minimize or maximize the reaction force at the desired bead contacts. Two design approaches are presented: introducing interstitial beads and prescribing initial plastic compression in the system. Using the intruders presence or lack thereof as the design variable is a discrete optimization problem. It is necessary to make the problem tractable by convexifying the design space. The intruders presence (or non-presence) are replaced by their volume fraction. A penalty term in the cost function is used to recover the discrete design representation wherein the volume fraction converges to 0,1 values. Constraints on the design space limit the total number of intruders, which is related to the total packing weight. Designs obtained from both the elastic and the elasto-plastic material response are compared.

In our second approach, we prescribe the initial plastic compression of the contact law in the beads which alters their stiffnesses. To do this the contact law is shifted by the amount of initial plastic compression and to ensure that all the beads are tightly packed, an upper bound on the initial plastic compression is imposed to limit the amount of plastic deformation between the beads.

To evaluate the response, we perform a transient analysis using an explicit Runge-Kutta algorithm with an adaptive time step scheme. Residual plasticity is modeled using an empirical one dimensional law that describes the history dependent contact interaction between the beads. A constitutive equation is required to evolve the state variables, i.e. the bead's plastic deformation and large displacements are considered. Sensitivities are calculated using an adjoint method for the coupled transient analysis.

To my mom, Isabel, and my dad, José Antonio

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List of Symbols

Notation

a	e.g. lower case letter denotes a scalar a
$\boldsymbol{a}$	e.g. italic bold font denotes a vector $\boldsymbol{a}$
$\boldsymbol{A}$	e.g. upper case bold font denotes a matrix $\boldsymbol{A}$

Abbreviations

MMA	Method of moving Asymptotes
IPOPT	Interior Point Optimization

Chapter 1

Introduction

Research on the design of granular materials is scarce due to their high complexity and difficulty to be properly modeled. This is especially true for disordered granular materials, which can show combined properties from solids, liquids and gases [9]. In this thesis, we focus on granular lattices whose characterization has been an active research area recently. This type of material show interesting dynamic properties that make them an ideal choice for specific applications such as impulse adsorption [5], energy trapping [4], and energy dissipation [13]. For example, the insertion of interstitial beads in select locations has been suggested as a mean to control energy propagation [17, 18]. Differences in the beads material properties also affect wave fronts [11] for so called energy wave tailoring. More recently, new approaches to design granular lattices for specific applications have been presented. In [7], using an evolutionary algorithm, bead size and material are optimized to minimize the transmitted force through a one-dimensional chain. Structural optimization tools [1] have also been successfully applied to the design of a two-dimensional bead packing [15].

Design approaches presented to date do not consider plastic deformation, an important issue in energy wave tailoring. Traditionally, contact between two spherical particles in a granular lattice has been modeled using Hertz's law, which assumes small deformation elastic behavior. While this theory has been validated for a wide range of materials [3], its applicability is somewhat limited. Notably, it cannot model the plastic deformation that incurs due to the high stress that develops in the small contact region between two beads. Such plasticity leads to the formation and merging of wave trains with different characteristics than those of elastic chains [12]. Thornton [19] developed one of the most widely used models for two spheres undergoing elasto-plastic contact. Unfortunately, this model under-predicts the experimental force-displacement behavior [22]. Other previous approaches to model plastic dissipation consider viscoelastic terms in the contact law [13, 14, 2] or use an empirical force-displacement law derived from finite element simulation [8, 20, 10, 12]. The studies in [20] and [10] are limited to small deformation and hence not appropriate for large deformations observed in our dynamically loaded lattice arrays. In this thesis, we incorporate the large deformation plasticity effects modeled by [12], that can accurately model initial loading, unloading and reloading.

In the following, we present an optimization framework for the design of bead packings which considers plastic dissipation. To simulate a given packing design, we model each contact between two beads via an elastic-plastic spring [12] making it amenable to the discrete element method (DEM). The dynamic nature of the problem necessitates an explicit time integration method. We employ a fifth-order explicit Runge-Kutta algorithm with an adaptive time step scheme to maintain the desired level of accuracy. State variables are evolved to describe the history dependent plasticity effects. The evolution equations are solved explicitly; thereby no nested loops are necessary despite the

coupling between the response, i.e. displacement and state variables. The cost and constraint function time integrals are evaluated during the primal analysis using the same adaptive time stepping scheme to reduce the error in these critical response measures. We use the adjoint method to evaluate the gradients of these functions with respect to the design variables, which are required by the gradient-based optimization algorithm that is used to solve the design problem.

Finally, we present two design problems. A discrete approach using intruder placement as design variables in a quadrangular packing is solved by means of a topology optimization scheme. The discrete design space, the presence (or absence) of intruders, is convexified by introducing intruder volume fractions. Penalization techniques are applied to obtain a discrete layout, wherein the volume fraction design variables converge to 0 or 1 values which indicate the intruder presence or lack thereof. Secondly, we design a hexagonal packing by means of optimizing the amount of residual plastic deformation in a bead pair contact. Such initial plastic deformation provides more contact area between beads and thusly extends the strain range in which they behave elastically. The initial plastic deformation also affects the contact law since it creates gaps between beads which reduces the order in the lattice. This latter effect is modeled by artificially shifting the contact law an amount equal to the initial plastic deformation. We present results for both approaches in Chapter 2 and we draw conclusions in Chapter 3.

Chapter 2

Design optimization for 2-D granular media with dissipation

2.1 Physical problem

The goal of this work is the design of granular systems, specifically a two-dimensional packing of spherical beads with tailored dynamic response. We use an optimization scheme to design the lattice to either maximize, i.e. focus, or minimize, i.e. disperse the contact force over a given space-time region. We consider two different types of lattices, cf. Figure 2.1. The quadrangular packing contains interstitial voids that will be selectively filled with small “intruder” beads (the red beads in Figure 2.1), i.e. the intruders distribution is optimized for this lattice. We also consider a hexagonal lattice on which the design variables are the level of initial plastic compression between every bead pair.

Simulating the lattice using a continuum mechanics approach would be highly costly. Each bead would have to be discretized by thousands of finite elements because of the high contact stress and the contact interfaces themselves would have to be modeled by hundreds of unilateral constraints equations. We simplify this analysis by representing the contact interaction between a bead pair with a one dimensional contact law. In this DEM approach, we disregard the information about the deformation within the beads. Rather, only the deformation between the centers of the contacting beads is modeled, cf. Figure 2.2.

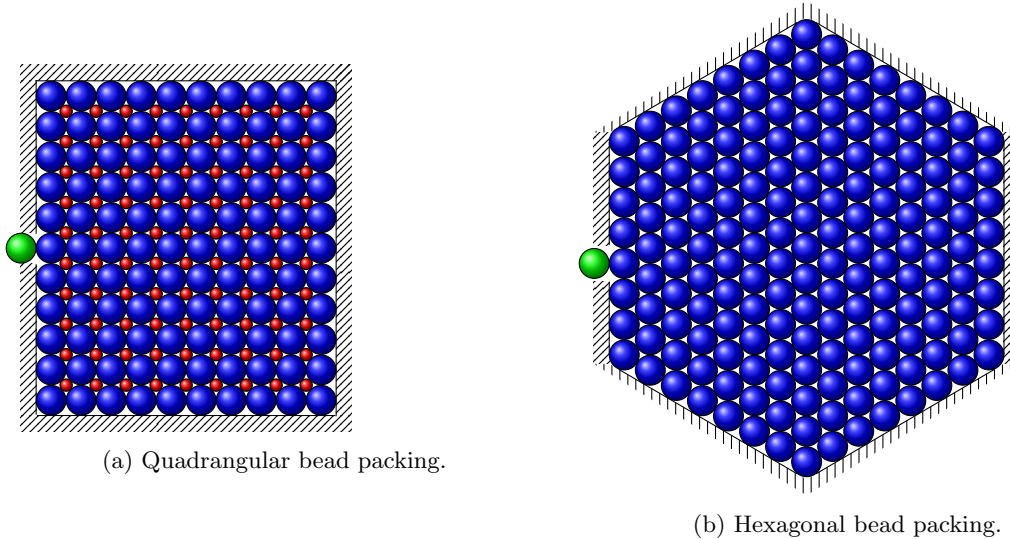


Figure 2.1: Bead packings.

With this simplification, we can model the bead packing as a spring-mass lattice, in which the bead centers serve as nodes. Springs interconnect the nodes of the adjacent, i.e. contacting, beads and the bead mass is assigned to its respective node. In Figure 2.3, we illustrate the lattice with two intruders (red beads).

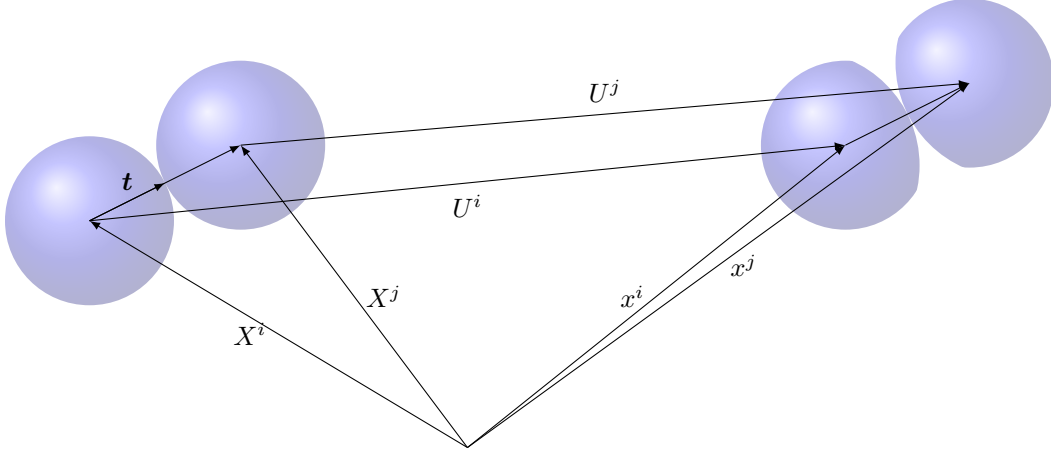


Figure 2.2: Displacements between two beads.

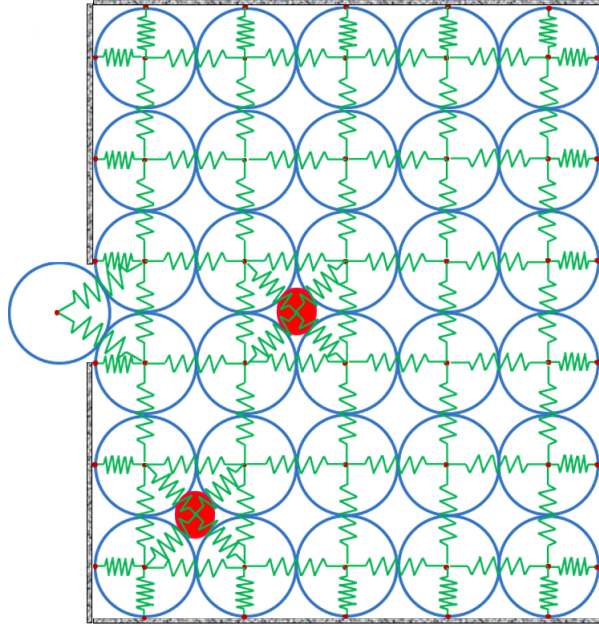


Figure 2.3: DEM for the bead packing.

2.2 Governing equations

The objective of the lattice simulation is to compute the bead displacement trajectories. To do so we define the relative displacement α_{ij} , i.e., the change in distance between the undeformed and deformed bead centers i and j , as:

$$\begin{aligned}
 \alpha_{ij} &= \|\mathbf{X}_i - \mathbf{X}_j\| - \|\mathbf{x}_i - \mathbf{x}_j\| \\
 &= \|\mathbf{X}_i - \mathbf{X}_j\| - \|\mathbf{X}_i + \mathbf{U}_i - (\mathbf{X}_j + \mathbf{U}_j)\| \\
 &= \sqrt{|\mathbf{X}_i - \mathbf{X}_j|^2} - \sqrt{|\mathbf{X}_i - \mathbf{X}_j|^2 + 2(\mathbf{X}_i - \mathbf{X}_j)(\mathbf{U}_i - \mathbf{U}_j) + |\mathbf{U}_i - \mathbf{U}_j|^2},
 \end{aligned} \tag{2.1}$$

where $\mathbf{X}_i$, $\mathbf{x}_i$ and $\mathbf{U}_i$ are the undeformed node coordinates, deformed coordinates and node displacement components for the bead i . Note that $\alpha_{ij} \geq 0$ implies beads i and j are in contact, whereas $\alpha_{ij} < 0$ implies they have separated.

The relative deformation α_{ij} is used to compute the interbead contact force F_{ij} , in much the same way that the strain (that is also obtained from the displacement) is used to compute the stress. Previous design frameworks have employed the classic Hertz's contact which restricts the design to very low load levels, which is not suitable for our situation. We do, however, apply this Hertz law before we have reached yielding; wherein:

$$F_{ij} = F_H(\alpha_{ij}) = \begin{cases} \frac{4}{3} E^* R^{*1/2} \alpha_{ij}^{3/2} & \text{if } \alpha_{ij} \geq 0 \\ 0 & \text{if } \alpha_{ij} < 0 \end{cases}, \quad (2.2)$$

in which E^* and R^* are the material and geometric parameters

$$\begin{aligned} R^* &= \frac{R_i R_j}{R_i + R_j} \\ \frac{1}{E^*} &= \frac{1 - \nu_1^2}{E_i} + \frac{1 - \nu_2^2}{E_j}, \end{aligned} \quad (2.3)$$

where R_i , E_i and ν_i are the bead i radius, Young modulus and Poisson ratio, respectively. In our study, we assume all the beads have the same material properties so that $E_i = E_j = E$ and $\nu_i = \nu_j = \nu$. Note that negative values of α_{ij} indicate bead separation and hence zero contact force.

The internal interbead forces, obtained from Equation (2.2) are decomposed into their components cf. Figure 2.4, such that the force $\mathbf{F}_{ij}$ acting on node i from node j is given by:

$$\mathbf{F}_{ij} = F_H(\alpha_{ij}) \mathbf{e}_{ij}, \quad (2.4)$$

where

$$\mathbf{e}_{ij} = \frac{\mathbf{x}_i - \mathbf{x}_j}{\|\mathbf{x}_i - \mathbf{x}_j\|}, \quad (2.5)$$

is the unit vector defined by the deformed locations of the bead centers. The force $\mathbf{F}_{ij}$ is added to the node i internal force vector while the opposite force, i.e. $\mathbf{F}_{ji} = -\mathbf{F}_{ij}$ is added to the node j internal force vector.

Having the constitutive law relating force to displacement, we next enforce the motion equation for the beads, i.e.

$$\begin{aligned} \mathbf{M}\ddot{\mathbf{u}} + \mathbf{n}(\mathbf{u}) &= \mathbf{F}^{ext} \\ \mathbf{u} &= \mathbf{0} \quad \text{at } t = 0 \\ \dot{\mathbf{u}} &= \mathbf{0} \quad \text{at } t = 0, \end{aligned} \quad (2.6)$$

where the mass matrix $\mathbf{M}$ is a diagonal matrix of bead masses; the vector $\mathbf{u}$ contains the node displacement x and y components for all the beads; the vector $\mathbf{F}^{ext}$ accounts for the external force components acting on each bead; and finally, the internal force vector $\mathbf{n}(\mathbf{u})$ collects the interbead contact force component contributions acting on each bead.

The high contact stress induces plasticity deformation even at low load levels. We model this plastic behavior in the context of our one-dimensional contact law by adopting an elasto-plastic contact law which is based on the finite element analysis of homogeneous isotropic elastic perfectly plastic contacting beads [12]. The law resembles that of a uniaxial stress strain law for ductile materials. To determine whether or not the beads yield, we compute

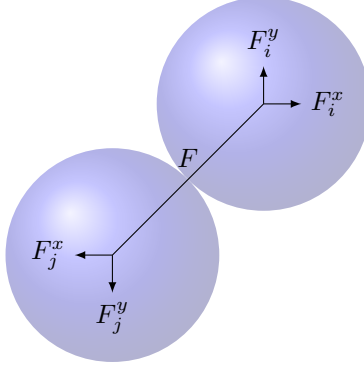


Figure 2.4: Force nodal contributions.

the relative displacement at the onset of yield.

$$\alpha_{ij}^y = \frac{\pi^2}{4} \left(\frac{1.6 \sigma_y}{E^*} \right)^2 R^* , \quad (2.7)$$

where σ_y is the bead yield strength (this is akin to the yield strain $\varepsilon_y = \sigma_y/E$). Assuming the initial plastic deformation for the bead $i-j$ contact is zero, the beads contact force is given by Hertz's law if $\alpha_{ij} < \alpha_{ij}^y$. Otherwise, we are in the plastic regime, whence:

$$F_{ij} = F_p(\alpha_{ij}) = \bar{p}_{ij} A_{ij} , \quad (2.8)$$

where

$$\bar{p}_{ij} = \sigma_y (2.48 - 1.41 \exp(-0.098 (\tilde{\alpha}_{ij} - 1))) , \quad (2.9)$$

$$A_{ij} = \begin{cases} A_y \tilde{\alpha}_{ij}^{1.14}, & \text{if } \tilde{\alpha}_{ij} < 177.6 \\ A_y (2.37 \tilde{\alpha}_{ij} - 59.59), & \text{otherwise} \end{cases} . \quad (2.10)$$

In the above $\bar{p}_{ij}$ is the average pressure and A_{ij} is the contact area between two beads with $\tilde{\alpha}_{ij} = \alpha_{ij}/\alpha_{ij}^y$ and $A_y = \pi R^* \alpha_{ij}^y$.

The permanent plastic deformation α_{ij}^R , which plays the role of the plastic strain, represents the flattening of the contacting surfaces cf. Figure 2.2. It evolves with deformation α_{ij} according to

$$\alpha_{ij}^R(t) = \max_{\tau \in [0, t]} \{0, 0.95 \alpha_{ij}(\tau) - 25.94 \alpha_{ij}^y + 25.0 \alpha_{ij}^y \exp(-0.015[\tilde{\alpha}_{ij}(\tau) - 1])\} . \quad (2.11)$$

In von Mises plasticity, the plastic equivalent strain $\bar{\varepsilon}$ is the internal state variable that quantifies the deformation history and path-dependent constitutive response. In our model, the analogous state variable is α_{ij}^R . However, because of the implicit relation between the maximum relative deformation, $\alpha_{ij}^m(t) = \max_{\tau \in [0, t]} \alpha_{ij}(\tau)$, and α_{ij}^R in Equation (2.11), it is preferable to use α_{ij}^m as the internal state variable and calculate α_{ij}^R using Equation (2.11). Note that while α_{ij}^m is not used to define F_p , it is used to define F_{ij} in the elastic regime for which $\alpha_{ij}^m < \alpha_{ij}^y$.

Once the plastic deformation α_{ij}^R exceeds zero, Equation (2.8) is used to define the yield criteria, rather than Equation (2.7), i.e. the bead pair yields if $F_p(\alpha_{ij}) > F_e(\alpha_{ij})$ as opposed to the Equation (2.7) criteria which indicates yielding if $F_H(\alpha_{ij}) > F_H(\alpha_{ij}^y)$. In the above, after the beads yield, i.e when $\alpha_{ij}^R > 0$, the elastic force response is

given by

$$F_{ij} = F_e(\alpha_{ij}, \alpha_{ij}^m) = \begin{cases} F_p(\alpha_{ij}^m) \left(\frac{\alpha_{ij} - \alpha_{ij}^R}{\alpha_{ij}^m - \alpha_{ij}^R} \right)^{1.35} & \text{if } \alpha_{ij} > \alpha_{ij}^R \\ 0 & \text{if } \alpha_{ij} \leq \alpha_{ij}^R \end{cases}. \quad (2.12)$$

Note the shift due to the permanent plastic deformation α_{ij}^R . This differs from the uniaxial case, wherein the same load curve is used for elastic behavior, i.e. $\sigma = E \varepsilon$ before yield and $\sigma = E(\varepsilon - \bar{\varepsilon})$ after yield. We express the elastic response as one conditional expression

$$F_E(\alpha_{ij}, \alpha_{ij}^m) = \begin{cases} F_H(\alpha_{ij}) & \text{if } \alpha_{ij}^m < \alpha_{ij}^y \\ F_e(\alpha_{ij}, \alpha_{ij}^m) & \text{else} \end{cases}. \quad (2.13)$$

We similarly summarize the yield function

$$f(\alpha_{ij}, \alpha_{ij}^R) = \begin{cases} F_H(\alpha_{ij}) - F_H(\alpha_{ij}^y) & \text{if } \alpha_{ij}^R = 0 \\ F_e(\alpha_{ij}, \alpha_{ij}^m) - F_p(\alpha_{ij}) & \text{if } \alpha_{ij}^R > 0 \end{cases}, \quad (2.14)$$

the force

$$F_{ij} = \begin{cases} F_E(\alpha_{ij}, \alpha_{ij}^m) & \text{if } f(\alpha_{ij}, \alpha_{ij}^R) \leq 0 \text{ and } \dot{\alpha}_{ij}^m = 0 \\ F_p(\alpha_{ij}) & \text{if } f(\alpha_{ij}, \alpha_{ij}^R) = 0 \text{ and } \dot{\alpha}_{ij}^m > 0 \end{cases}, \quad (2.15)$$

and the state variable evolution

$$\dot{\alpha}_{ij}^m = g(\mathbf{u}, \alpha_{ij}^m) = \begin{cases} 0, & \text{if } f(\alpha_{ij}, \alpha_{ij}^R) \leq 0 \\ \dot{\alpha}_{ij} & \text{if } f(\alpha_{ij}, \alpha_{ij}^R) = 0 \end{cases}. \quad (2.16)$$

In Figure 2.5, we plot the elasto-plastic contact law for several loading cycles. The blue line represents the plastic loading, while the red line represents the elastic regime. Note the continuity of the load curves obtained by the model [12].

We need to incorporate the state variable and its evolution Equation (2.16) with the governing Equations (2.6) to complete the problem description, i.e. we now need to evaluate $\mathbf{u}$ and $\boldsymbol{\alpha}^m$ such that

$$\begin{aligned} \mathbf{M}\ddot{\mathbf{u}} + \mathbf{n}(\mathbf{u}, \boldsymbol{\alpha}^m) &= \mathbf{F}^{ext} \\ \dot{\boldsymbol{\alpha}}^m &= \mathbf{g}(\mathbf{u}, \boldsymbol{\alpha}_{ij}^m) \\ \mathbf{u} &= \mathbf{0} \quad \text{at } t = 0 \\ \dot{\mathbf{u}} &= \mathbf{0} \quad \text{at } t = 0 \\ \boldsymbol{\alpha}^m &= \mathbf{0} \quad \text{at } t = 0, \end{aligned} \quad (2.17)$$

where $\boldsymbol{\alpha}^m$ contains the spring α_{ij}^m . There are as many state variable equations as springs in our DEM, however the evolution equations are not coupled.

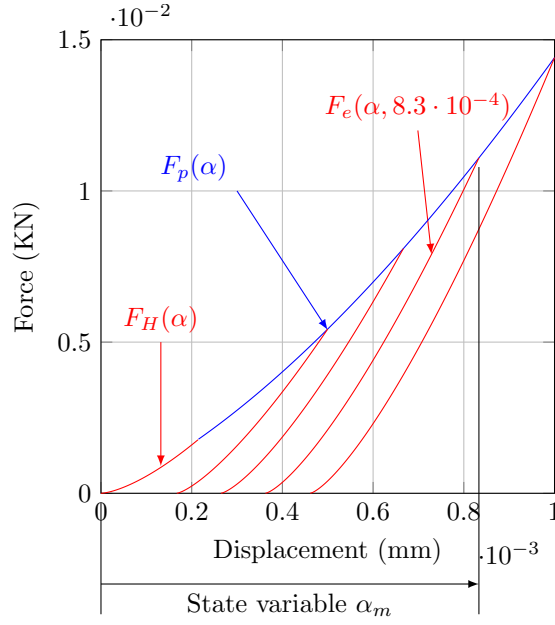


Figure 2.5: Elasto-plastic contact law.

2.3 Optimization

Our intention is to obtain a desired response from the lattice. To do this we formulate and solve the optimization problem:

$$\begin{aligned} \min_{\mathbf{p} \in [a, b]} \quad & \Psi_0(\mathbf{p}) \\ \text{such that} \quad & \Psi_k(\mathbf{p}) \leq 0, \quad k = 1, \dots, M, \end{aligned} \quad (2.18)$$

in which we are optimizing the design variable vector $\mathbf{p}$ to minimize the cost function Ψ_0 and satisfy the constraints $\Psi_k(\mathbf{p}) \leq 0$. The design variables quantify either the interstitial volume fraction or bead precompression. The cost function Ψ_0 reflects the force based quantity we want to minimize and the constraints $\Psi_k(\mathbf{p}) \leq 0$ are used to enforce desired limitations in the design space, for instance, an upper bound on the number of interstitial beads.

The cost and constraint functions are defined as integrals over the space-time domain, i.e.

$$\Psi(\mathbf{p}) = \int_{\mathcal{I}} \int_{\Omega} \Psi(t, \mathbf{p}) \, d\Omega \, dt \quad . \quad (2.19)$$

We integrate them using the same adaptive time stepping integration scheme that we use in the primal analysis to ensure a desired level of accuracy. In Equation (2.19), the space region Ω is the lattice region and $\mathcal{I} = [0, t_f]$ is the time interval of interest. For our purpose, Ω is the contact interface between certain bead pairs which we model with springs. As such, Equation (2.19) is replaced

$$\Psi(\mathbf{p}) = \int_{\mathcal{I}} \sum_{j=1}^{NTe} \Psi_j(t, \mathbf{p}) \, dt = \int_{\mathcal{I}} r(t, \mathbf{p}) \, dt \quad , \quad (2.20)$$

where NTe is the number of contacts and $\Psi_j(t, \mathbf{p})$ is the restriction of Ψ to the contact region Ω_j . For instance, in Figure 2.6, the contact between beads 1 – 4 and the wall is subjected to a force maximization. As such Ψ_j is replaced

with F_{jw} with $j = 1, 2, 3, 4$, w being the fixed wall and $NTe = 4$.

For numerical computation, we isolate the integrand in Equation (2.20) and define

$$\dot{q}(t, \mathbf{p}) = r(t, \mathbf{p}) , \quad (2.21)$$

which allows us to evaluate:

$$\Psi(\mathbf{p}) = q(t_f, \mathbf{p}) , \quad (2.22)$$

assuming $q(0, \mathbf{p}) = 0$.

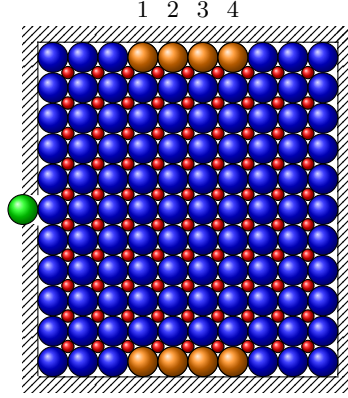


Figure 2.6: Target beads.

We add the function integrations to the primal analysis, which now reads

$$\begin{aligned} \mathbf{M}(\mathbf{p})\ddot{\mathbf{u}}(t, \mathbf{p}) + \mathbf{n}(\mathbf{u}(t, \mathbf{p}), \boldsymbol{\alpha}^m(t, \mathbf{p}), \mathbf{p}) &= \mathbf{F}^{ext}(t, \mathbf{p}) \\ \dot{\boldsymbol{\alpha}}^m(t, \mathbf{p}) &= \mathbf{g}(\mathbf{u}(t, \mathbf{p}), \mathbf{p}) \\ \mathbf{u}(0, \mathbf{p}) &= \mathbf{0} \\ \dot{\mathbf{u}}(0, \mathbf{p}) &= \mathbf{0} \\ \boldsymbol{\alpha}^m(0, \mathbf{p}) &= \mathbf{0} \\ \dot{q}_k(t, \mathbf{p}) &= r_k(t, \mathbf{p}) \quad k = 0 \dots M , \end{aligned} \quad (2.23)$$

where we have added the dependency on the design variables $\mathbf{p}$ in anticipation of the sensitivity analysis to follow.

2.4 Numerical approach

We solve the transient problem with a fifth-order explicit Runge-Kutta method, specifically, the Dormand-Prince method. This requires us to reformulate Equation (2.23) in a state-space form which is.

$$\begin{aligned}
\dot{\mathbf{y}}(t, \mathbf{p}) &= \mathbf{F}(\mathbf{y}(t, \mathbf{p}), \boldsymbol{\alpha}^m(t, \mathbf{p}), \mathbf{p}) \\
\dot{\boldsymbol{\alpha}}^m(t, \mathbf{p}) &= \mathbf{g}(\mathbf{y}(t, \mathbf{p}), \mathbf{p}) \\
\dot{\mathbf{p}} &= \mathbf{0} \\
\mathbf{y}(0, \mathbf{p}) &= \mathbf{0} \\
\boldsymbol{\alpha}^m(0, \mathbf{p}) &= \mathbf{0} \\
\dot{q}_k(\mathbf{y}(t, \mathbf{p}), \boldsymbol{\alpha}^m(t, \mathbf{p}), t, \mathbf{p}) &= r_k(\mathbf{y}(t, \mathbf{p}), \boldsymbol{\alpha}^m(t, \mathbf{p}), t, \mathbf{p}) \quad k = 0 \dots M,
\end{aligned} \tag{2.24}$$

The state-space form is readily obtained because the mass matrix $\mathbf{M}$ is diagonal. To ensure the design variables remain constant throughout the simulation, we enforce $\dot{\mathbf{p}} = \mathbf{0}$ and thusly we suppress the arguments on $\mathbf{p}$ for conciseness. This seemingly unnecessary equation is included to simplify the adjoint sensitivity analysis. In the above:

$$\mathbf{y} = \begin{bmatrix} \mathbf{v} \\ \mathbf{u} \end{bmatrix}, \tag{2.25}$$

with $\mathbf{v} = \dot{\mathbf{u}}$, and

$$\mathbf{F} = \begin{bmatrix} \mathbf{M}^{-1} (\mathbf{F}^{ext} - \mathbf{n}) \\ \mathbf{v} \end{bmatrix}. \tag{2.26}$$

Discretizing the above via the Runge-Kutta method yields the update formulas for $\mathbf{y}, \boldsymbol{\alpha}^m$ and q^k .

For $n = 1 \dots N$

$$\begin{aligned}
\mathbf{y}_n &= \mathbf{y}_{n-1} + h \sum_{i=1}^s b_i [\mathbf{F}(\mathbf{y}_{n-1}^i, \boldsymbol{\alpha}_{n-1}^m, t_{n-1} + c_i h, \mathbf{p}_{n-1}^i)] \\
\mathbf{y}_{n-1}^i &= \mathbf{y}_{n-1} + h \sum_{j=1}^s a_{ij} [\mathbf{F}(\mathbf{y}_{n-1}^j, \boldsymbol{\alpha}_{n-1}^m, t_{n-1} + c_j h, \mathbf{p}_{n-1}^j)] \quad i = 1 \dots s \\
\mathbf{p}_n &= \mathbf{p}_{n-1} \\
\mathbf{p}_{n-1}^i &= \mathbf{p}_{n-1} \quad i = 1 \dots s \\
\boldsymbol{\alpha}_n^m &= \mathbf{g}(\boldsymbol{\alpha}_{n-1}^m, \mathbf{y}_n, \mathbf{p}_{n-1}) \\
q_n^k &= q_{n-1}^k + h \sum_{i=1}^s b_i [r^k(\mathbf{y}_{n-1}^i, \boldsymbol{\alpha}_{n-1}^m, t_{n-1} + c_i h, \mathbf{p}_{n-1}^i)] \quad k = 0, 1, \dots M \\
(q_{n-1}^k)^i &= q_{n-1}^k \quad i = 1 \dots s,
\end{aligned} \tag{2.27}$$

where $t_f = t_N$, $s = 7$ is the number of stages; $\mathbf{y}_{n-1}^i, \mathbf{p}_{n-1}^i$ and $(q_{n-1}^k)^i$ are the auxiliary stage i variables at time step t_{n-1} ; $h = t_n - t_{n-1}$ is the time step size; and the state variable $\boldsymbol{\alpha}^m$ is integrated directly because $\mathbf{g}(\boldsymbol{\alpha}_{n-1}^m, \mathbf{y}_n, \mathbf{p}_{n-1})$ is either equal to $\boldsymbol{\alpha}_{n-1}^m$ or $\boldsymbol{\alpha}_n$ depending on whether we are in the elastic or plastic regime.

As we stated before, we use the Dormand-Prince explicit Runge-Kutta scheme. The Equation (2.27) coefficients

b_i , c_i and a_{ij} are obtained from the Butcher table:

$$\begin{array}{c|cccc}
 c_1 & a_{11} & a_{12} & \dots & a_{1s} \\
 c_2 & a_{21} & a_{22} & \dots & a_{2s} \\
 \vdots & \vdots & \vdots & \ddots & \vdots \\
 c_s & a_{s1} & a_{s2} & \dots & a_{ss} \\
 \hline
 & b_1 & b_2 & \dots & b_s \\
 & b_1^* & b_2^* & \dots & b_s^*
 \end{array} \tag{2.28}$$

which in our fifth-order seven-stage scheme is as follows:

$$\begin{array}{c|cccccc}
 0 & & & & & \\
 1/5 & 1/5 & & & & \\
 3/10 & 3/40 & 9/40 & & & \\
 4/5 & 44/45 & -56/15 & 32/9 & & \\
 8/9 & 19372/6561 & -25360/2187 & 64448/6561 & -212/729 & \\
 1 & 9017/3168 & -355/33 & 46732/5247 & 49/176 & -5103/18656 \\
 1 & 35/384 & 0 & 500/1113 & 125/192 & -2187/6784 & 11/84 \\
 \hline
 & 35/384 & 0 & 500/1113 & 125/192 & -2187/6784 & 11/84 & 0 \\
 & 5179/57600 & 0 & 7571/16695 & 393/640 & -92097/339200 & 187/2100 & 1/40
 \end{array} \tag{2.29}$$

where, e.g. $a_{31} = 3/40$. The b_i^* coefficients (the last row of the Table 2.29) are required to implement the adaptive time stepping scheme as described in [6]. For our simulation, it is important to have an adaptive scheme because the initial high concentration of momentum dissipates considerably as the simulation progresses. Thusly, initially small time steps give way to larger ones.

2.5 Sensitivity analysis

To solve Equation (2.18) we invoke an iterative nonlinear programming algorithm. In each iteration of the algorithm, we solve the nonlinear transient dynamics problem to compute the response variables and the cost and constraint function. Next we run the adjoint sensitivity analysis to evaluate the cost and constraint function derivatives with respect to the design variables $\mathbf{p}$. The optimization algorithm uses this information to check for convergence and update the design variables when necessary. Figure 2.7 represents the described process.

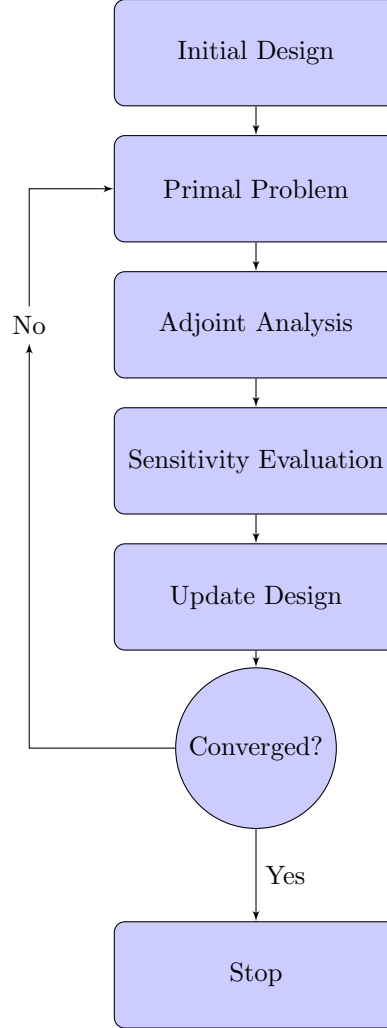


Figure 2.7: Optimization scheme.

2.5.1 Infinity-norm optimization

In this optimization problem, we intend to minimize, maximize or constrain the maximum value f_{max} of a given function f over a given space-time domain. Unfortunately, such a function is non-differentiable with respect to the design and thereby it precludes the use of gradient-based optimization algorithms when solving Equation (2.18). For

this reason, we approximate the maximum function with the p -norm.

$$f_{\max}(\mathbf{p}) = \|f\|_{L^\infty(\Omega \times \mathcal{I})}(\mathbf{p}) \approx \|f\|_{L^p(\Omega \times \mathcal{I})}(\mathbf{p}) = \left(\int_{\mathcal{I}} \left(\int_{\Omega} |f(\mathbf{p}, t)|^S d\Omega \right)^{T/S} dt \right)^{1/T}. \quad (2.30)$$

As seen above the p -norm encompasses both the spatial Ω and time domain $\mathcal{I} = [0, t_f]$. The coefficients S and T correspond to the p -norm coefficients for the space and time domains; they are chosen to be sufficiently large to accurately approximate the ∞ -norm, but not too large so as to adversely affect the optimization via ill-conditioning. Note the value of $T(S) = 1$ captures the average magnitude of f over the time(spatial) domain.

To evaluate $\|f\|_{L^p}$ We apply the same discretization in space as we do in Equation (2.20) to define a generic response function, i.e.

$$\Psi(\mathbf{p}) = \|f\|_{L^p(\Omega \times \mathcal{I})}(\mathbf{p}) = \left(\int_{\mathcal{I}} \left(\sum_{j=1}^{N_{Te}} (f_j(t, \mathbf{p}))^S \right)^{T/S} dt \right)^{1/T}. \quad (2.31)$$

Next we extract the integrand that we evolve in the primal analysis, i.e.

$$\dot{q}(t, \mathbf{p}) = r(t, \mathbf{p}) = \left(\sum_{j=1}^{N_{Te}} (f_j(t, \mathbf{p}))^S \right)^{T/S}. \quad (2.32)$$

With this, we compute the response function value as

$$\Psi(\mathbf{p}) = (q(\mathbf{p}, t_f))^{(1/T)}. \quad (2.33)$$

To accommodate a likely need to optimize different response functions, i.e to simultaneously maximize the reaction force in different regions, we define the multiobjective response function as

$$\Psi(\mathbf{p}) = \sum_{l=1}^{N_{obj}} \beta_l \Psi^l(\mathbf{p}), \quad (2.34)$$

where the β_l are the weighting coefficients for the N_{obj} cost functions $\Psi^l = (q^l)^{(1/T)}$.

For the sensitivity analysis we differentiate Ψ with respect to a scalar design variable p_i

$$D_i \Psi = \left(\sum_{l=1}^{N_{obj}} \beta_l \frac{1}{T} [q_N^l]^{\frac{1}{T}-1} D_i q^l \right) \Big|_{t=t_f} = \sum_{l=1}^{N_{obj}} \Phi^l D_i q_N^l, \quad (2.35)$$

where

$$\Phi^l = \beta_l \frac{1}{T} [q_N^l]^{\frac{1}{T}-1}, \quad (2.36)$$

and $D_i q_N^l$ is the derivative of q^l with respect to p_i at time $t = t_f$, i.e. at time step N . To calculate the sensitivity, we use the direct differentiation and adjoint methods.

2.5.2 Direct differentiation

The direct differentiation solves the so called pseudo problems to evaluate $D_i q_N^l$. These problems are obtained by differentiating the governing Equations (2.27) with respect to each design variable p_i , i.e.

For $n = 1 \dots N$

$$D\mathbf{y}_n = D\mathbf{y}_{n-1} + h \sum_{i=1}^s b_i \left[\frac{\partial \mathbf{F}(\mathbf{y}_{n-1}^i, t + c_i h)}{\partial \mathbf{y}_{n-1}^i} D\mathbf{y}_{n-1}^i + \frac{\partial \mathbf{F}(\mathbf{y}_{n-1}^i, t + c_i h)}{\partial \mathbf{p}_{n-1}^i} D\mathbf{p}_{n-1}^i + \frac{\partial \mathbf{F}(\mathbf{y}_{n-1}^i, t + c_i h)}{\partial \boldsymbol{\alpha}_{n-1}^m} D\boldsymbol{\alpha}_{n-1}^m \right]$$

$$D\mathbf{y}_{n-1}^i = D\mathbf{y}_{n-1} + h \sum_{j=1}^s a_{ij} \left[\frac{\partial \mathbf{F}(\mathbf{y}_{n-1}^j, t + c_j h)}{\partial \mathbf{y}_{n-1}^j} D\mathbf{y}_{n-1}^j + \frac{\partial \mathbf{F}(\mathbf{y}_{n-1}^j, t + c_j h)}{\partial \mathbf{p}_{n-1}^j} D\mathbf{p}_{n-1}^j + \frac{\partial \mathbf{F}(\mathbf{y}_{n-1}^j, t + c_j h)}{\partial \boldsymbol{\alpha}_{n-1}^m} D\boldsymbol{\alpha}_{n-1}^m \right] \quad i = 1 \dots s$$

$$D\mathbf{p}_n = D\mathbf{p}_{n-1}$$

$$D\mathbf{p}_{n-1}^i = D\mathbf{p}_{n-1} \quad i = 1 \dots s$$

$$D\boldsymbol{\alpha}_n^m = \frac{\partial g(\boldsymbol{\alpha}_{n-1}^m, \mathbf{y}_n, \mathbf{p}_{n-1})}{\partial \boldsymbol{\alpha}_{n-1}^m} D\boldsymbol{\alpha}_{n-1}^m + \frac{\partial g(\boldsymbol{\alpha}_{n-1}^m, \mathbf{y}_n, \mathbf{p}_{n-1})}{\partial \mathbf{y}_n} D\mathbf{y}_n + \frac{\partial g(\boldsymbol{\alpha}_{n-1}^m, \mathbf{y}_n, \mathbf{p}_{n-1})}{\partial \mathbf{p}_{n-1}} D\mathbf{p}_{n-1}$$

For $l = 1, \dots, NObj$

$$Dq_n^l = Dq_{n-1}^l + h \sum_{i=1}^s b_i \left[\frac{\partial r^l(\mathbf{y}_{n-1}^i, t + c_i h)}{\partial \mathbf{y}_{n-1}^i} D\mathbf{y}_{n-1}^i + \frac{\partial r^l(\mathbf{y}_{n-1}^i, t + c_i h)}{\partial \mathbf{p}_{n-1}^i} D\mathbf{p}_{n-1}^i + \frac{\partial r^l(\mathbf{y}_{n-1}^i, t + c_i h)}{\partial \boldsymbol{\alpha}_{n-1}^m} D\boldsymbol{\alpha}_{n-1}^m \right]$$

$$Dq_{n-1}^{i,l} = Dq_{n-1}^l \quad i = 1 \dots s,$$

(2.37)

Once the $D_i q^l$ are computed, the sensitivity is evaluated from Equation (2.35).

In the above, the variables $\mathbf{p}$ and $\boldsymbol{\alpha}^m$ are evaluated at the same time steps as $\mathbf{y}$ for the functions $\mathbf{F}$, q^l and r^l , i.e. $\mathbf{F}(\mathbf{y}_{n-1}^i, t + c_i h) = \mathbf{F}(\mathbf{y}_{n-1}^i, \boldsymbol{\alpha}_{n-1}^m, t + c_i h, \mathbf{p}_{n-1}^i)$. We suppress them for conciseness. We also neglect the time step controller derivatives because it is non differentiable. In the same vein, we note that the response is nondifferentiable if a spring is exactly on elastic-plastic or contact-no-contact interface. In practice, we find the occurrence of these situations are rare, so we neglect them. Should they occur, we merely define the sensitivity using a single directional derivative, i.e. we neglect the other.

2.5.3 Adjoint Analysis

In the adjoint method, we annihilate the implicitly defined derivatives $D\mathbf{y}_n, D\mathbf{y}_{n-1}^i, D\mathbf{p}_n, D\mathbf{p}_{n-1}^i, Dq_n^l, Dq_{n-1}^{i,l}, D\boldsymbol{\alpha}_n^m$ and $D\boldsymbol{\alpha}_{n-1}^m$. To do so, we augment the pseudo equation to the sensitivity Equation (2.35). The vector valued equations terms derived from Equation (2.37) are multiplied by the convolved adjoint variables $\boldsymbol{\lambda}^{(N-n+1)}, \boldsymbol{\Lambda}_i^{(N-n+1)}, \boldsymbol{\mu}^{(N-n+1)}, \boldsymbol{\Upsilon}_i^{(N-n+1)}, \boldsymbol{\theta}^{(N-n+1)}, \boldsymbol{\Theta}_i^{(N-n+1)}$ and $\boldsymbol{\gamma}^{(N-n+1)}$, and their resulting zero expressions are added to Equation

(2.35) rendering:

$$\begin{aligned}
D_{,i}\Psi = & \sum_{l=1}^{Nobj} \Phi^l Dq_N^l \\
& - \sum_{n=1}^N \lambda^{(N-n+1)} \left(D\mathbf{y}_n - D\mathbf{y}_{n-1} \right. \\
& \quad \left. - h \sum_{i=1}^s b_i \left[\frac{\partial \mathbf{F}(\mathbf{y}_{n-1}^i, t + c_i h)}{\partial \mathbf{y}_{n-1}^i} D\mathbf{y}_{n-1}^i + \frac{\partial \mathbf{F}(\mathbf{y}_{n-1}^i, t + c_i h)}{\partial \mathbf{p}_{n-1}^i} D\mathbf{p}_{n-1}^i + \frac{\partial \mathbf{F}(\mathbf{y}_{n-1}^i, t + c_i h)}{\partial \boldsymbol{\alpha}_{n-1}^m} D\boldsymbol{\alpha}_{n-1}^m \right] \right) \\
& - \sum_{n=1}^N \sum_{i=1}^s \Lambda_i^{(N-n+1)^T} \left(D\mathbf{y}_{n-1}^i - D\mathbf{y}_{n-1} \right. \\
& \quad \left. - h \sum_{j=1}^s a_{ij} \left[\frac{\partial \mathbf{F}(\mathbf{y}_{n-1}^j, t + c_j h)}{\partial \mathbf{y}_{n-1}^j} D\mathbf{y}_{n-1}^j + \frac{\partial \mathbf{F}(\mathbf{y}_{n-1}^j, t + c_j h)}{\partial \mathbf{p}_{n-1}^j} D\mathbf{p}_{n-1}^j + \frac{\partial \mathbf{F}(\mathbf{y}_{n-1}^j, t + c_j h)}{\partial \boldsymbol{\alpha}_{n-1}^m} D\boldsymbol{\alpha}_{n-1}^m \right] \right) \\
& - \sum_{n=1}^N \boldsymbol{\mu}^{(N-n+1)^T} (D\mathbf{p}_n - D\mathbf{p}_{n-1}) \\
& - \sum_{n=1}^N \sum_{i=1}^s \mathbf{r}_i^{(N-n+1)^T} (D\mathbf{p}_{n-1}^i - D\mathbf{p}_{n-1}) \\
& - \sum_{l=1}^{Nobj} \sum_{n=1}^N \boldsymbol{\theta}_l^{(N-n+1)^T} (Dq_n^l - Dq_{n-1}^l \\
& \quad - h \sum_{i=1}^s b_i \left[\frac{\partial r^l(\mathbf{y}_{n-1}^i, t + c_i h)}{\partial \mathbf{y}_{n-1}^i} D\mathbf{y}_{n-1}^i + \frac{\partial r^l(\mathbf{y}_{n-1}^i, t + c_i h)}{\partial \mathbf{p}_{n-1}^i} D\mathbf{p}_{n-1}^i + \frac{\partial r^l(\mathbf{y}_{n-1}^i, t + c_i h)}{\partial \boldsymbol{\alpha}_{n-1}^m} D\boldsymbol{\alpha}_{n-1}^m \right]) \\
& - \sum_{l=1}^{Nobj} \sum_{n=1}^N \sum_{i=1}^s \boldsymbol{\Theta}_{i,l}^{(N-n+1)^T} (Dq_n^{i,l} - Dq_{n-1}^l) \\
& - \sum_{n=1}^N \gamma^{(N-n+1)^T} \left(D\boldsymbol{\alpha}_n^m - \frac{\partial \mathbf{g}(\boldsymbol{\alpha}_{n-1}^m, \mathbf{y}_n, \mathbf{p}_{n-1})}{\partial \boldsymbol{\alpha}_{n-1}^m} D\boldsymbol{\alpha}_{n-1}^m - \frac{\partial \mathbf{g}(\boldsymbol{\alpha}_{n-1}^m, \mathbf{y}_n, \mathbf{p}_{n-1})}{\partial \mathbf{y}_n} D\mathbf{y}_n \right. \\
& \quad \left. - \frac{\partial \mathbf{g}(\boldsymbol{\alpha}_{n-1}^m, \mathbf{y}_n, \mathbf{p}_{n-1})}{\partial \mathbf{p}_{n-1}} D\mathbf{p}_{n-1} \right), \tag{2.38}
\end{aligned}$$

Factoring the implicit derivatives and some manipulation yields.

$$\begin{aligned}
D_{,i}\Psi = & \sum_{n=1}^N D\mathbf{y}_n^T \left(-\boldsymbol{\lambda}^{(N-n+1)} + \frac{\partial \mathbf{g}(\boldsymbol{\alpha}_{n-1}^m, \mathbf{y}_n, \mathbf{p}_{n-1})}{\partial \mathbf{y}_n} \boldsymbol{\gamma}^{(N-n+1)} + \boldsymbol{\lambda}^{(N-n)} + \sum_{i=1}^s \boldsymbol{\Lambda}_i^{(N-n)} \right) \\
& + \sum_{n=1}^N \sum_{i=1}^s D\mathbf{y}_n^i{}^T \left(-\boldsymbol{\Lambda}_i^{(N-n)} + h \frac{\partial \mathbf{F}(\mathbf{y}_n^i, t + c_i h)}{\partial \mathbf{y}_n^i} \left[\sum_{j=1}^s a_{ji} \boldsymbol{\Lambda}_j^{(N-n)} + b_i \boldsymbol{\lambda}^{(N-n)} \right] \right. \\
& \quad \left. + b_i h \sum_{l=1}^{Nobj} \frac{\partial r^l(\mathbf{y}_n^i, t + c_i h)}{\partial \mathbf{y}_n^i} \boldsymbol{\theta}_l^{(N-n)T} \right) \\
& + \sum_{n=1}^N D\mathbf{p}_n^T \left(-\boldsymbol{\mu}^{(N-n+1)} + \boldsymbol{\mu}^{(N-n)} + \sum_{i=1}^s \boldsymbol{\Upsilon}_i^{(N-n)} \right) \\
& + \sum_{n=1}^N \sum_{i=1}^s D\mathbf{p}_n^i{}^T \left(-\boldsymbol{\Upsilon}_i^{(N-n)} + h \frac{\partial \mathbf{F}(\mathbf{y}_n^i, t + c_i h)}{\partial \mathbf{p}_n^i} \left[\sum_{j=1}^s a_{ji} \boldsymbol{\Lambda}_j^{(N-n)} + b_i \boldsymbol{\lambda}^{(N-n)} \right] \right. \\
& \quad \left. + b_i h \sum_{l=1}^{Nobj} \frac{\partial r^l(\mathbf{y}_n^i, t + c_i h)}{\partial \mathbf{p}_n^i} \boldsymbol{\theta}_l^{(N-n)T} \right) \\
& + \sum_{l=1}^{Nobj} \sum_{n=1}^N Dq_n^l{}^T \left(-\boldsymbol{\theta}_l^{(N-n+1)} + \boldsymbol{\theta}_l^{(N-n)} + \sum_{i=1}^s \boldsymbol{\Theta}_i^{(N-n)} \right) \\
& + \sum_{l=1}^{Nobj} \sum_{n=1}^N \sum_{i=1}^s Dq_n^{i,l}{}^T \left(\boldsymbol{\Theta}_{i,l}^{(N-n)} \right) \\
& + \sum_{n=1}^N D\boldsymbol{\alpha}_n^m{}^T \left(-\boldsymbol{\gamma}^{(N-n+1)} + \frac{\partial \mathbf{g}(\boldsymbol{\alpha}_n^m, \mathbf{y}_{n+1}, \mathbf{p}_n)}{\partial \boldsymbol{\alpha}_n^m} \boldsymbol{\gamma}^{(N-n)} \right. \\
& \quad \left. + h \sum_{i=1}^s \frac{\partial \mathbf{F}(\mathbf{y}_n^i, t + c_i h)}{\partial \boldsymbol{\alpha}_n^m} \left[b_i \boldsymbol{\lambda}^{(N-n)} + \sum_{j=1}^s a_{ji} \boldsymbol{\Lambda}_j^{(N-n)} \right] + b_i h \sum_{l=1}^{Nobj} \frac{\partial r^l(\mathbf{y}_n^i, t + c_i h)}{\partial \boldsymbol{\alpha}_n^m} \boldsymbol{\theta}_l^{(N-n)T} \right) \\
& + D\mathbf{y}_N^T \left[-\boldsymbol{\lambda}^{(1)} + \frac{\partial \mathbf{g}(\boldsymbol{\alpha}_{N-1}^m, \mathbf{y}_N, \mathbf{p}_{N-1})}{\partial \mathbf{y}_N} \boldsymbol{\gamma}^{(1)} \right] + D\mathbf{p}_N^T \left[-\boldsymbol{\mu}^{(1)} \right] + \sum_{l=1}^{Nobj} Dq_N^l \left[\Phi^l - \boldsymbol{\theta}_l^{(1)} \right] + D\boldsymbol{\alpha}_N^m \left[-\boldsymbol{\gamma}^{(1)} \right] \\
& + D\mathbf{y}_0 \left[\boldsymbol{\lambda}^N + \sum_{i=1}^s \boldsymbol{\Lambda}_i^N \right] + D\mathbf{p}_0 \left[\boldsymbol{\mu}^N + \sum_{i=1}^s \boldsymbol{\Upsilon}_i^N \right] \\
& + \sum_{l=1}^{Nobj} Dq_0^l \left[\boldsymbol{\theta}_l^N + \sum_{i=1}^s \boldsymbol{\Theta}_{i,l}^N \right] \\
& + D\boldsymbol{\alpha}_0^m \left[\frac{\partial \mathbf{g}(\boldsymbol{\alpha}_0^m, \mathbf{y}_1, \mathbf{p}_0)}{\partial \boldsymbol{\alpha}_0^m} \boldsymbol{\gamma}^{(N)} + h \sum_{i=1}^s \frac{\partial \mathbf{F}(\mathbf{y}_0^i, t + c_i h)}{\partial \boldsymbol{\alpha}_0^m} \left(b_i \boldsymbol{\lambda}^{(N)} + \sum_{j=1}^s a_{ji} \boldsymbol{\Lambda}_j^{(N)} \right) \right. \\
& \quad \left. + b_i \sum_{l=1}^{Nobj} \frac{\partial r^l(\mathbf{y}_0^i, t + c_i h)}{\partial \boldsymbol{\alpha}_0^m} \boldsymbol{\theta}_l^{(N)T} \right].
\end{aligned} \tag{2.39}$$

Note the initial condition derivatives, e.g. $D\mathbf{y}_0$, are known. To annihilate the remaining implicit derivatives, e.g. $D\mathbf{y}_n$, we solve the following adjoint problem

$$\begin{aligned}
\lambda^{(N-n+1)} &= \lambda^{(N-n)} + \frac{\partial g(\alpha_{n-1}^m, \mathbf{y}_n, \mathbf{p}_{n-1})}{\partial \mathbf{y}_n} \gamma^{(N-n+1)} + \sum_{i=1}^s \Lambda_i^{(N-n)} \\
\Lambda_i^{(N-n)} &= h \frac{\partial \mathbf{F}(\mathbf{y}_n^i, t + c_i h)}{\partial \mathbf{y}_n^i}^T \left[\sum_{j=1}^s a_{ji} \Lambda_j^{(N-n)} + b_i \lambda^{(N-n)} \right] + b_i h \sum_{l=1}^{Nobj} \frac{\partial r^l(\mathbf{y}_n^i, t + c_i h)}{\partial \mathbf{y}_n^i} \boldsymbol{\theta}^{(N-n)} \quad i = 1 \dots s \\
\mu^{(N-n+1)} &= \mu^{(N-n)} + \sum_{i=1}^s \Upsilon_i^{(N-n)} \\
\Upsilon_i^{(N-n)} &= h \frac{\partial \mathbf{F}(\mathbf{y}_n^i, t + c_i h)}{\partial \mathbf{p}_n^i}^T \left[\sum_{j=1}^s a_{ji} \Lambda_j^{(N-n)} + b_i \lambda^{(N-n)} \right] + b_i h \sum_{l=1}^{Nobj} \frac{\partial r^l(\mathbf{y}_n^i, t + c_i h)}{\partial \mathbf{p}_n^i} \boldsymbol{\theta}^{(N-n)} \quad i = 1 \dots s \\
\gamma^{(N-n+1)} &= \frac{\partial g(\alpha_n^m, \mathbf{y}_{n+1}, \mathbf{p}_n)}{\partial \alpha_n^m} \gamma^{(N-n)} + h \sum_{i=1}^s \frac{\partial \mathbf{F}(\mathbf{y}_n^i, t + c_i h)}{\partial \alpha_n^m}^T \left[b_i \lambda^{(N-n)} + \sum_{j=1}^s a_{ji} \Lambda_j^{(N-n)} \right] \\
&\quad + b_i h \sum_{l=1}^{Nobj} \frac{\partial r^l(\mathbf{y}_n^i, t + c_i h)}{\partial \alpha_n^m} \boldsymbol{\theta}^{(N-n)}
\end{aligned}$$

For $l = 1 \dots Nobj$

$$\begin{aligned}
\theta_l^{(N-n+1)} &= \theta_l^{(N-n)} + \sum_{i=1}^s \Theta_{i,l}^{(N-n)} \\
\Theta_{i,l}^{(N-n)} &= 0 \quad i = 1 \dots s,
\end{aligned} \tag{2.40}$$

with the following “initial” conditions, for $t = t_N$

$$\begin{aligned}
\lambda^{(1)} &= \frac{\partial g(\alpha_{N-1}^m, \mathbf{y}_N, \mathbf{p}_{N-1})}{\partial \mathbf{y}_N} \gamma^{(1)} = \mathbf{0} \\
\mu^{(1)} &= \mathbf{0} \\
\gamma^{(1)} &= \mathbf{0} \\
\theta_l^{(1)} &= \Phi^l,
\end{aligned} \tag{2.41}$$

where $\lambda^1 = \mathbf{0}$ follows from $\gamma^1 = \mathbf{0}$. Noting that $\Theta_{i,l}^{(N-n)} = \mathbf{0}$ we obtain the result $\theta_l^{(N-n+1)} = \theta_l^{(N-n)}$ is a constant, which from Equation (2.41) we know to be Φ^l , i.e.

$$\theta_l^{(N-n+1)} = \Phi^l \text{ for all } n \text{ and } l, \tag{2.42}$$

where Φ^l is defined in Equation (2.35). Using this simplification and transforming $n \rightarrow N - n$ reduces the adjoint problem to

For $n = 1 \dots N - 1$

$$\begin{aligned}
\lambda^{(n+1)} &= \lambda^{(n)} + \frac{\partial g(\alpha_{N-n-1}^m, \mathbf{y}_{N-n}, \mathbf{p}_{N-n-1})}{\partial \mathbf{y}_{N-n}} \gamma^{(n+1)} + \sum_{i=1}^s \Lambda_i^{(n)} \\
\Lambda_i^{(n)} &= h \frac{\partial \mathbf{F}(\mathbf{y}_{N-n}^i, t + c_i h)^T}{\partial \mathbf{y}_{N-n}^i} \left[\sum_{j=1}^s a_{ji} \Lambda_j^{(n)} + b_i \lambda^{(n)} \right] + b_i h \sum_{l=1}^{Nobj} \frac{\partial r^l(\mathbf{y}_{N-n}^i, t + c_i h)}{\partial \mathbf{y}_{N-n}^i} \Phi^l \\
\mu^{(n+1)} &= \mu^{(n)} + \sum_{i=1}^s \Upsilon_i^{(n)} \\
\Upsilon_i^{(n)} &= h \frac{\partial \mathbf{F}(\mathbf{y}_{N-n}^i, t + c_i h)^T}{\partial \mathbf{p}_{N-n}^i} \left[\sum_{j=1}^s a_{ji} \Lambda_j^{(n)} + b_i \lambda^{(n)} \right] + b_i h \sum_{l=1}^{Nobj} \frac{\partial r^l(\mathbf{y}_{N-n}^i, t + c_i h)}{\partial \mathbf{p}_{N-n}^i} \Phi^l \\
\gamma^{(n+1)} &= \frac{\partial g(\alpha_{N-n}^m, \mathbf{y}_{N-n+1}, \mathbf{p}_{N-n})}{\partial \alpha_{N-n}^m} \gamma^{(n)} + h \sum_{i=1}^s \frac{\partial \mathbf{F}(\mathbf{y}_{N-n}^i, t + c_i h)^T}{\partial \alpha_{N-n}^m} \left[b_i \lambda^{(n)} + \sum_{j=1}^s a_{ji} \Lambda_j^{(n)} \right] \\
&\quad + b_i h \sum_{l=1}^{Nobj} \frac{\partial r^l(\mathbf{y}_{N-n}^i, t + c_i h)}{\partial \alpha_{N-n}^m} \Phi^l,
\end{aligned} \tag{2.43}$$

with the following initial conditions, for $n = 1$

$$\begin{aligned}
\lambda^{(1)} &= \mathbf{0} \\
\mu^{(1)} &= \mathbf{0} \\
\gamma^{(1)} &= \mathbf{0}.
\end{aligned} \tag{2.44}$$

We must solve the primal problem before solving the adjoint problem. Indeed the adjoint problem is solved backwards in time; e.g. it requires the primal response at time t_N to define its initial condition, cf. Equation (2.44). Once we have solved the adjoint variables, the sensitivity reduces to

$$\begin{aligned}
D\Psi &= D\mathbf{y}_0 \left(\lambda^N + \sum_{i=1}^s \Lambda_i^N \right) + D\mathbf{p}_0 \left(\mu^N + \sum_{i=1}^s \Upsilon_i^N \right) + D\alpha_0^m \left[\frac{\partial g(\alpha_0^m, \mathbf{y}_1, \mathbf{p}_0)}{\partial \alpha_0^m} \gamma^{(N)^T} \right. \\
&\quad \left. + h \sum_{i=1}^s \frac{\partial \mathbf{F}(\mathbf{y}_0^i, t + c_i h)^T}{\partial \alpha_0^m} \left[b_i \lambda^{(N)^T} + \sum_{j=1}^s a_{ji} \Lambda_j^{(N)^T} \right] + b_i \sum_{l=1}^{Nobj} \frac{\partial r^l(\mathbf{y}_0^i, t + c_i h)}{\partial \alpha_0^m} \Phi^l \right].
\end{aligned} \tag{2.45}$$

The adjoint variables that multiply $D\mathbf{y}_0$ and $D\alpha_0^m$ are the sensitivities with respect to the primal problem initial conditions, whereas the ones that multiply $D\mathbf{p}_0 = \mathbf{1}$ are the sensitivity with respect to the design variables. Thanks to having added the equation $\dot{\mathbf{p}} = \mathbf{0}$ to the governing equations, the adjoint variable μ collects the explicit derivatives terms and integrates them throughout the adjoint problem. Otherwise, we would have had a more complicated sensitivity expression.

2.6 Examples

2.6.1 Problem setup

As previously mentioned we are optimizing rectangular or hexagonal bead lattices, cf. Figure 2.1. The beads are made of brass and exhibit the material characteristics provided in Table 2.1. In each case, a striker bead, represented

as a green bead in Figure 2.1, impacts the initially quiescent lattices. This force is modeled via a one period sinusoidal signal, cf. Figure 2.8. Fixed wall boundaries constrain the lattices and the total analysis time is at least $400 \mu s$.

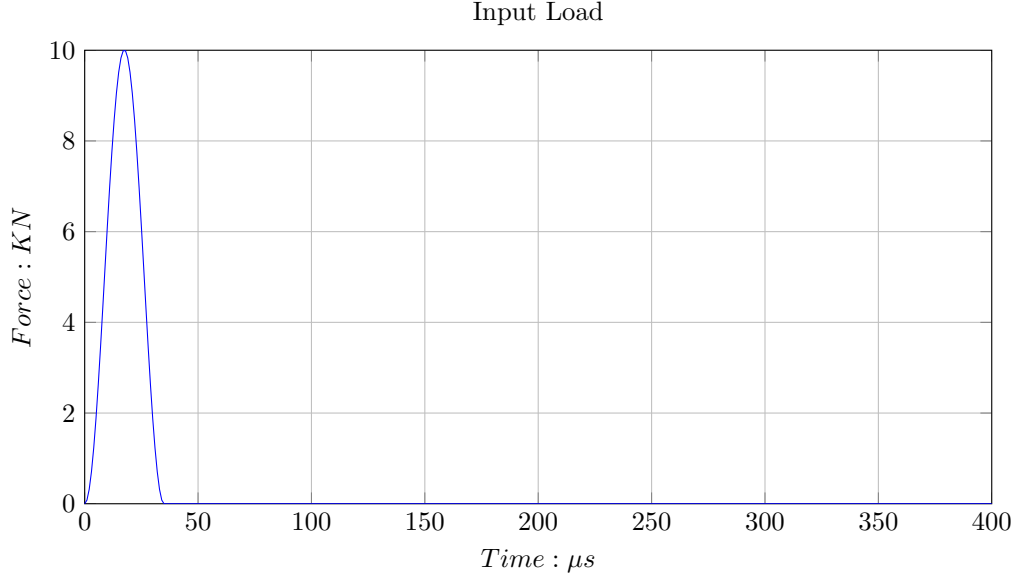


Figure 2.8: Input load.

Young Modulus E	115 GPa
Poisson coefficient ν	0.3
Density ρ	$8000 \text{ kg}/\text{m}^3$
Yield strength σ_y	550 MPa
Diameter	9.525 mm
Diameter (Intruders)	3.945 mm

Table 2.1: Bead characteristics.

2.6.2 Intruders

In this design, we optimize the 11x10 rectangular bead-packing illustrated in Figure 2.10 by selectively filling the interstitial voids with smaller intruder beads to achieve our design goals.

Where to place the intruders and how many we need constitutes a discrete optimization problem. The design variable needed for each potential interstitial site has the range $\{0, 1\}$, i.e. indicating either the presence (1) or lack (0) of an intruder. In order to make the problem tractable, we convexify the design space by replacing the discrete valued variables with volume fraction variables to indicate the “amount” of intruder at each site and use strategies to recover the originally sought discrete variable representation.

Using the interstitial volume fraction p_i , we assign interstitial bead i Young’s modulus and density as

$$\begin{aligned} E_i &= p_i E \\ \rho_i &= p_i \rho , \end{aligned} \tag{2.46}$$

where

$$\epsilon \leq p_i \leq 1 . \quad (2.47)$$

As seen above, for a volume fraction $p_i = 1$, the interstitial bead is assigned the nominal brass properties, i.e. Young's modulus E and density ρ . To avoid zero stiffness and mass values that would otherwise cause the analysis to diverge, we assign minimal values to the “void” interstitial beads, i.e. $p_i = \epsilon = 10^{-4}$. Representing the absence of intruders by small volume fraction beads is not a problem for our simulation. In Figure 2.9, we compare simulations for packings with no-intruders, i.e. $p_i = 0$ to those with small volume fraction, i.e. $p_i = \epsilon = 10^{-4}$. We plot the contact force at the rightmost bead-wall contact in the striker bead row. As seen in the plot, the responses are quite similar.

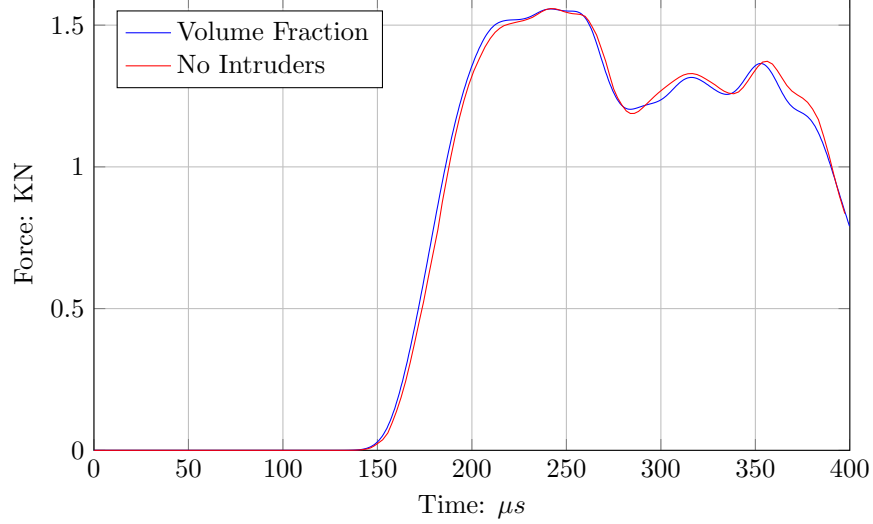


Figure 2.9: Contact force comparison for small volume fraction and no-intruders.

Using the same cost function defined in Section 2.5.1, we intend to maximize the reaction force at the contacts between the eight beads marked in orange and the wall (Figure 2.10), i.e.

$$\Psi_0(\mathbf{p}) = \left(\int_{\mathcal{I}} \left(\sum_{j=1}^8 (F_{jw}(t, \mathbf{p}))^S \right)^{T/S} dt \right)^{1/T} , \quad (2.48)$$

where F_{jw} is the reaction force at the orange bead j -wall contacts in Figure 2.10.

The single constraint we employ in our designs limits the total number of intruders in the packing, i.e.

$$\Psi_1(\mathbf{p}) = \sum_{i=1}^N p_i - (n + (N - n)\epsilon) , \quad (2.49)$$

where N is the total number of variables, i.e. interstitial bead sites, and n the maximum number of beads allowed in the packing. The second term on the right hand side accommodates the design variable lower bound ϵ .

If we solve the optimization problem as given, we do not obtain a discrete layout. Rather, we obtain values of p_i between 0 and 1. To recover the discrete design, i.e. one in which the design variables attain their originally sought

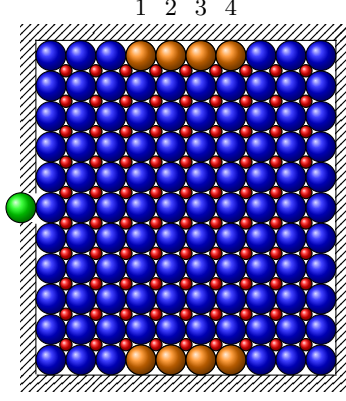


Figure 2.10: Target beads.

0 or 1 values, we impose the constraint

$$\sum_{i=1}^N (p_i - \epsilon)(1.0 - p_i) = 0, \quad (2.50)$$

which requires $p_i = \epsilon$ or $p_i = 1$ at all interstitial beads sites. Rather than imposing this constraint explicitly, we approximate it by using the penalty method. The optimization problems now reads

$$\begin{aligned} \min_{\mathbf{p} \in [\epsilon, 1]} \quad & \tilde{\Psi}(\mathbf{p}) = \Psi_0(\mathbf{p}) + w \sum_{i=1}^N (p_i - \epsilon)(1.0 - p_i) \\ \text{such that} \quad & \Psi_1(\mathbf{p}) = 0, \end{aligned} \quad (2.51)$$

where penalty coefficient w is sufficiently large to obtain the discrete layout.

2.6.2.1 Results

We present three examples to demonstrate the capabilities of the optimization. We use the IPOPT [21] optimization algorithm to solve Equation (2.51) and enforce geometric symmetry by initializing all intruder design variable values to $p_i = 0.5$.

We run the first optimization with a constraint of $n = 10$ intruders in the packing. Figures 2.11 and 2.12 show the optimal packing and the reaction forces corresponding to the upper orange beads in Figure 2.10. The force peak is two orders of magnitude smaller than the input load partially due to the dissipation in the system; however, it is much larger than a design with zero intruders for which these forces are zero.

We obtain inferior results if we design with $n = 30$ intruders. The optimal packing is plotted in Figure 2.13 and the reaction force is plotted in Figure 2.14. Note that the peak force is obtained in a different bead than that of the ten intruders case. However, this is not important since we are interested in the overall peak, regardless which bead it occurs. As seen here, more beads results in more dissipation.

Finally, we remove the number of beads constraint and observe that fewer intruders, i.e. two, yield an increased force, cf. Figures 2.16 and 2.15. Indeed, each intruder transmits its input force into two directions, with smaller magnitudes. Therefore, the more intruders result is less force to the desired regions. We obtain the same design for the elastic case, i.e. with no plasticity, but as expected, the force for this elastic design is greater than that for the plastic design, with its dissipative response, cf. Figure 2.17. Both in Figures 2.16 and 2.17, only the reaction force

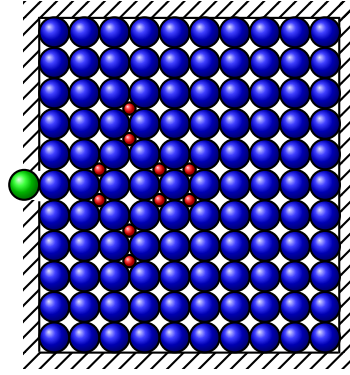


Figure 2.11: Optimal packing for the 10 intruders design.

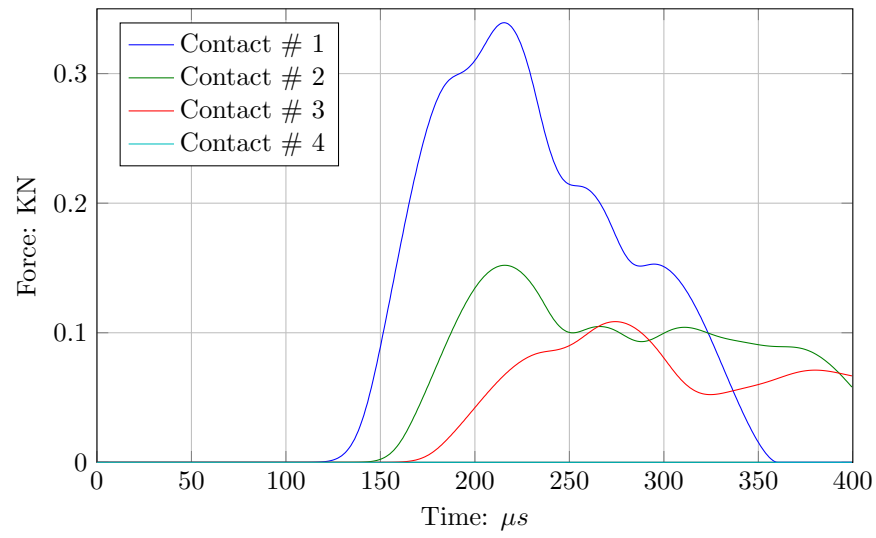


Figure 2.12: Reaction force at the target contacts for the 10 intruders design.

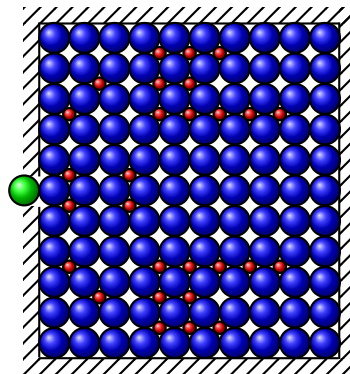


Figure 2.13: Optimal packing for the 30 intruder design.

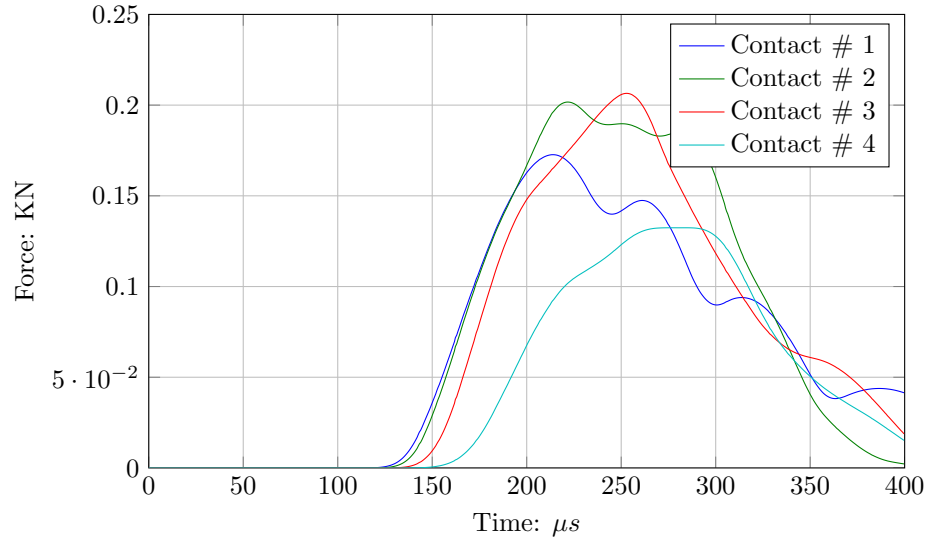


Figure 2.14: Reaction force at the target contact for the 30 intruders design.

at the bead-wall contact number 1 is shown. The reaction force is zero for the other contacts.

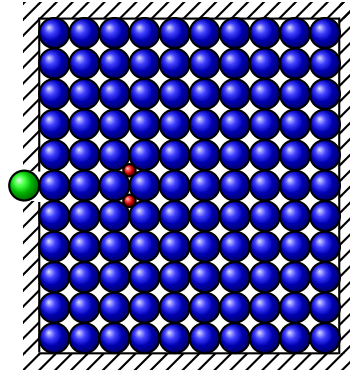


Figure 2.15: Optimal packing for the unconstrained design.

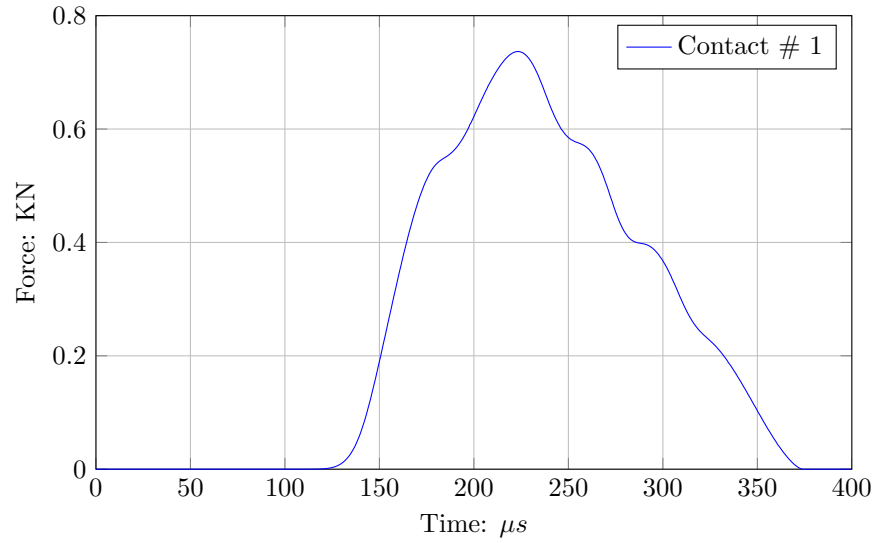


Figure 2.16: Reaction force at the target contacts for the unconstrained design.

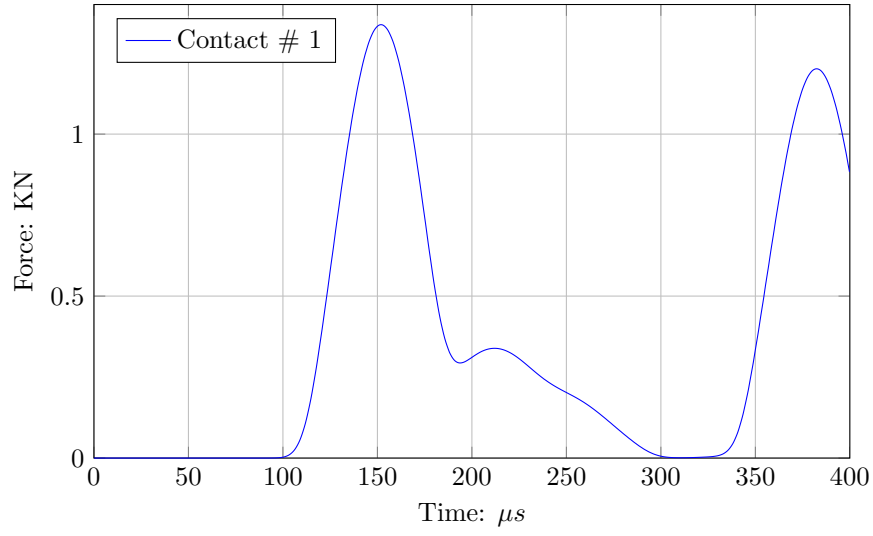


Figure 2.17: Reaction force at the target contacts for the elastic unconstrained design.

We obtain a more interesting result if instead of looking for the maximum force over all bead contacts, we look for a trade-off solution that optimizes all bead contact reaction forces equally. We group the bead–wall contacts in pairs. Each pair is represented with the same color in Figure 2.18. And we define the cost function

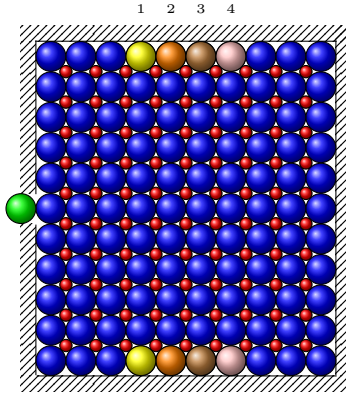


Figure 2.18: Optimal packing for the unconstrained design.

$$\Psi_0^l(\mathbf{p}) = \left(\int_{\mathcal{I}} \sum_{k \in l} (F_{kw}(t, \mathbf{p}))^T dt \right)^{1/T}, \quad (2.52)$$

with the index l iterating through the bead–wall contact pairs, and w being the fixed wall. We assign equal weights to each bead cost function to obtain the multi objective cost function we optimize

$$\Psi_0(\mathbf{p}) = \sum_{l=1}^{NTe} \Psi_0^l(\mathbf{p}). \quad (2.53)$$

No constraints are enforced in this design problem. As seen in Figures 2.19 and 2.20, the optimized design needs more intruders to obtain a more uniform peak reaction force.

We have shown that the intruders can effectively change the way the force propagates through the packing.

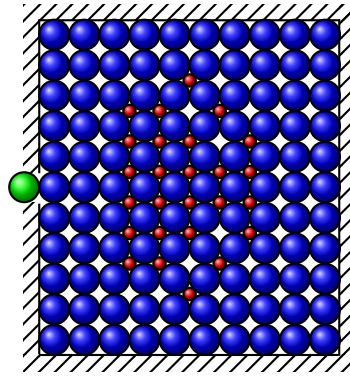


Figure 2.19: Multi-Objective result.

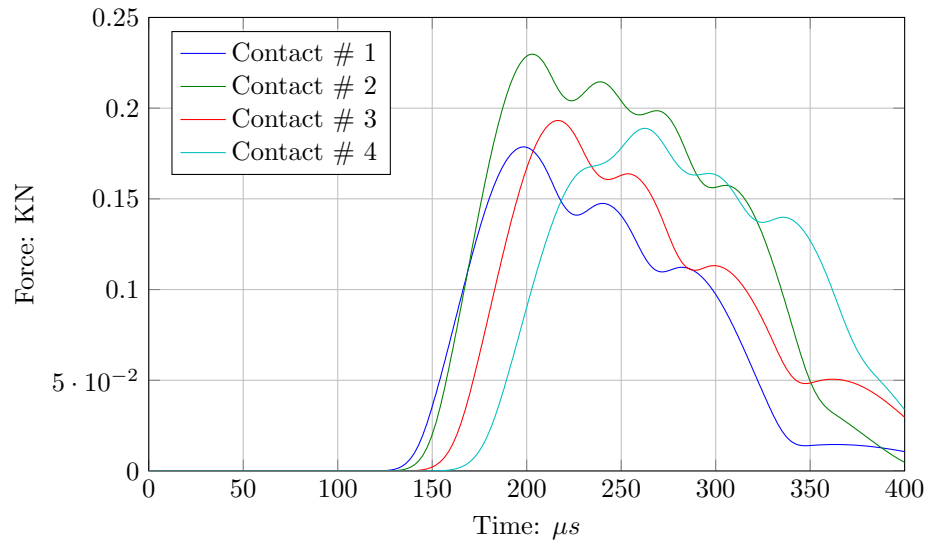


Figure 2.20: Reaction force at the target contacts for the multi objective design.

Unfortunately, the plasticity effects dissipate much of the energy and as a consequence, limits the force that can be focused on the target areas and although we can constrain the weight by limiting the total number of intruders, this is not necessary, as the optimal design actually requires fewer intruders.

2.6.3 Precompression

Our second design concerns the hexagonal packing of Figure 2.1, wherein the initial plastic deformation of the bead contacts is optimized, i.e. $\mathbf{p} = \boldsymbol{\alpha}_{ij}^m(0)$. Adding plastic compression to the bead contacts creates a problem; however, because precompressing the bead contacts, i.e. distorting the beads, creates gaps in the packing which complicates the analysis. We overcome this problem by assuming that the beads are in contact at the beginning of the simulation by shifting the contact law with the initial plastic compression, i.e.

$$\alpha_{ij} \rightarrow \alpha_{ij} + \alpha^R(\alpha_{ij}^m(0)) . \quad (2.54)$$

We limit the amount of initial plastic compression to avoid unrealistic situations by imposing the constraint

$$\alpha_{ij}^m(0) \in [0, 5] \text{ mm} \quad (2.55)$$

which is equivalent to $\alpha_{ij}^R(0) \in [0, 4.741] \text{ mm}$, cf. Equation (2.11).

We use the same cost function that we had for the previous example, but we change the target areas to maximize the reaction force at the red contact in Figure 2.21. At the same time, we want to minimize the reaction force at the blue contact. Therefore, we use the multiobjective function, cf. Equation (2.34), with

$$\Psi^l(\boldsymbol{\alpha}^m(0)) = \left(\int_{\mathcal{I}} (F_{lw}(t, \boldsymbol{\alpha}^m(0)))^T dt \right)^{1/T} , \quad (2.56)$$

where β_l equals 1 for the blue bead contact l we want to minimize and -1 for the red bead contact l we want to maximize. Note that there is no need for the penalty term in the cost function because this is not a discrete problem.

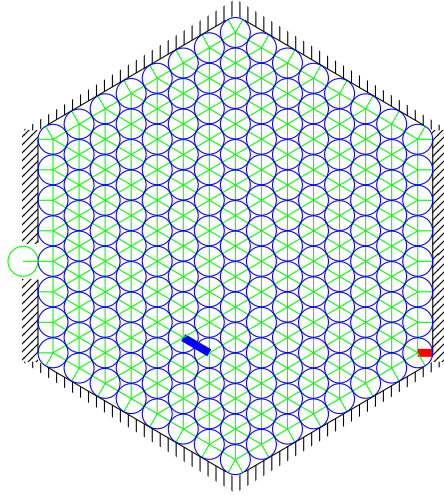


Figure 2.21: Target areas.

2.6.3.1 Results

In this problem, we use an input load with the same sinusoidal shape and period as in the previous example, but an increased 22 KN amplitude. The optimization problem is solved with the MMA [16].

Figure 2.22 depicts the optimized design wherein the rectangle color and width indicates the values of the design variable $\alpha_{ij}^m(0)$. The target contacts are highlighted with a blue ellipse for the minimization and a red ellipse for the maximization.

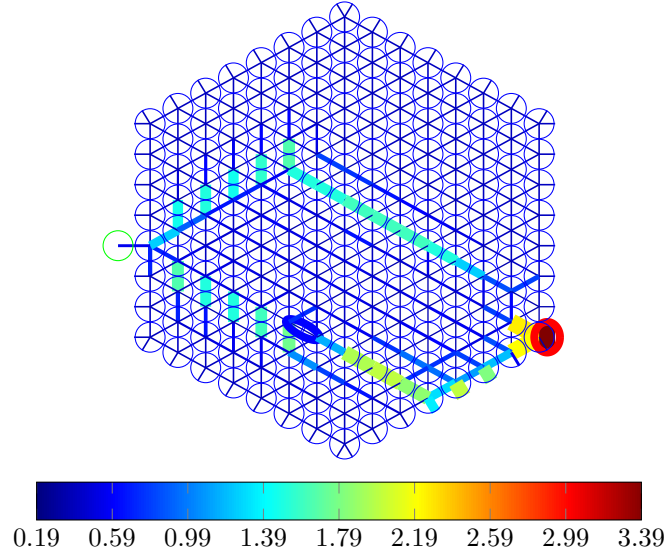


Figure 2.22: Optimized precompression.

The force at the target contacts are plotted in Figure 2.23. The blue and red colors correspond to the contact forces we want to minimize and maximize. Dashed lines correspond to the multiobjective optimization, whereas dotted lines correspond to an optimization in which we only maximize the force at the red contact. The continuous lines correspond to a non-optimal bead packing, where all of the bead initial plastic compression equal 0.3. In comparing the dashed and dotted lines, we see that we are able to achieve a large force in the red contact even while minimizing the force in the blue contact. Note also that the peak force is the same order as the input load since little dissipation is induced in the system because the elastic regime is increased by means of adding initial plastic compression.

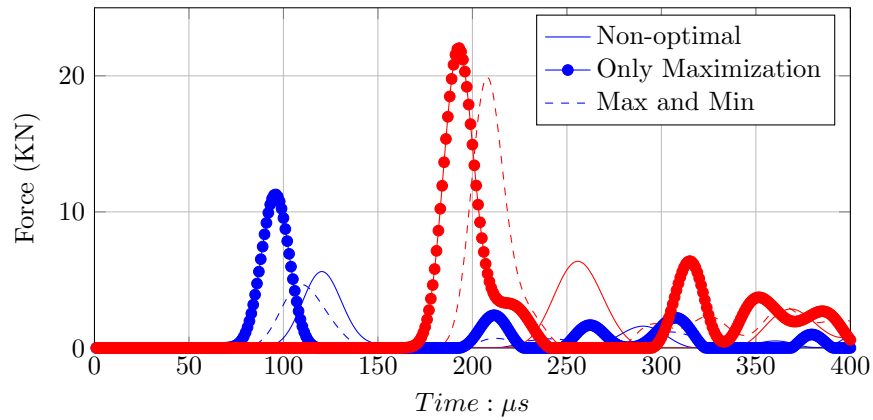


Figure 2.23: Reaction forces at target contacts .

Chapter 3

Conclusions

In this thesis, we have presented an optimization scheme for the tailored force propagation through a two-dimensional packing of spherical beads. We have used a DEM with an empirical contact law that describes the history dependent contact interaction between the beads. The problem analysis does not require a nested loop because the state variables are obtained explicitly.

Two designs were presented. First, a rectangular packing was optimized by introducing interstitial beads, i.e. intruders. This discrete problem was convexified to make it amenable to a nonlinear programming solver. To these ends, the intruders indicator functions were replaced by volume fraction functions and a penalization technique was employed to recover the discrete design. Plastic deformation significantly dissipates energy in the system, limiting the amount of force that we can redirect to our target regions. Thusly, introducing intruders creates even more dissipation, and hence the optimized design uses relatively few intruders. In the second design, we optimize initial plastic compression between each bead contact. Increasing the initial plastic compression also increases the elastic regime in the bead contacts and thus less dissipation is created. There is one clear pitfall for this approach, however as the initial plastic compression creates gaps in the packing. To resolve this otherwise difficult analysis problem, we add an artificial shift in the contact law to ensure an initially tightly packed array. This feature cannot be translated to experiments.

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