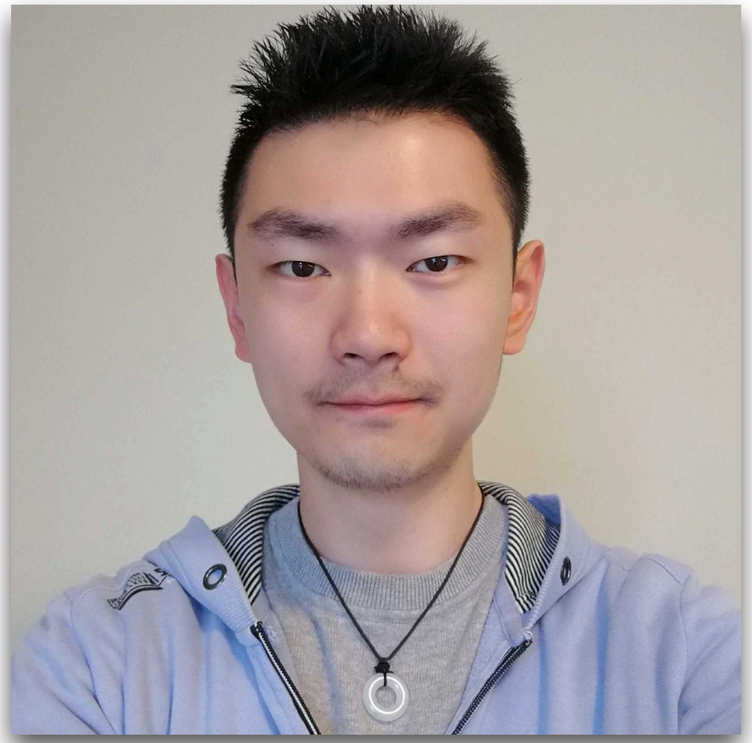
Introduction to Optimization Time Integration for Solids and Fluids

SGP 2024 Graduate School

Speakers: Minchen Li (CMU), Jiayi (Eris) Zhang (Stanford)

Speakers



Minchen Li
Assistant Professor
Carnegie Mellon University

Jiayi (Eris) Zhang
PhD student
Stanford University

Topics Today

Part I: Fundamentals and The Big Picture (Minchen)

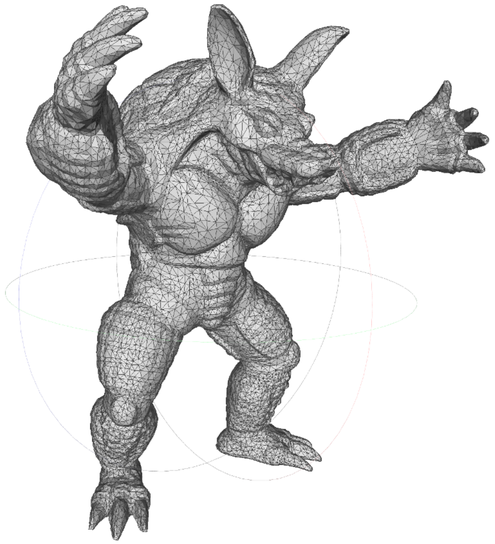
- Distortion Minimization
- Elastodynamics Simulation via Optimization Time Integration
- Case Study: Mass-Spring System
- More Topics on Optimization Time Integration

Part II: Advanced Topics (Eris)

- Constrained System
- Reduced-Order System
- Multilevel System
- Adaptive Simulation

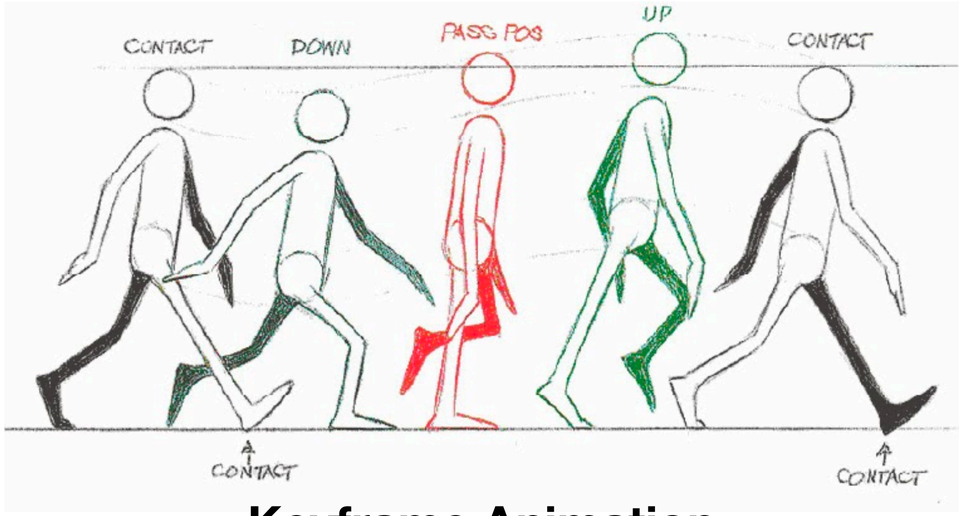
Computer Graphics:

Generating Realistic Visual Effects via Computing

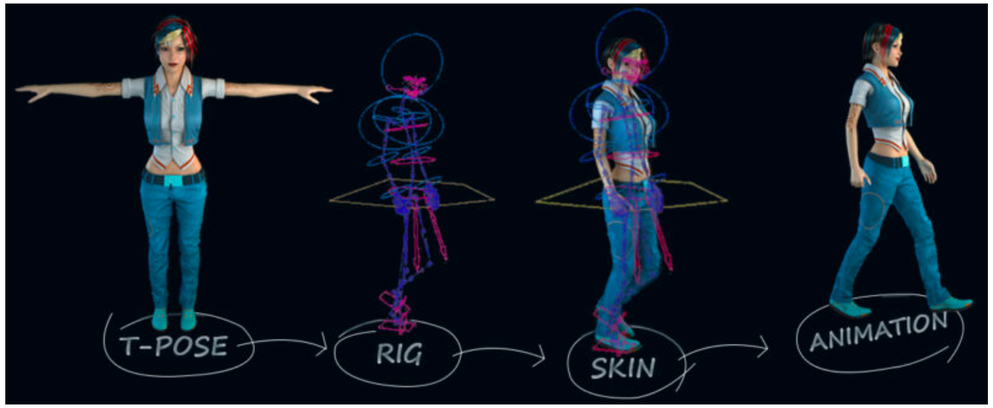


Geometry → Appearance → Animation

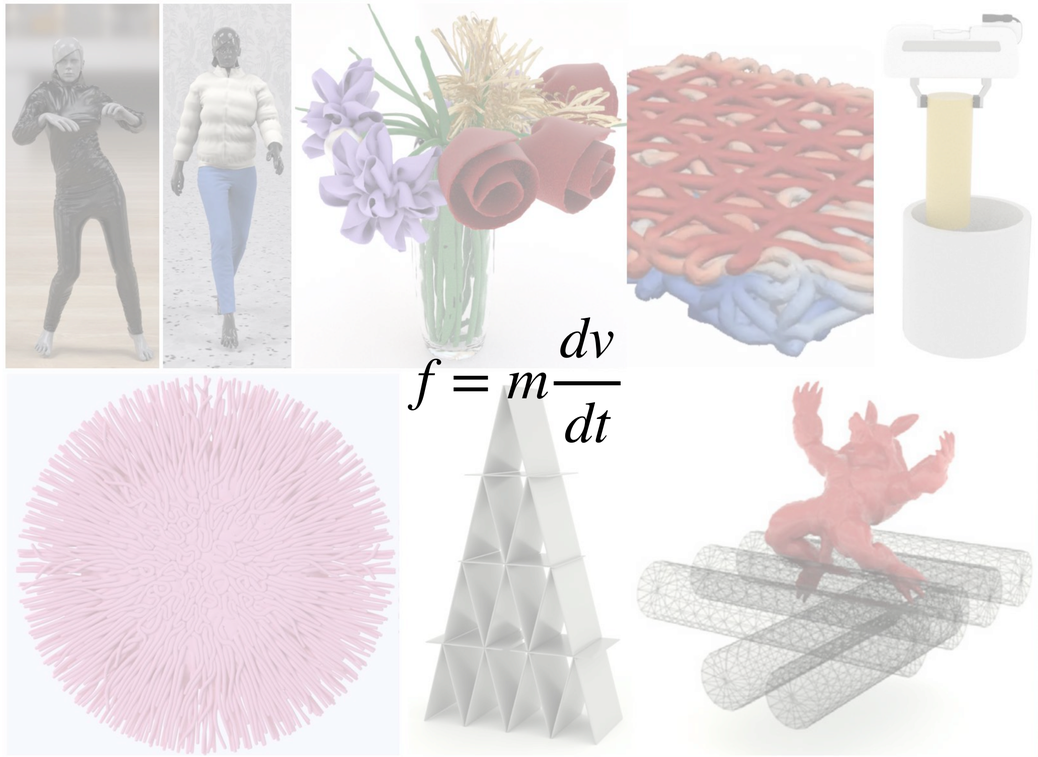
Animation



Keyframe Animation

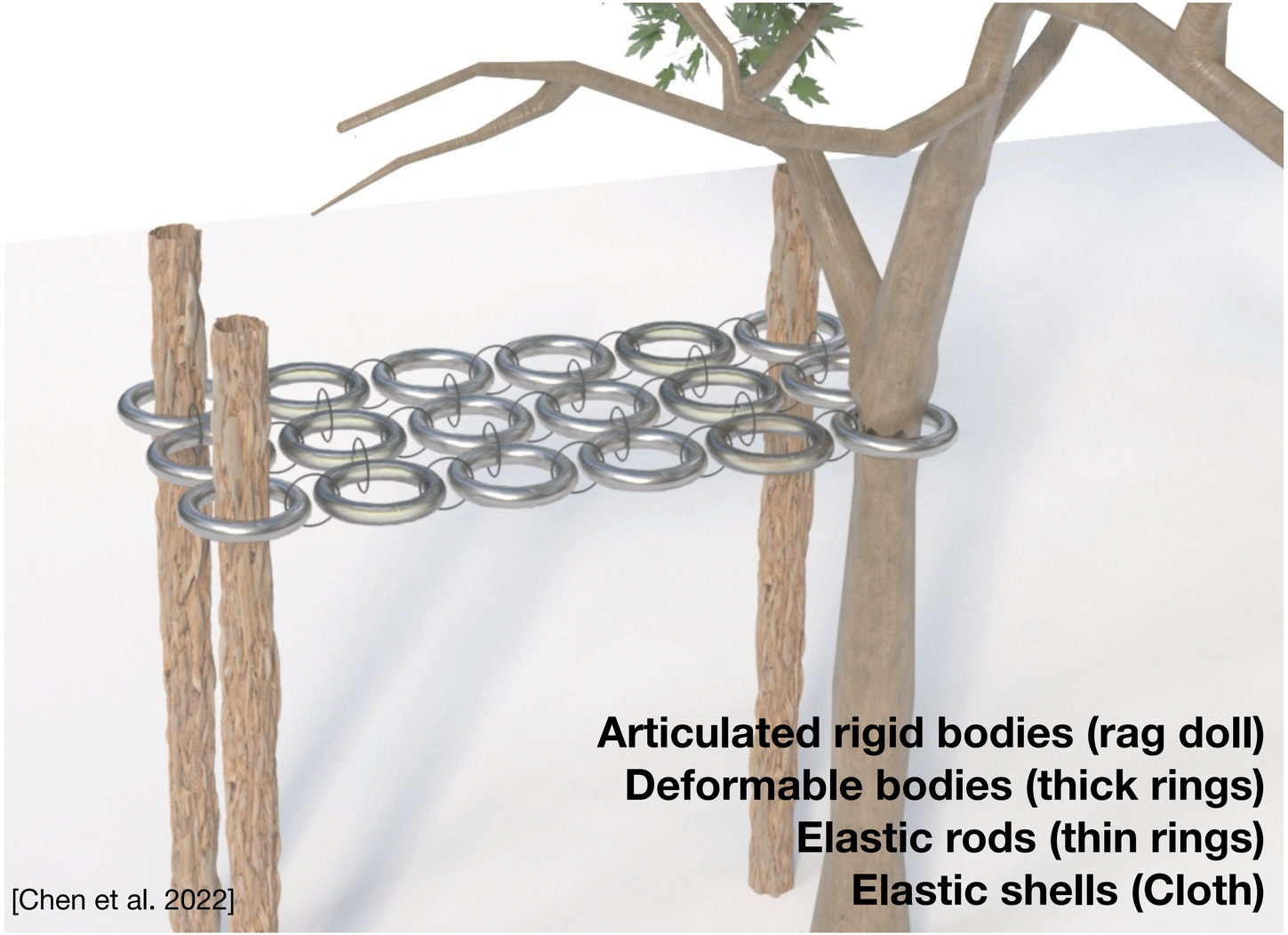


Skinning Animation



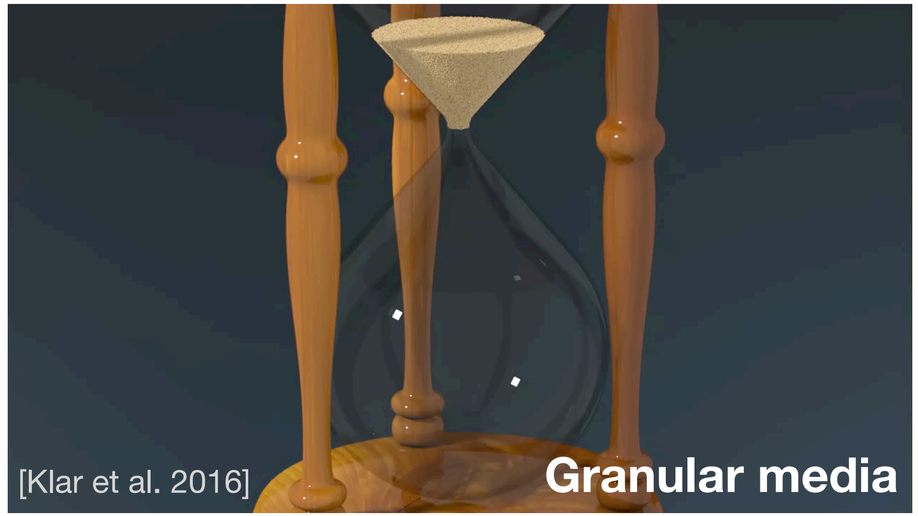
Physics-based Animation

Physics-based Animation



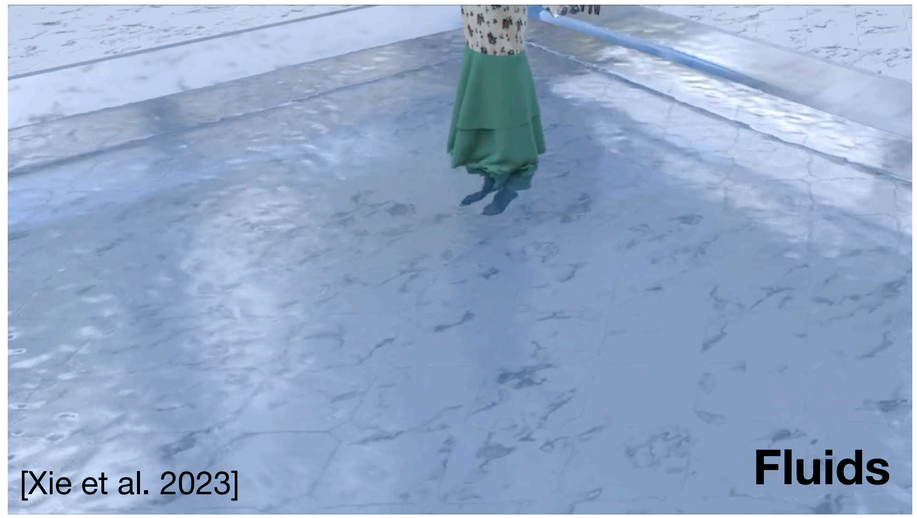
Articulated rigid bodies (rag doll)
Deformable bodies (thick rings)
Elastic rods (thin rings)
Elastic shells (Cloth)

[Chen et al. 2022]



[Klar et al. 2016]

Granular media



[Xie et al. 2023]

Fluids

Optimization Time Integration

A Reliable Simulation Approach based on Numerical Optimization

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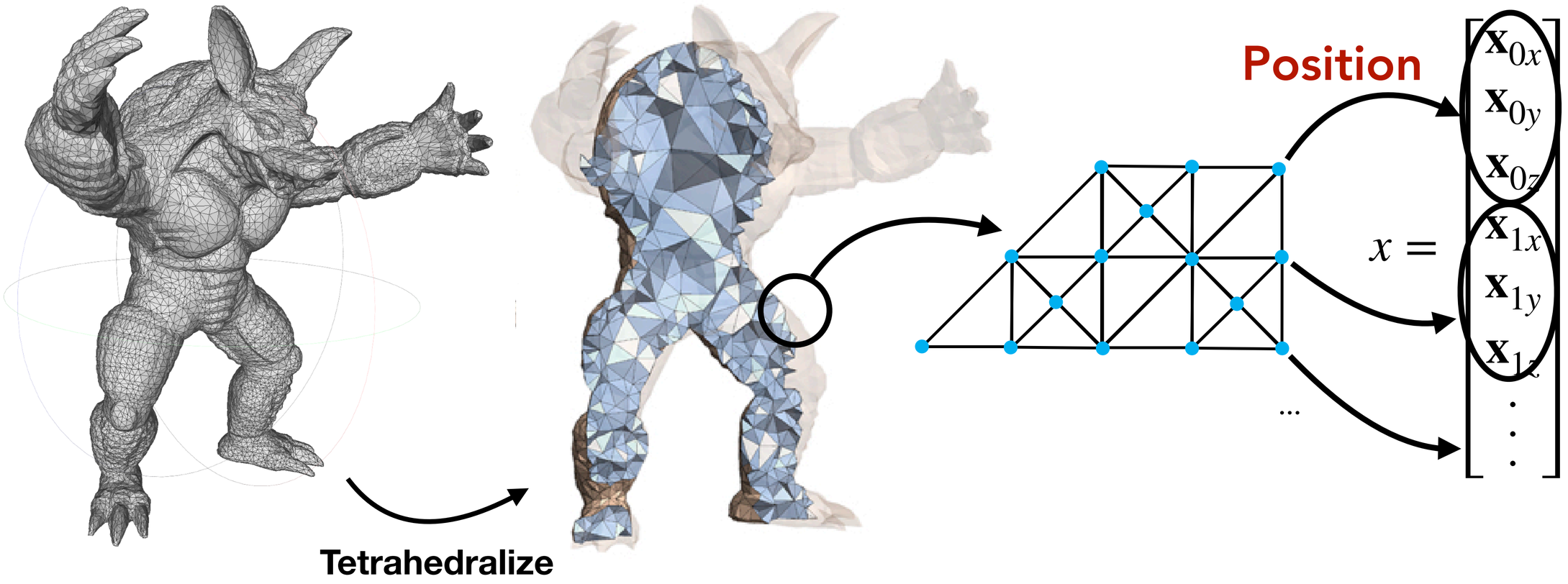
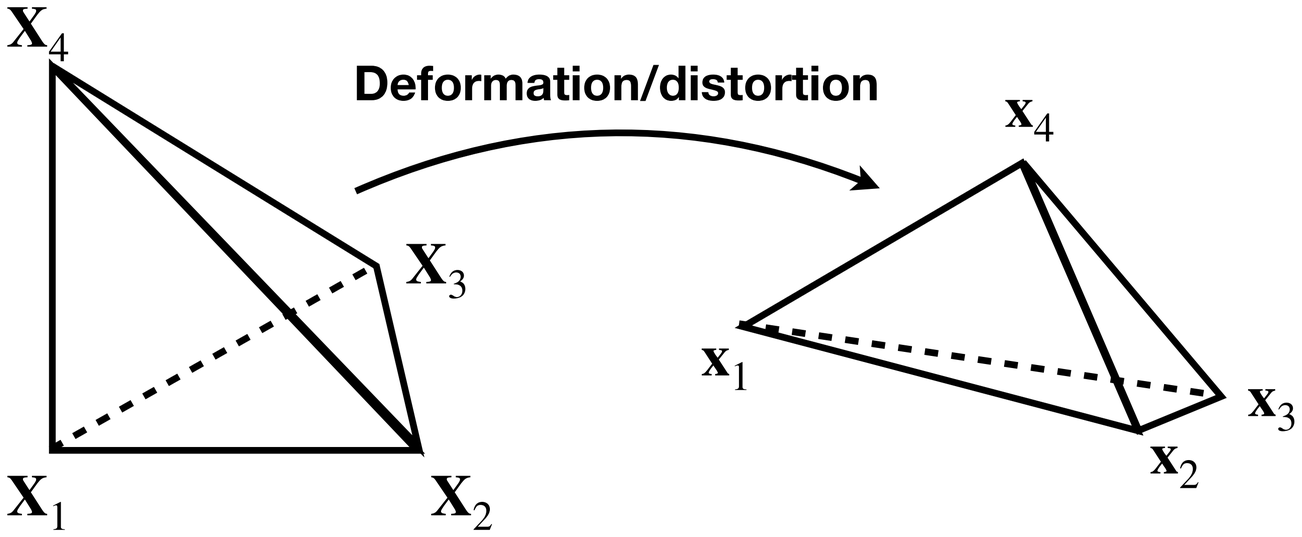
Spatial Discretization



Measure Distortion Locally



Distortion energy, e.g. $\Psi(\mathbf{F}) = \mu\|\mathbf{F} - \mathbf{R}\|_F^2$

- $\mathbf{R} = \mathbf{U}\mathbf{V}^T$ **is the closest rotation to** $\mathbf{F}$
- $\mathbf{F} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$ **is the SVD**

— As-Rigid-As-Possible (ARAP) [Igarashi et al. 2005]

Assume uniform deformation

Distortion over the whole mesh: $\sum_e V_e \Psi(\mathbf{F}_e)$

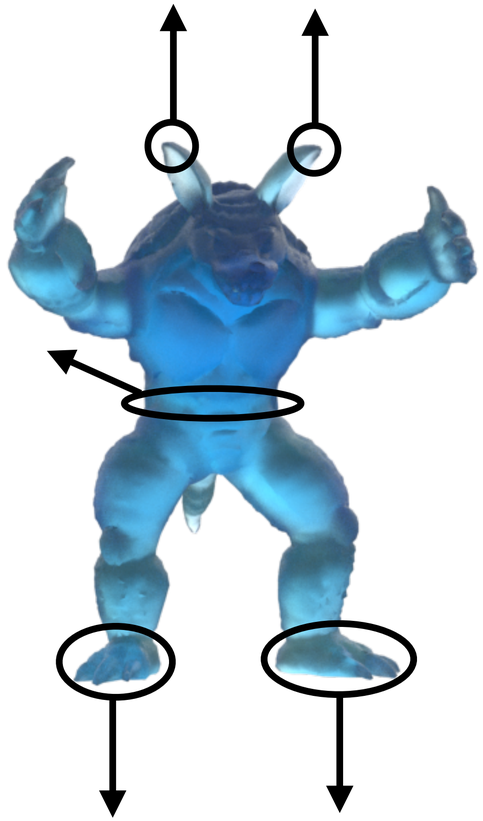
Affine transformation:

$$\mathbf{F} = [\mathbf{x}_2 - \mathbf{x}_1, \mathbf{x}_3 - \mathbf{x}_1, \mathbf{x}_4 - \mathbf{x}_1][\mathbf{X}_2 - \mathbf{X}_1, \mathbf{X}_3 - \mathbf{X}_1, \mathbf{X}_4 - \mathbf{X}_1]^{-1}$$

$$\forall \mathbf{X},\ \mathbf{x}(\mathbf{X}) = \mathbf{F}(\mathbf{X} - \mathbf{X}_1) + \mathbf{x}_1$$

(V_e **is the volume of tetrahedron element e)**

Mesh Deformation via Distortion Minimization



- S selects the anchors
- $\hat{x}$ contains the target position

$$\min_x \sum_e V_e \Psi(\mathbf{F}_e) \quad s.t. \quad Sx = \hat{x}$$

We could move the anchors to the target position, and only optimize for the free vertices

$$\min_x \sum_e V_e \Psi(\mathbf{F}_e)$$

Newton's Method for Distortion Minimization

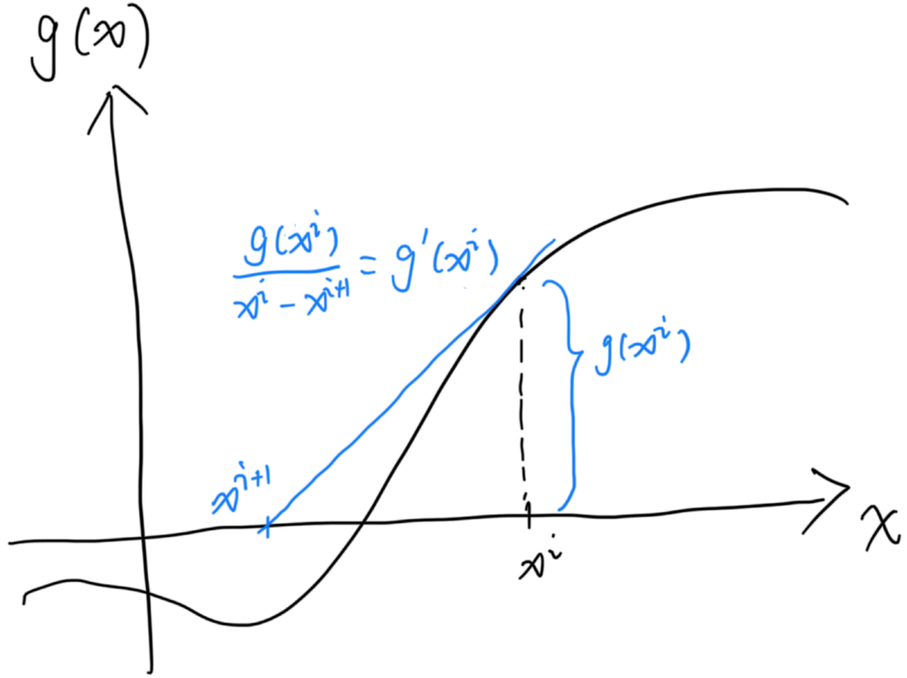
Formulation

Let $g(x) = \nabla E(x)$, $E(x) = \sum_e V_e \Psi(\mathbf{F}_e)$

We want to solve $g(x) = 0$

Newton's method in 1D:

- **Start from initial guess** x^0
- **For each iteration (until convergence)**
  - $x^{i+1} \leftarrow x^i - g(x^i)/g'(x^i)$



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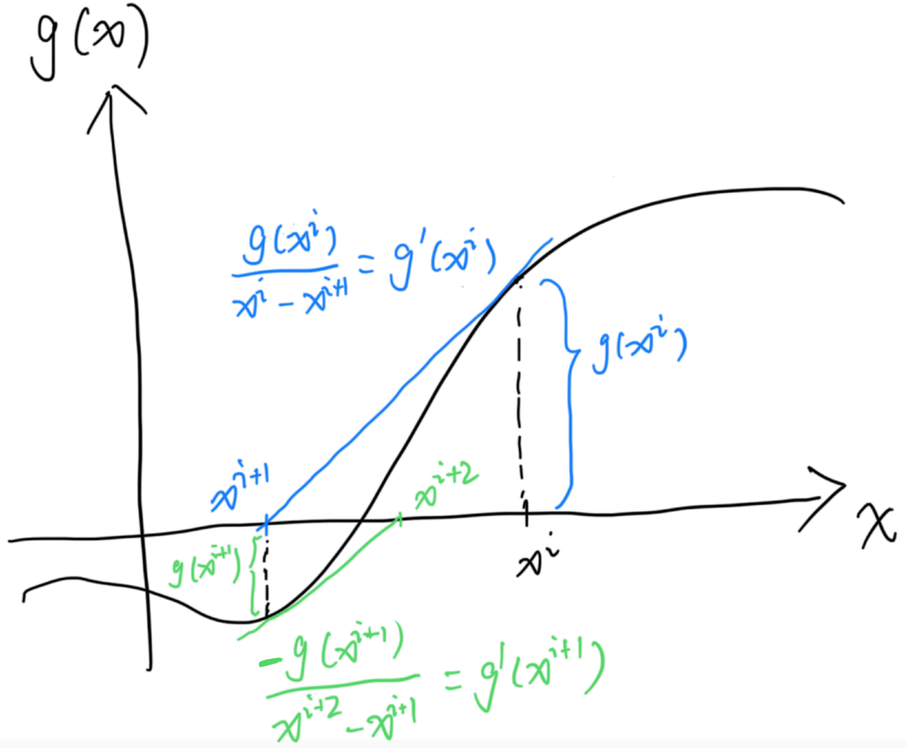
In higher dimensions:

$$x^{i+1} \leftarrow x^i - (\nabla g(x^i))^{-1} g(x^i)$$



Derivation:

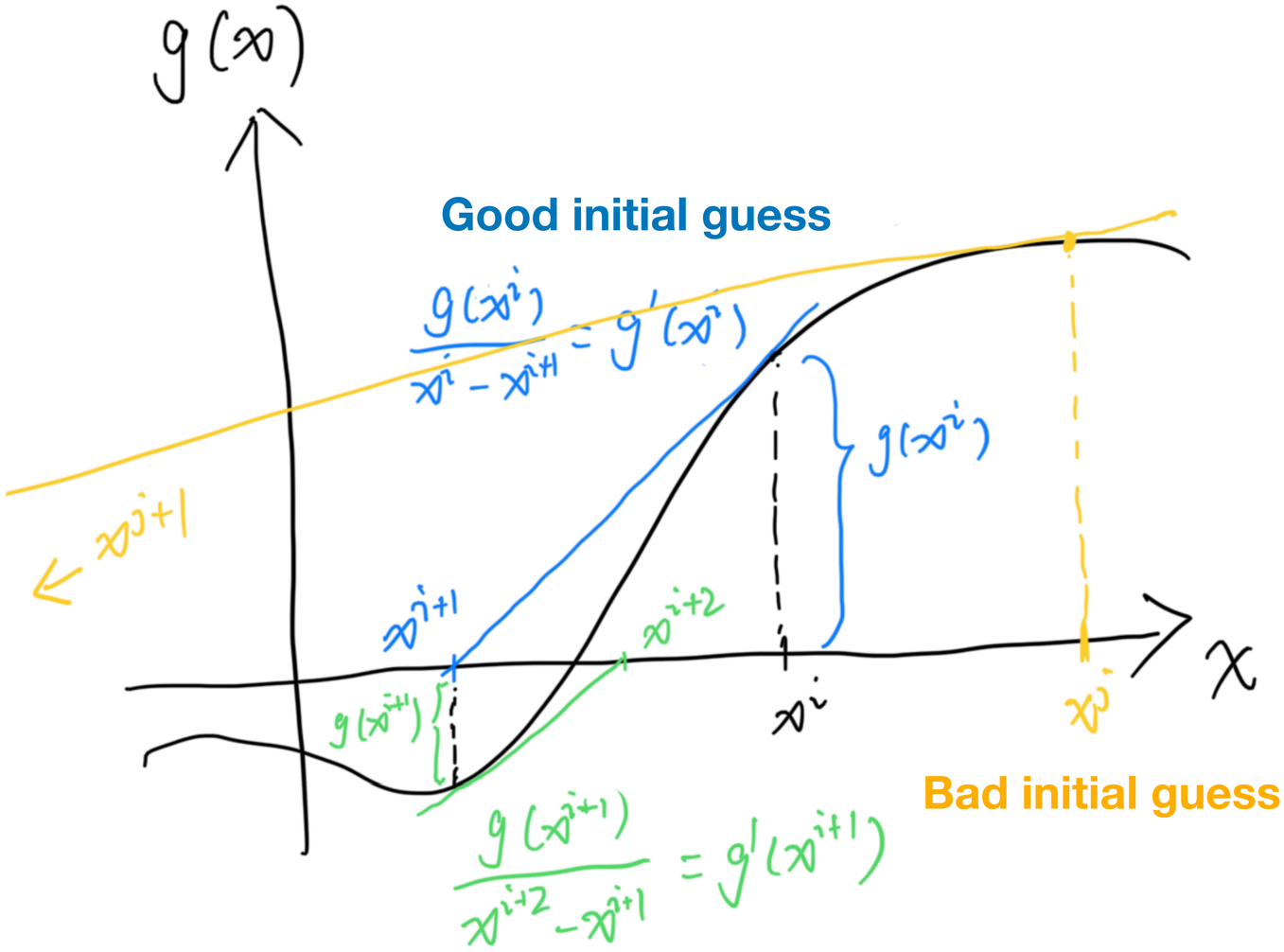
Linearly approximate $g(x) = 0$ **at** x^i **:**

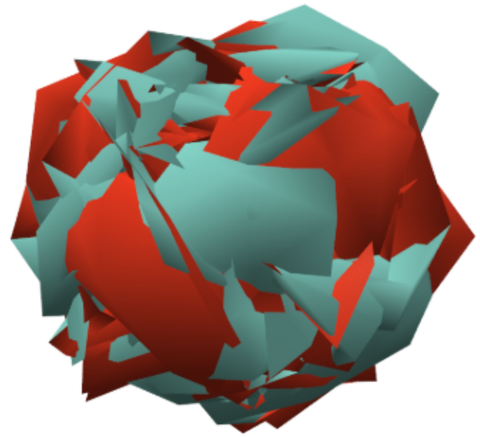
$$g(x) = g(x^i) + \nabla g(x^i)(x - x^i)$$

$$g(x^{i+1}) \approx g(x^i) + \nabla g(x^i)(x^{i+1} - x^i) = 0$$

Convergence Issue of Newton's Method

Over-shooting





Bad initial guess → Numerical explosion!

Robust Distortion Minimization

Newton's Method with Line Search

We want to solve $\nabla E(x) = 0$

Newton's method:

- **Start from initial guess** x^0
- **For each iteration (until convergence)**
  - $x^{i+1} \leftarrow x^i - (\nabla^2 E(x^i))^{-1} \nabla E(x^i)$

Let $p = -(\nabla^2 E(x^i))^{-1} \nabla E(x^i)$

Line Search along direction p**:**

$$\min_{\alpha} E(x^i + \alpha p)$$

$$x^{i+1} \leftarrow x^i + \alpha p$$

Theory:

If p **is a descent direction at** $x = x^i$ **(like** $-\nabla E(x^i)$**),**

$$\exists \alpha > 0,\ s.t.\ E(x^i + \alpha p) < E(x^i)$$

— need $\nabla^2 E(x)$ **to be symmetric positive-definite**

Idea:

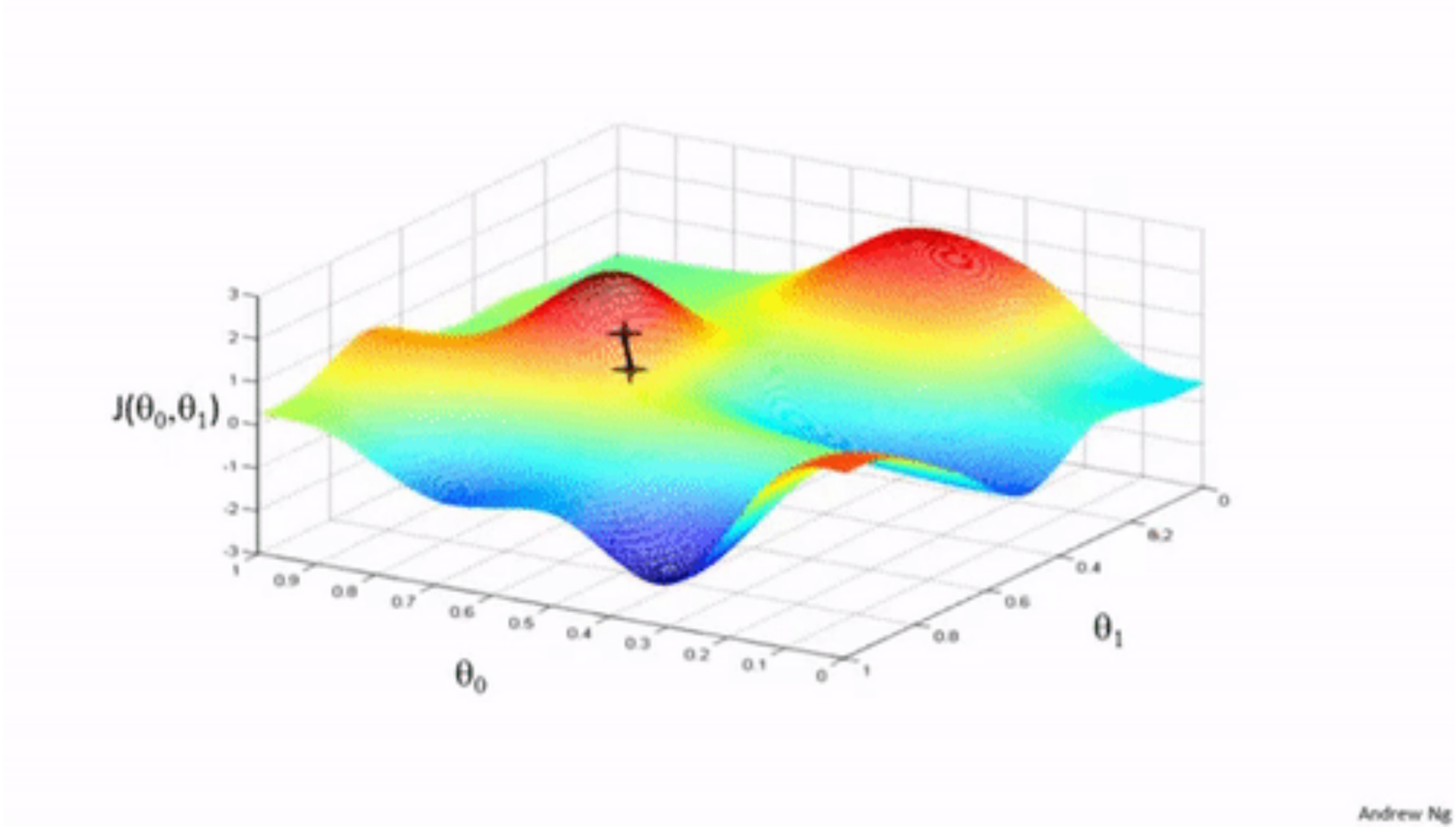
We can project $\nabla^2 E(x)$ **to a nearby SPD matrix for computing** p

Then we can ensure $E(x^{i+1}) < E(x^i)\ \forall i$

— no explosion!

Robust Distortion Minimization

Newton's Method with Line Search, 2D Illustration



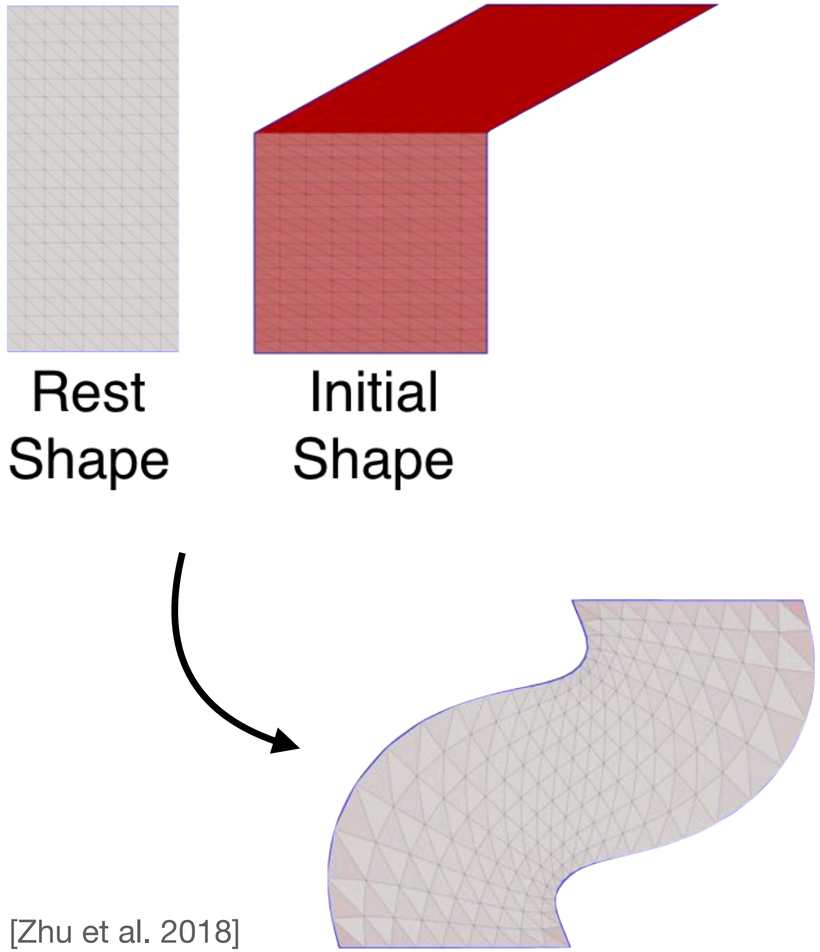
Andrew Ng

Robust Distortion Minimization

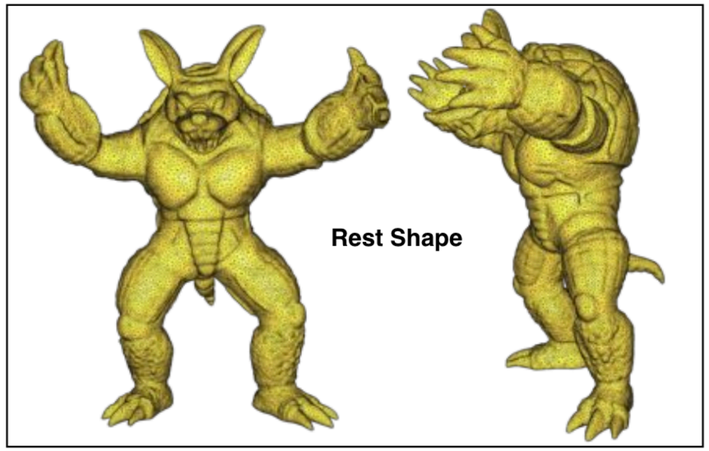
Pseudo-code

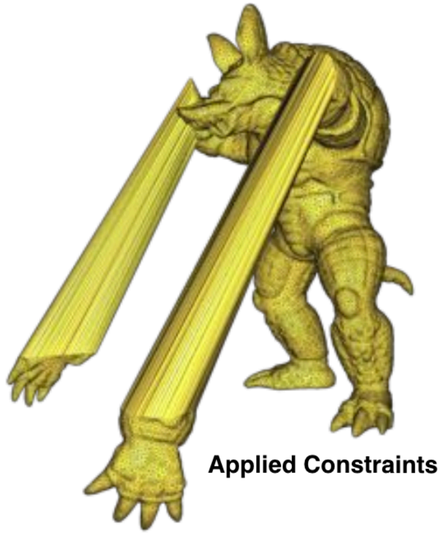
- $x \leftarrow$ initial guess
- Do
  - $P \leftarrow$ projectSPD($\nabla^2 E(x)$)
  - $p \leftarrow P^{-1} \nabla E(x)$
  - $\alpha \leftarrow 1$
  - While $E(x + \alpha p) > E(x)$
    - $\alpha \leftarrow \alpha/2$
  - $x \leftarrow x + \alpha p$
- While $\|p\| < \epsilon$

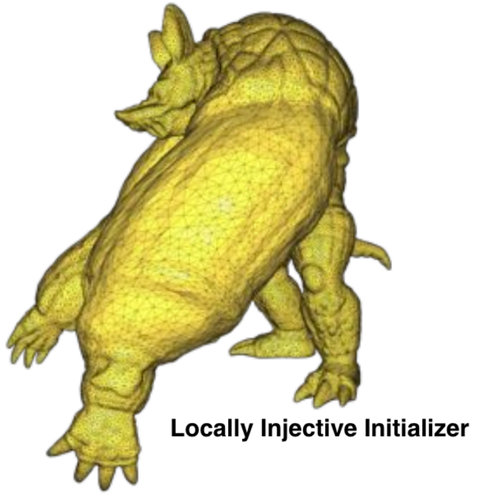
Distortion Minimization Examples



[Zhu et al. 2018]







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Adding Dynamics

Distortion minimization: $\min_x E(x)$ $\quad E(x) = \sum_e V_e \Psi(\mathbf{F}_e)$

Elastodynamic simulation: $\min_x E(x)$ $\quad E(x) = \sum_e V_e \Psi(\mathbf{F}_e) + \boxed{\frac{1}{2\Delta t^2} \|x - (x^n + \Delta t v^n)\|_M^2}$

Inertia term

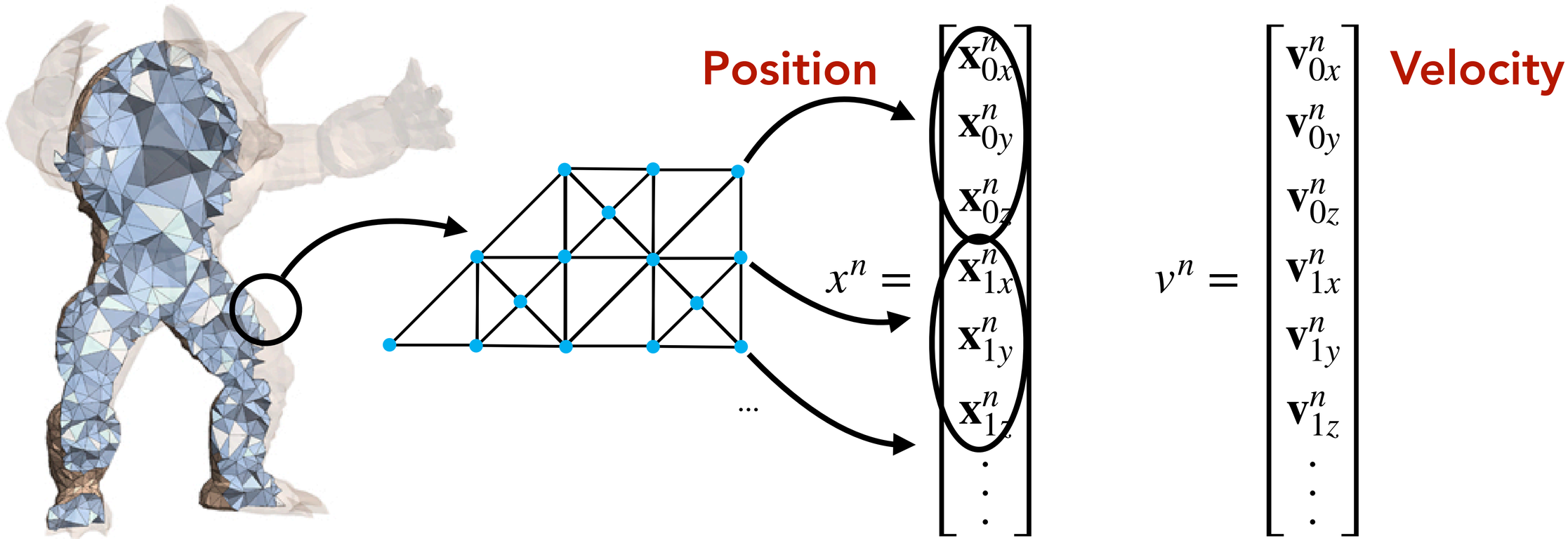
Δt: time step size

x^n: vertex positions at previous time step

v^n: velocity at previous time step

M: mass matrix

Spatial Discretization with Dynamics



Governing Equation (Conservation of Momentum)

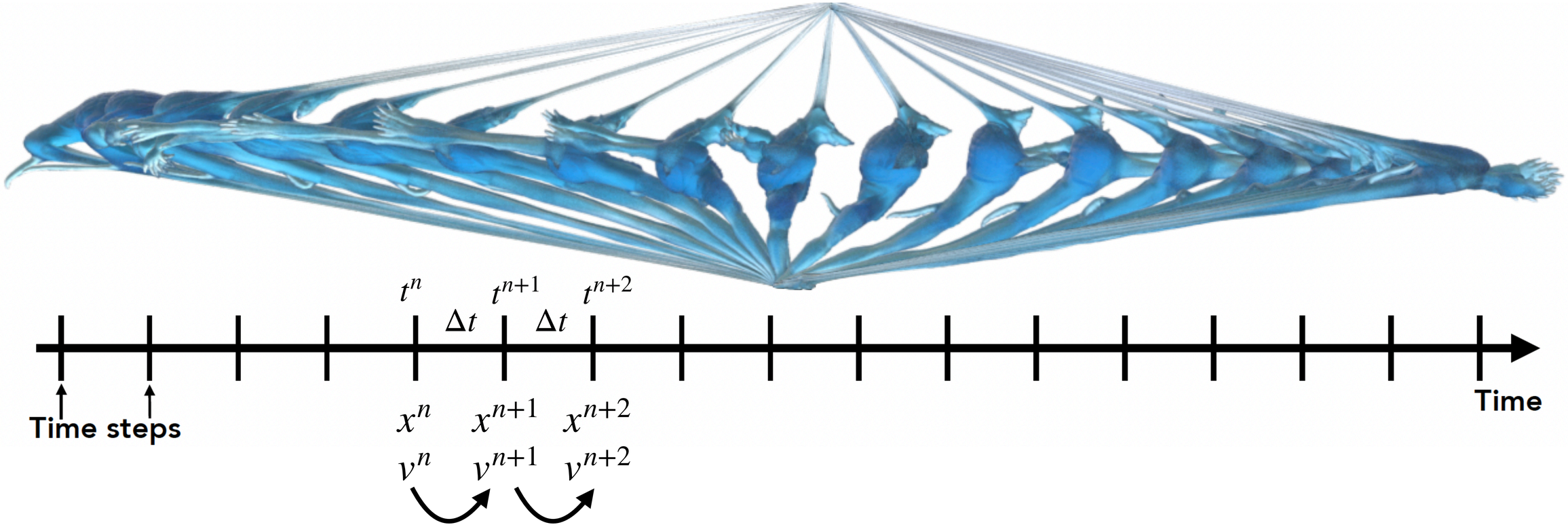
- The spatially discrete, temporally continuous form

$$\frac{dx}{dt} = v,$$
$$M\frac{dv}{dt} = f.$$

- Mass matrix (for now)

$$M = \begin{pmatrix} m_1 & & & \\ & m_1 & & \\ & & m_2 & \\ & & & m_2 \end{pmatrix}$$

Time Stepping (Time Integration)



Governing Equation (Temporally Discrete)

Forward Difference, Forward Euler

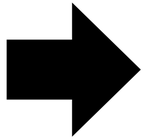
- Forward difference approximation on velocity and acceleration

$$\left(\frac{\mathbf{d}x}{\mathbf{d}t}\right)^n \approx \frac{x^{n+1}-x^n}{\Delta t} \qquad \left(\frac{\mathbf{d}v}{\mathbf{d}t}\right)^n \approx \frac{v^{n+1}-v^n}{\Delta t}$$

$$\left(f(t^n+\Delta t) = f(t^n) + \frac{\mathbf{d}f}{\mathbf{d}t}(t^n)\Delta t + O(\Delta t^2)\right)$$

Taylor's expansion

$$\frac{x^{n+1}-x^n}{\Delta t} = v^n,$$
$$M\frac{v^{n+1}-v^n}{\Delta t} = f^n.$$



$$x^{n+1} = x^n + \Delta t v^n,$$
$$v^{n+1} = v^n + \Delta t M^{-1} f^n$$

Newton's 2nd Law (Temporally Discrete)

Forward and Backward Difference, Symplectic Euler

- Forward difference on acceleration, backward difference on velocity

$$x^{n+1} = x^n + \Delta t v^{n+1}$$

$$v^{n+1} = v^n + \Delta t M^{-1} f^n$$

Newton's 2nd Law (Temporally Discrete)

Backward Difference, Backward Euler (or Implicit Euler)

- Backward difference approximation on velocity and acceleration

$$x^{n+1} = x^n + \Delta t v^{n+1},$$
$$v^{n+1} = v^n + \Delta t M^{-1} f^{n+1}$$

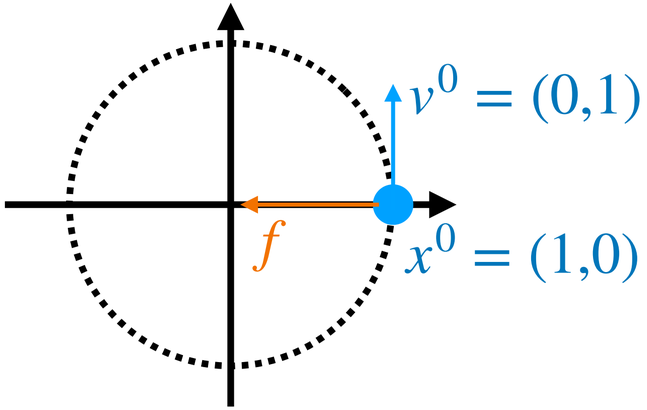
$$f^{n+1} = f(x^{n+1})$$

Needs to solve a system of equations:

$$M(x^{n+1} - (x^n + \Delta t v^n)) - \Delta t^2 f(x^{n+1}) = 0.$$

Stability of Forward, Symplectic, and Backward Euler

Example on a uniform circular motion



Problem Setup

$$x^{n+1} = x^n + \Delta t v^n,$$
$$v^{n+1} = v^n + \Delta t M^{-1} f^n$$

$$x^{n+1} = x^n + \Delta t v^{n+1}$$
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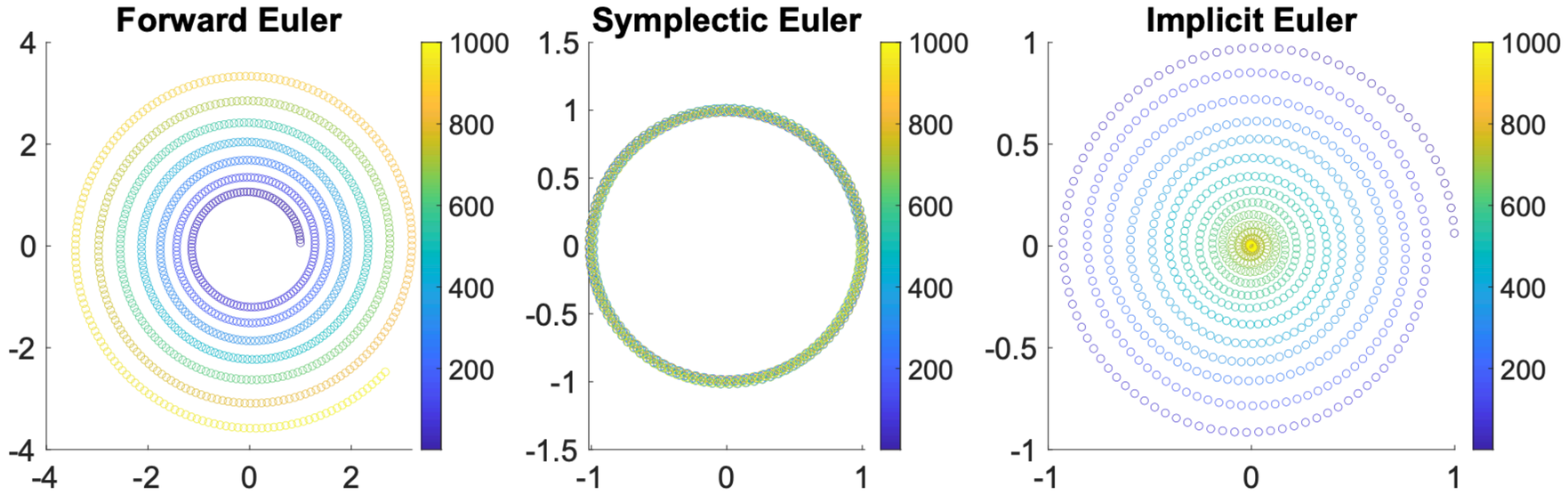


Newton's Method for Backward Euler

Formulation

Let $g(x) = M(x - (x^n + \Delta t v^n)) - \Delta t^2 f(x)$

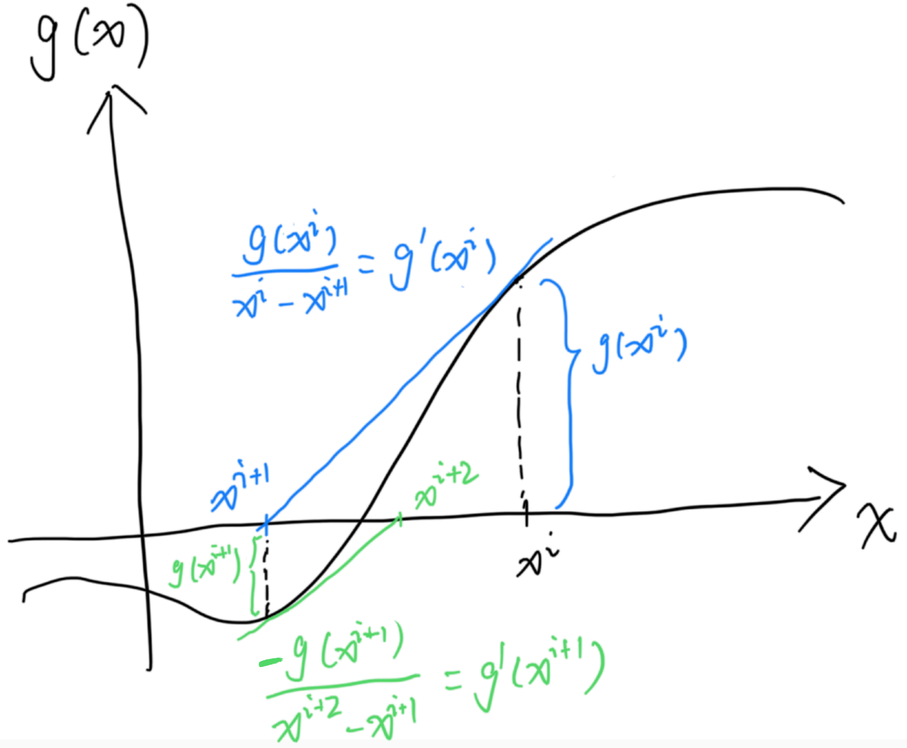
We want to solve $g(x) = 0$

Newton's method in 1D:

- **Start from initial guess** x^0
- **For each iteration (until convergence)**
  - $x^{i+1} \leftarrow x^i - g(x^i)/g'(x^i)$

In higher dimensions:

$$x^{i+1} \leftarrow x^i - (\nabla g(x^i))^{-1} g(x^i)$$



Derivation:

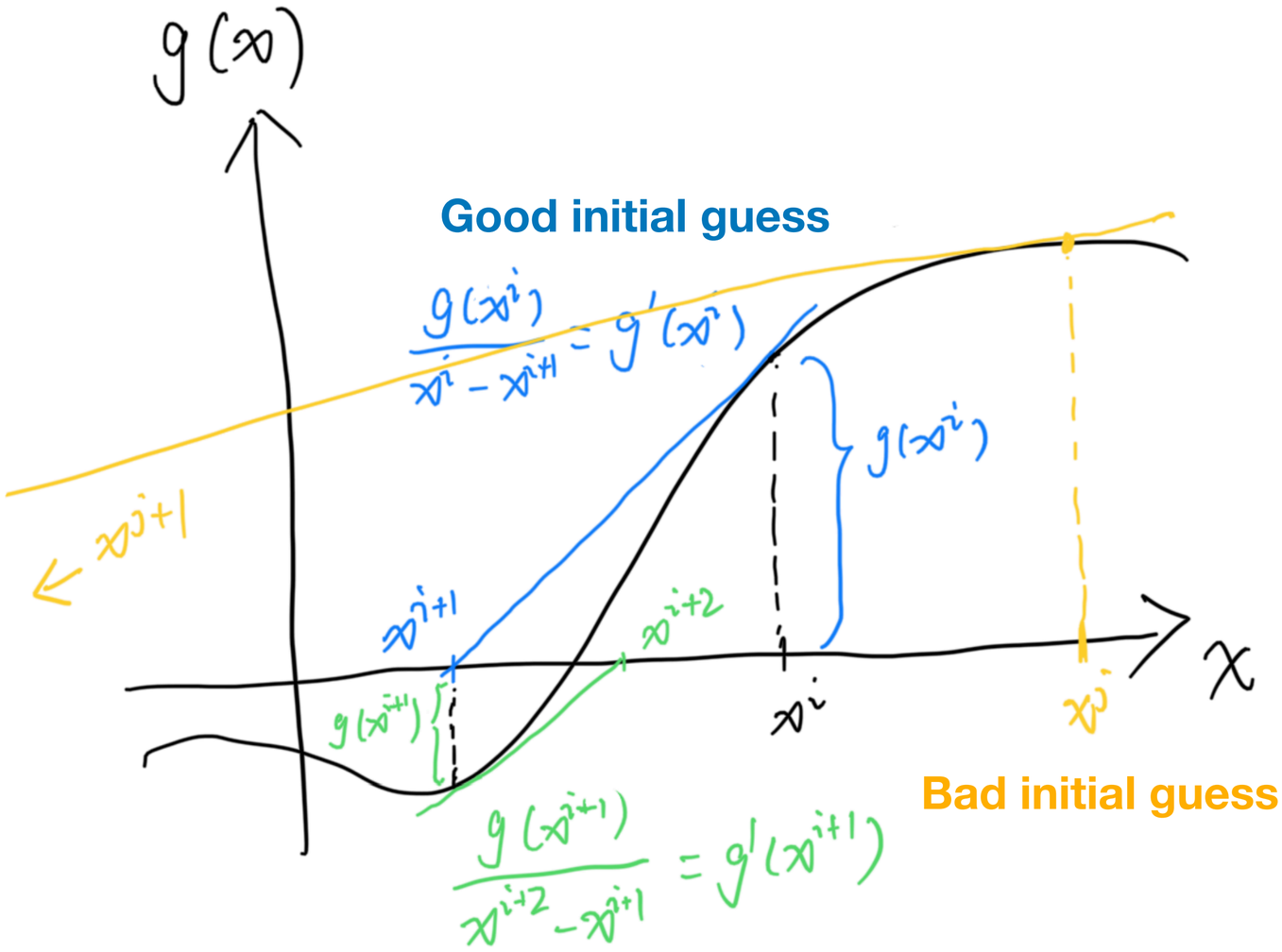
Linearly approximate $g(x) = 0$ **at** x^i **:**

$$g(x) = g(x^i) + \nabla g(x^i)(x - x^i)$$

$$g(x^{i+1}) \approx g(x^i) + \nabla g(x^i)(x^{i+1} - x^i) = 0$$

Convergence Issue of Newton's Method

Over-shooting



Simulation explodes!

Optimization Time Integration

$$x^{n+1} = \arg\min_x E(x)$$

$$\text{where } E(x) = \frac{1}{2}\|x - \tilde{x}^n\|_M^2 + \Delta t^2 P(x).$$

$$\tilde{x}^n = x^n + \Delta t v^n$$

$$\tfrac{1}{2}\|x - \tilde{x}^n\|_M^2 = \tfrac{1}{2}(x - \tilde{x}^n)^T M (x - \tilde{x}^n)$$

$$\tfrac{\partial P}{\partial x}(x) = -f(x)$$

At the local minimum of $E(x)$, $\tfrac{\partial E}{\partial x}(x^{n+1}) = 0$

$$M(x^{n+1} - (x^n + \Delta t v^n)) - \Delta t^2 f(x^{n+1}) = 0.$$

Global Convergence with Line Search

Pseudo-code

Algorithm 3: Projected Newton Method for Backward Euler Time Integration

Result: x^{n+1}, v^{n+1}

$x^i \leftarrow x^n$;
do
  $P \leftarrow \text{SPDProjection}(\nabla^2 E(x^i))$;
  $p \leftarrow -P^{-1}\nabla E(x^i)$;
  $\alpha \leftarrow \text{BackTrackingLineSearch}(x^i, p)$; //
  $x^i \leftarrow x^i + \alpha p$;
while $\|p\|_\infty / h > \epsilon$;
$x^{n+1} \leftarrow x^i$;
$v^{n+1} \leftarrow (x^{n+1} - x^n)/\Delta t$;

Algorithm 2: Backtracking Line Search

Result: α

$\alpha \leftarrow 1$;
while $E(x^i + \alpha p) > E(x^i)$ **do**
  $\alpha \leftarrow \alpha/2$;

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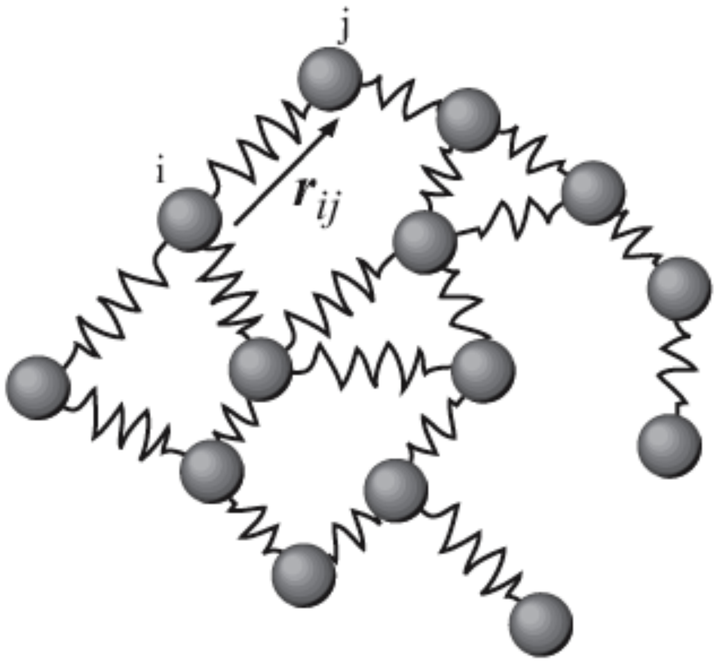
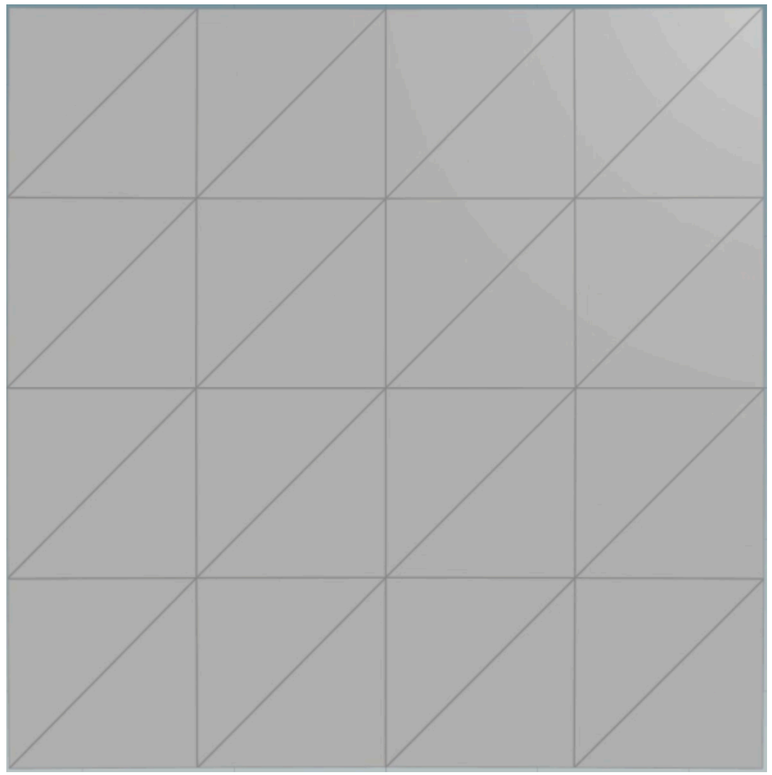
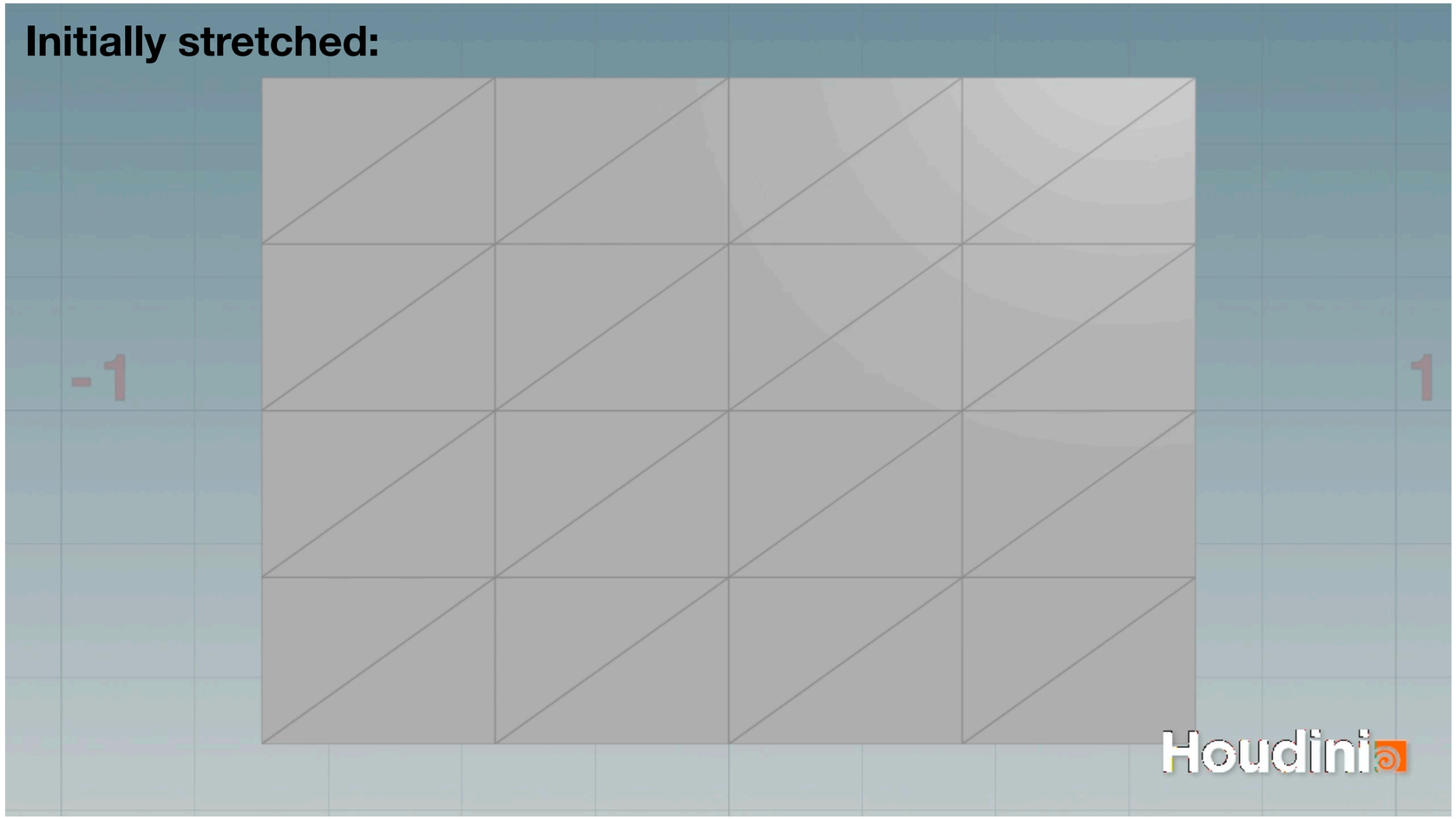


Case Study — Mass-Spring Simulation

An Initially Stretched Elastic Square

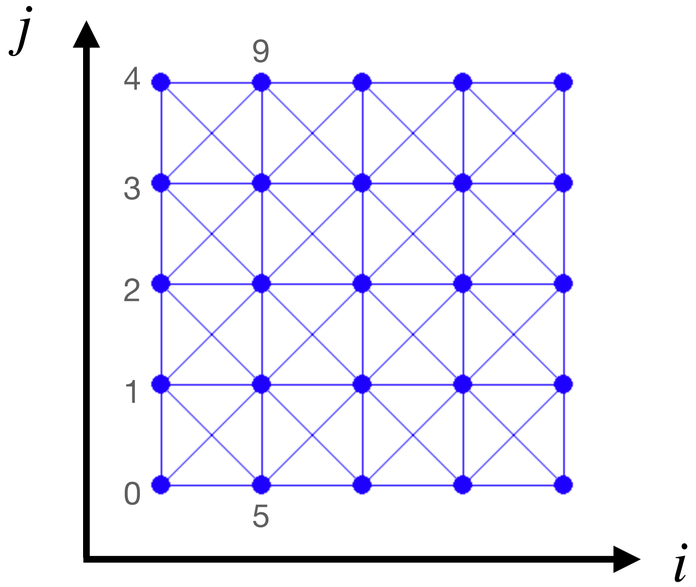


Rest shape



Mass-Spring Representation of Solids

- Mass particles connected by springs
  - square_mesh.py




```python
import numpy as np

def generate(side_length, n_seg):
    # sample nodes uniformly on a square
    x = np.array([[0.0, 0.0]] * ((n_seg + 1) ** 2))
    step = side_length / n_seg
    for i in range(0, n_seg + 1):
        for j in range(0, n_seg + 1):
            x[i * (n_seg + 1) + j] = [-side_length / 2 + i *
    step, -side_length / 2 + j * step]
```

```python
    # connect the nodes with edges
    e = []
    # horizontal edges
    for i in range(0, n_seg):
        for j in range(0, n_seg + 1):
            e.append([i * (n_seg + 1) + j, (i + 1) * (n_seg +
    1) + j])
```

```python
    # vertical edges
    for i in range(0, n_seg + 1):
        for j in range(0, n_seg):
            e.append([i * (n_seg + 1) + j, i * (n_seg + 1) + j
     + 1])
```

```python
    # diagonals
    for i in range(0, n_seg):
        for j in range(0, n_seg):
            e.append([i * (n_seg + 1) + j, (i + 1) * (n_seg +
    1) + j + 1])
            e.append([(i + 1) * (n_seg + 1) + j, i * (n_seg +
    1) + j + 1])

    return [x, e]
```

Time Integration

Optimization-based Implicit Euler

$$x^{n+1} = x^n + \Delta t v^{n+1},$$
$$v^{n+1} = v^n + \Delta t M^{-1} f^{n+1}$$

$\Longleftrightarrow$

Inertia term — Elasticity

$$E(x) = \frac{1}{2}\|x - (x^n + h v^n)\|_M^2 + h^2 P(x).$$

Incremental Potential

$$\frac{\partial P}{\partial x}(x) = -f(x)$$

Algorithm 3: Projected Newton Method for Backward Euler Time Integration

Result: x^{n+1}, v^{n+1}

$x^i \leftarrow x^n$;
do
  $P \leftarrow \text{SPDProjection}(\nabla^2 E(x^i))$; // Energy Hessian
  $p \leftarrow -P^{-1}\nabla E(x^i)$; // Energy Gradient
  $\alpha \leftarrow \text{BackTrackingLineSearch}(x^i, p)$;
  $x^i \leftarrow x^i + \alpha p$;
while $\|p\|_\infty / h > \epsilon$;
$x^{n+1} \leftarrow x^i$;
$v^{n+1} \leftarrow (x^{n+1} - x^n)/\Delta t$;

Algorithm 2: Backtracking Line Search

Result: α

$\alpha \leftarrow 1$;
while $E(x^i + \alpha p) > E(x^i)$ **do** // Energy Value
  $\alpha \leftarrow \alpha/2$;

Incremental Potential

Inertia Term

$$\text{with } \tilde{x}^n = x^n + hv^n$$

$$E_I(x) = \frac{1}{2}\|x - \tilde{x}^n\|_M^2$$

$$\nabla E_I(x) = M(x - \tilde{x}^n)$$

$$\nabla^2 E_I(x) = M \quad \text{– SPD}$$

InertiaEnergy.py

```python
import numpy as np

def val(x, x_tilde, m):
    sum = 0.0
    for i in range(0, len(x)):
        diff = x[i] - x_tilde[i]
        sum += 0.5 * m[i] * diff.dot(diff)
    return sum

def grad(x, x_tilde, m):
    g = np.array([[0.0, 0.0]] * len(x))
    for i in range(0, len(x)):
        g[i] = m[i] * (x[i] - x_tilde[i])
    return g

def hess(x, x_tilde, m):
    IJV = [[0] * (len(x) * 2), [0] * (len(x) * 2), np.array
    ([0.0] * (len(x) * 2))]
    for i in range(0, len(x)):
        for d in range(0, 2):
            IJV[0][i * 2 + d] = i * 2 + d
            IJV[1][i * 2 + d] = i * 2 + d
            IJV[2][i * 2 + d] = m[i]
    return IJV
```

Incremental Potential

Mass-Spring Elasticity Energy

- Hooke's Law in 1D:
  - $E = \frac{1}{2} k (\Delta x)^2$

Spring stiffness

Spring displacement

- In higher dimensions:

  - $\frac{1}{2} k (\|x_1 - x_2\| - l)^2$ or $l^2 \frac{1}{2} k (\frac{\|x_1 - x_2\|}{l} - 1)^2$

Current length

Rest length

A strain measure

- To avoid computing square root, we define

Area weighting

$$P_e(x) = l^2 \frac{1}{2} k (\frac{\|\boldsymbol{x}_1 - \boldsymbol{x}_2\|^2}{l^2} - 1)^2$$

Elasticity energy density
(elasticity energy per unit area)

Continuous setting:

$$P = \int_{\Omega^0} \Psi dX$$

Incremental Potential

Mass-Spring Elasticity Energy Gradient and Hessian

$$P_e(x) = l^2 \frac{1}{2} k (\frac{\|\boldsymbol{x}_1 - \boldsymbol{x}_2\|^2}{l^2} - 1)^2$$

$$\frac{\partial P_e}{\partial \boldsymbol{x}_1}(x) = -\frac{\partial P_e}{\partial \boldsymbol{x}_2}(x) = 2k(\frac{\|\boldsymbol{x}_1 - \boldsymbol{x}_2\|^2}{l^2} - 1)(\boldsymbol{x}_1 - \boldsymbol{x}_2)$$

$$\begin{aligned}
\frac{\partial^2 P_e}{\partial \boldsymbol{x}_1^2}(x) = \frac{\partial^2 P_e}{\partial \boldsymbol{x}_2^2}(x) = -\frac{\partial^2 P_e}{\partial \boldsymbol{x}_1 \boldsymbol{x}_2}(x) = -\frac{\partial^2 P_e}{\partial \boldsymbol{x}_2 \boldsymbol{x}_1}(x) \\
= \frac{4k}{l^2}(\boldsymbol{x}_1 - \boldsymbol{x}_2)(\boldsymbol{x}_1 - \boldsymbol{x}_2)^T + 2k(\frac{\|\boldsymbol{x}_1 - \boldsymbol{x}_2\|^2}{l^2} - 1)\boldsymbol{I} \\
= \frac{2k}{l^2}(2(\boldsymbol{x}_1 - \boldsymbol{x}_2)(\boldsymbol{x}_1 - \boldsymbol{x}_2)^T + (\|\boldsymbol{x}_1 - \boldsymbol{x}_2\|^2 - l^2)\boldsymbol{I})
\end{aligned}$$

MassSpringEnergy.py

```python
import numpy as np
import utils

def val(x, e, l2, k):
    sum = 0.0
    for i in range(0, len(e)):
        diff = x[e[i][0]] - x[e[i][1]]
        sum += l2[i] * 0.5 * k[i] * (diff.dot(diff) / l2[i] - 1) ** 2
    return sum

def grad(x, e, l2, k):
    g = np.array([[0.0, 0.0]] * len(x))
    for i in range(0, len(e)):
        diff = x[e[i][0]] - x[e[i][1]]
        g_diff = 2 * k[i] * (diff.dot(diff) / l2[i] - 1) * diff
        g[e[i][0]] += g_diff
        g[e[i][1]] -= g_diff
    return g
```

Incremental Potential

Mass-Spring Elasticity Energy Hessian Implementation

$$\begin{aligned}\frac{\partial^2 P_e}{\partial \boldsymbol{x}_1^2}(x) &= \frac{\partial^2 P_e}{\partial \boldsymbol{x}_2^2}(x) = -\frac{\partial^2 P_e}{\partial \boldsymbol{x}_1 \boldsymbol{x}_2}(x) = -\frac{\partial^2 P_e}{\partial \boldsymbol{x}_2 \boldsymbol{x}_1}(x) \\ &= \frac{4k}{l^2}(\boldsymbol{x}_1 - \boldsymbol{x}_2)(\boldsymbol{x}_1 - \boldsymbol{x}_2)^T + 2k(\frac{\|\boldsymbol{x}_1 - \boldsymbol{x}_2\|^2}{l^2} - 1)\boldsymbol{I} \\ &= \frac{2k}{l^2}(2(\boldsymbol{x}_1 - \boldsymbol{x}_2)(\boldsymbol{x}_1 - \boldsymbol{x}_2)^T + (\|\boldsymbol{x}_1 - \boldsymbol{x}_2\|^2 - l^2)\boldsymbol{I})\end{aligned}$$

MassSpringEnergy.py

```
20 def hess(x, e, l2, k):
21     IJV = [[0] * (len(e) * 16), [0] * (len(e) * 16), np.array
       ([0.0] * (len(e) * 16))]
22     for i in range(0, len(e)):
23         diff = x[e[i][0]] - x[e[i][1]]
24         H_diff = 2 * k[i] / l2[i] * (2 * np.outer(diff, diff)
       + (diff.dot(diff) - l2[i]) * np.identity(2))
25         H_local = utils.make_PD(np.block([[H_diff, -H_diff],
       [-H_diff, H_diff]]))
26         # add to global matrix
27         for nI in range(0, 2):
28             for nJ in range(0, 2):
29                 indStart = i * 16 + (nI * 2 + nJ) * 4
30                 for r in range(0, 2):
31                     for c in range(0, 2):
32                         IJV[0][indStart + r * 2 + c] = e[i][nI
       ] * 2 + r
33                         IJV[1][indStart + r * 2 + c] = e[i][nJ
       ] * 2 + c
34                         IJV[2][indStart + r * 2 + c] = H_local
       [nI * 2 + r, nJ * 2 + c]
35     return IJV
```

Incremental Potential

Mass-Spring Elasticity Energy Hessian Projection (make_PSD)

$$\min_P \|P - \nabla^2 E(x^i)\|_{\mathrm{F}} \quad s.t. \quad v^T P v \geq 0 \;\; \forall v \neq 0$$

Solution: $\hat{A} = Q\hat{\Lambda}Q^{-1}, \quad \hat{\Lambda}_{ij} = \Lambda_{ij} > 0 \; ? \; \Lambda_{ij} : 0$

Definition (Eigendecomposition). The eigendecomposition of a square matrix $A \in R^{n \times n}$ is

$$A = Q\Lambda Q^{-1}$$

where $Q = [q_1, q_2, ..., q_n]$ is composed of the eigenvectors q_i of A, $\|q_i\| = 1$; $\Lambda = [\lambda_1, \lambda_2, ..., \lambda_n]$, $\lambda_1 \geq \lambda_2 \geq ..., \lambda_n$ are the eigenvalues of A; and $Aq_i = \lambda_i q_i$.

utils.py

```python
import numpy as np
import numpy.linalg as LA

def make_PD(hess):
    [lam, V] = LA.eigh(hess)    # Eigen decomposition on symmetric matrix
    # set all negative Eigenvalues to 0
    for i in range(0, len(lam)):
        lam[i] = max(0, lam[i])
    return np.matmul(np.matmul(V, np.diag(lam)), np.transpose(V))
```

Incremental Potential

Gradient and Hessian

time_integrator.py

```
38 def IP_val(x, e, x_tilde, m, l2, k, h):
39     return InertiaEnergy.val(x, x_tilde, m) + h * h *
       MassSpringEnergy.val(x, e, l2, k)      # implicit Euler
40
41 def IP_grad(x, e, x_tilde, m, l2, k, h):
42     return InertiaEnergy.grad(x, x_tilde, m) + h * h *
       MassSpringEnergy.grad(x, e, l2, k)    # implicit Euler
43
44 def IP_hess(x, e, x_tilde, m, l2, k, h):
45     IJV_In = InertiaEnergy.hess(x, x_tilde, m)
46     IJV_MS = MassSpringEnergy.hess(x, e, l2, k)
47     IJV_MS[2] *= h * h     # implicit Euler
48     IJV = np.append(IJV_In, IJV_MS, axis=1)
49     H = sparse.coo_matrix((IJV[2], (IJV[0], IJV[1])), shape=(
       len(x) * 2, len(x) * 2)).tocsr()
50     return H
```

Time Integration

Algorithm 3: Projected Newton Method for Backward Euler Time Integration

Result: x^{n+1}, v^{n+1}

$x^i \leftarrow x^n$;
do
  $P \leftarrow \text{SPDProjection}(\nabla^2 E(x^i))$;
  $p \leftarrow -P^{-1}\nabla E(x^i)$;
  $\alpha \leftarrow \text{BackTrackingLineSearch}(x^i, p)$; //
  $x^i \leftarrow x^i + \alpha p$;
while $\|p\|_\infty / h > \epsilon$;
$x^{n+1} \leftarrow x^i$;
$v^{n+1} \leftarrow (x^{n+1} - x^n)/\Delta t$;

Algorithm 2: Backtracking Line Search

Result: α

$\alpha \leftarrow 1$;
while $E(x^i + \alpha p) > E(x^i)$ **do**
  $\alpha \leftarrow \alpha/2$;

time_integrator.py

```python
import copy
from cmath import inf

import numpy as np
import numpy.linalg as LA
import scipy.sparse as sparse
from scipy.sparse.linalg import spsolve

import InertiaEnergy
import MassSpringEnergy
```

```python
def step_forward(x, e, v, m, l2, k, h, tol):
    x_tilde = x + v * h     # implicit Euler predictive position
    x_n = copy.deepcopy(x)

    # Newton loop
    iter = 0
    E_last = IP_val(x, e, x_tilde, m, l2, k, h)
    p = search_dir(x, e, x_tilde, m, l2, k, h)
    while LA.norm(p, inf) / h > tol:
        print('Iteration', iter, ':')
        print('residual =', LA.norm(p, inf) / h)

        # line search
        alpha = 1
        while IP_val(x + alpha * p, e, x_tilde, m, l2, k, h) > E_last:
            alpha /= 2
        print('step size =', alpha)

        x += alpha * p
        E_last = IP_val(x, e, x_tilde, m, l2, k, h)
        p = search_dir(x, e, x_tilde, m, l2, k, h)
        iter += 1

    v = (x - x_n) / h   # implicit Euler velocity update
    return [x, v]
```

```python
def search_dir(x, e, x_tilde, m, l2, k, h):
    projected_hess = IP_hess(x, e, x_tilde, m, l2, k, h)
    reshaped_grad = IP_grad(x, e, x_tilde, m, l2, k, h).reshape(len(x) * 2, 1)
    return spsolve(projected_hess, -reshaped_grad).reshape(len(x), 2)
```

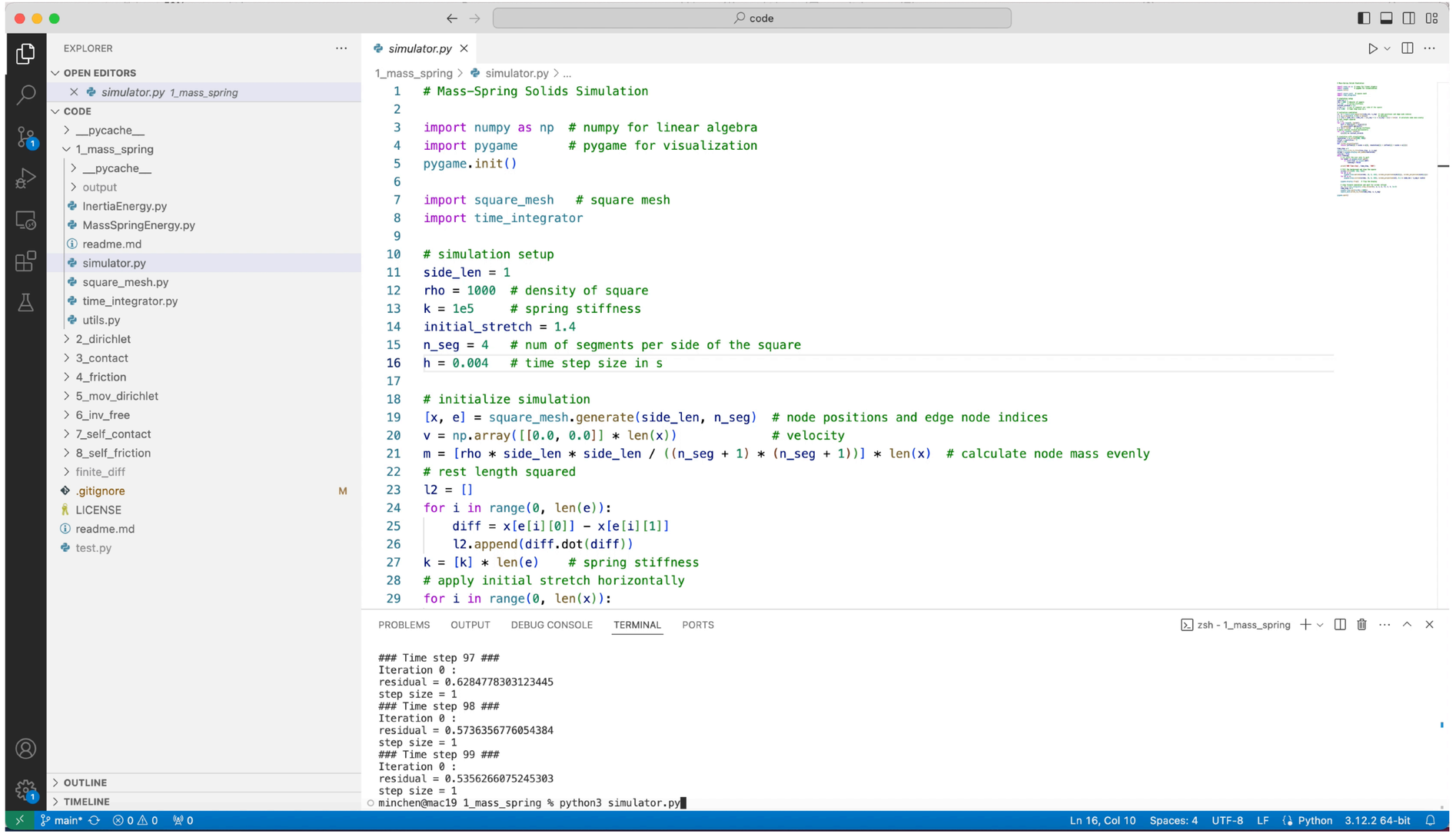
Simulator with Visualization

Simulator.py

```python
# Mass-Spring Solids Simulation

import numpy as np  # numpy for linear algebra
import pygame       # pygame for visualization
pygame.init()

import square_mesh   # square mesh
import time_integrator

# simulation setup
side_len = 1
rho = 1000  # density of square
k = 1e5     # spring stiffness
initial_stretch = 1.4
n_seg = 4   # num of segments per side of the square
h = 0.004   # time step size in s

# initialize simulation
[x, e] = square_mesh.generate(side_len, n_seg)  # node positions and edge node indices
v = np.array([[0.0, 0.0]] * len(x))             # velocity
m = [rho * side_len * side_len / ((n_seg + 1) * (n_seg + 1))] * len(x)  # calculate node mass evenly
# rest length squared
l2 = []
for i in range(0, len(e)):
    diff = x[e[i][0]] - x[e[i][1]]
    l2.append(diff.dot(diff))
k = [k] * len(e)    # spring stiffness
# apply initial stretch horizontally
for i in range(0, len(x)):
    x[i][0] *= initial_stretch
```

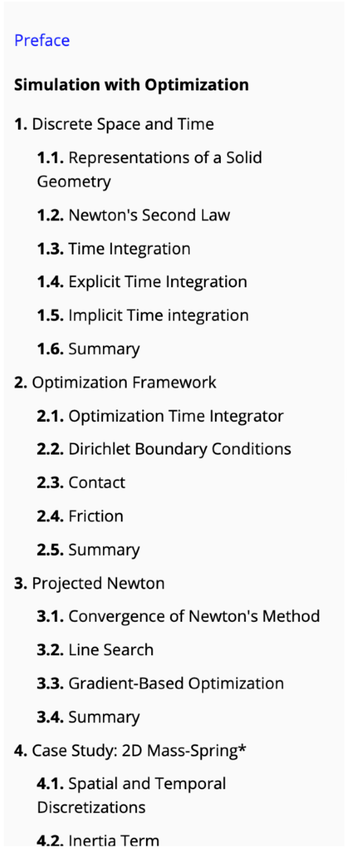
```python
# simulation with visualization
resolution = np.array([900, 900])
offset = resolution / 2
scale = 200
def screen_projection(x):
    return [offset[0] + scale * x[0], resolution[1] - (offset[1] + scale * x[1])]

time_step = 0
screen = pygame.display.set_mode(resolution)
running = True
while running:
    # run until the user asks to quit
    for event in pygame.event.get():
        if event.type == pygame.QUIT:
            running = False

    print('### Time step', time_step, '###')

    # fill the background and draw the square
    screen.fill((255, 255, 255))
    for eI in e:
        pygame.draw.aaline(screen, (0, 0, 255), screen_projection(x[eI[0]]), screen_projection(x[eI[1]]))
    for xI in x:
        pygame.draw.circle(screen, (0, 0, 255), screen_projection(xI), 0.1 * side_len / n_seg * scale)

    pygame.display.flip()   # flip the display

    # step forward simulation and wait for screen refresh
    [x, v] = time_integrator.step_forward(x, e, v, m, l2, k, h, 1e-2)
    time_step += 1
    pygame.time.wait(int(h * 1000))

pygame.quit()
```

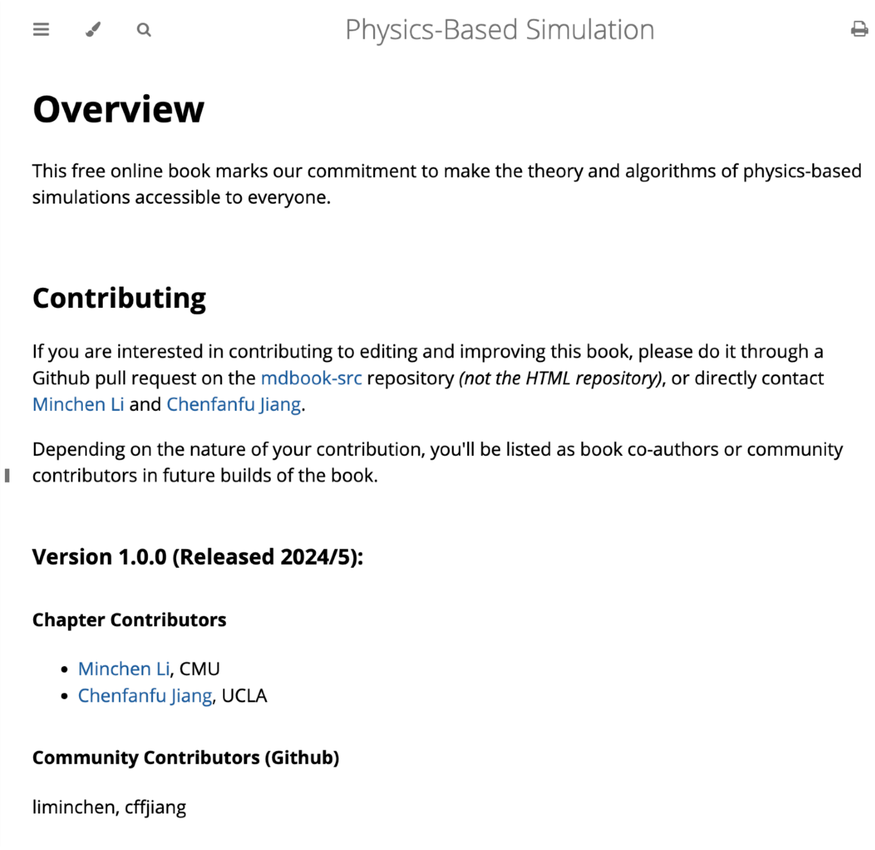
Demo

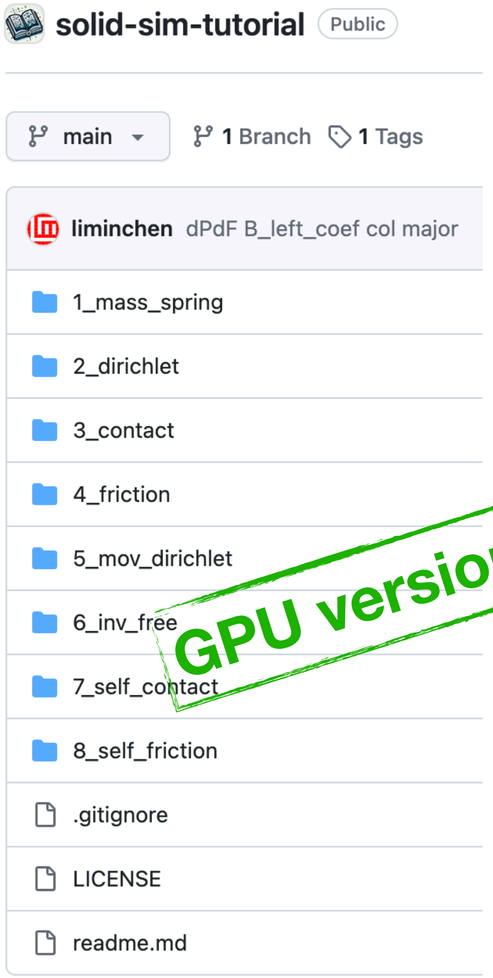

code
EXPLORER
OPEN EDITORS
simulator.py 1_mass_spring
CODE
__pycache__
1_mass_spring
__pycache__
output
InertiaEnergy.py
MassSpringEnergy.py
readme.md
simulator.py
square_mesh.py
time_integrator.py
utils.py
2_dirichlet
3_contact
4_friction
5_mov_dirichlet
6_inv_free
7_self_contact
8_self_friction
finite_diff
.gitignore
M
LICENSE
readme.md
test.py
OUTLINE
TIMELINE
simulator.py
1_mass_spring > simulator.py > ...
1 # Mass-Spring Solids Simulation
2
3 import numpy as np # numpy for linear algebra
4 import pygame # pygame for visualization
5 pygame.init()
6
7 import square_mesh # square mesh
8 import time_integrator
9
10 # simulation setup
11 side_len = 1
12 rho = 1000 # density of square
13 k = 1e5 # spring stiffness
14 initial_stretch = 1.4
15 n_seg = 4 # num of segments per side of the square
16 h = 0.004 # time step size in s
17
18 # initialize simulation
19 [x, e] = square_mesh.generate(side_len, n_seg) # node positions and edge node indices
20 v = np.array([[0.0, 0.0]] * len(x)) # velocity
21 m = [rho * side_len * side_len / ((n_seg + 1) * (n_seg + 1))] * len(x) # calculate node mass evenly
22 # rest length squared
23 l2 = []
24 for i in range(0, len(e)):
25 diff = x[e[i][0]] - x[e[i][1]]
26 l2.append(diff.dot(diff))
27 k = [k] * len(e) # spring stiffness
28 # apply initial stretch horizontally
29 for i in range(0, len(x)):
PROBLEMS
OUTPUT
DEBUG CONSOLE
TERMINAL
PORTS
zsh - 1_mass_spring
Time step 97
Iteration 0 :
residual = 0.6284778303123445
step size = 1
Time step 98
Iteration 0 :
residual = 0.5736356776054384
step size = 1
Time step 99
Iteration 0 :
residual = 0.5356266075245303
step size = 1
minchen@mac19 1_mass_spring % python3 simulator.py
main*
0 0 0
Ln 16, Col 10
Spaces: 4
UTF-8
LF
Python
3.12.2 64-bit

Free Online Book and Python Tutorial

Code: github.com/phys-sim-book/solid-sim-tutorial







GPU version coming!

Free online book: phys-sim-book.github.io

Topics Today

Part I: Fundamentals and The Big Picture (Minchen)

- Distortion Minimization
- Elastodynamics Simulation via Optimization Time Integration
- Case Study: Mass-Spring System
- More Topics on Optimization Time Integration

Part II: Advanced Topics (Eris)

- Constrained System
- Reduced-Order System
- Multilevel System
- Adaptive Simulation

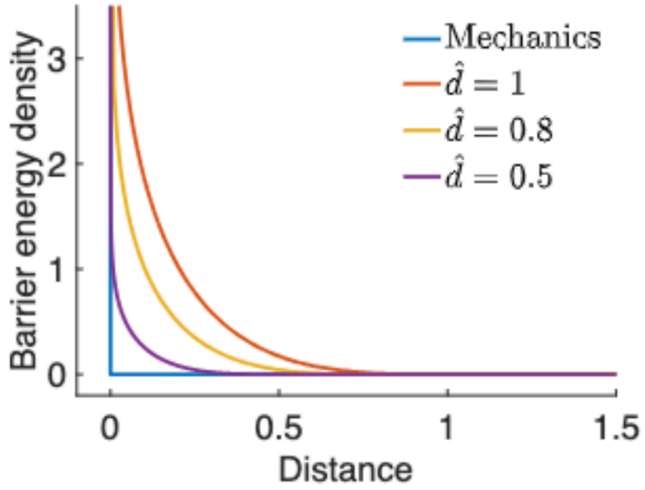
Self-Contact (Briefly)

$$x^{n+1} = arg\min_{x} E(x)$$
$$s.t. \quad \forall ij,\ d_{ij}(x) > 0$$

ij iterates non-adjacent surface primitive pairs

$$x^{n+1} = arg\min_{x} E(x) + \Delta t^2 \sum_{ij} w_{ij} b(d_{ij}(x))$$

$$b(d_{ij}(x)) = \begin{cases} \frac{\kappa}{2}\left(\frac{d_{ij}}{\hat{d}} - 1\right)\ln\frac{d_{ij}}{\hat{d}} & d_{ij} < \hat{d} \\ 0 & d_{ij} \geq \hat{d} \end{cases}$$



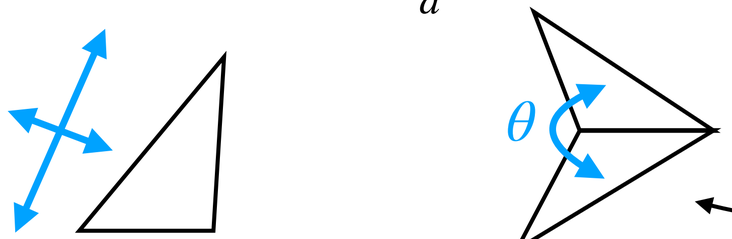
[Li et al. 2020]

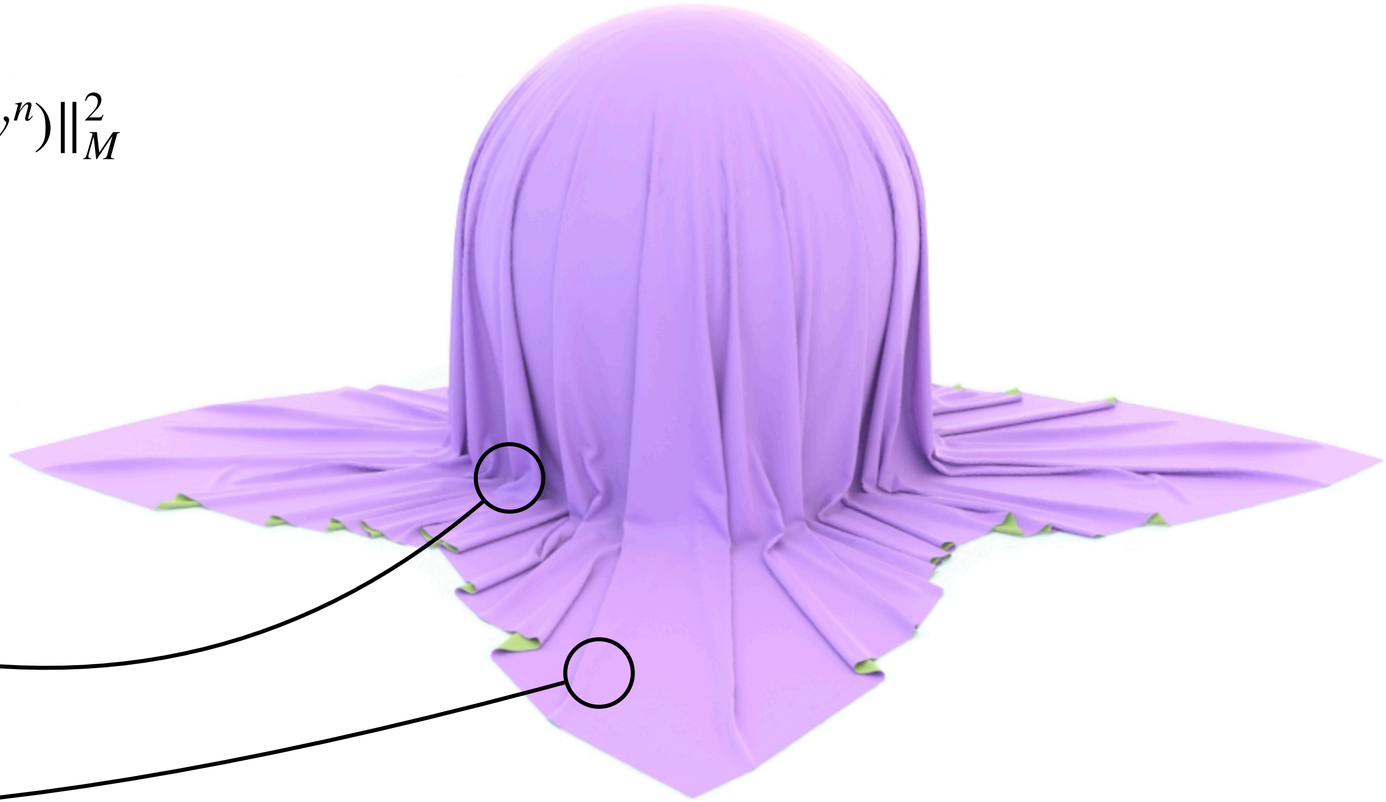
Thin Objects (Briefly)

$$x^{n+1} = \arg\min_x E(x)$$

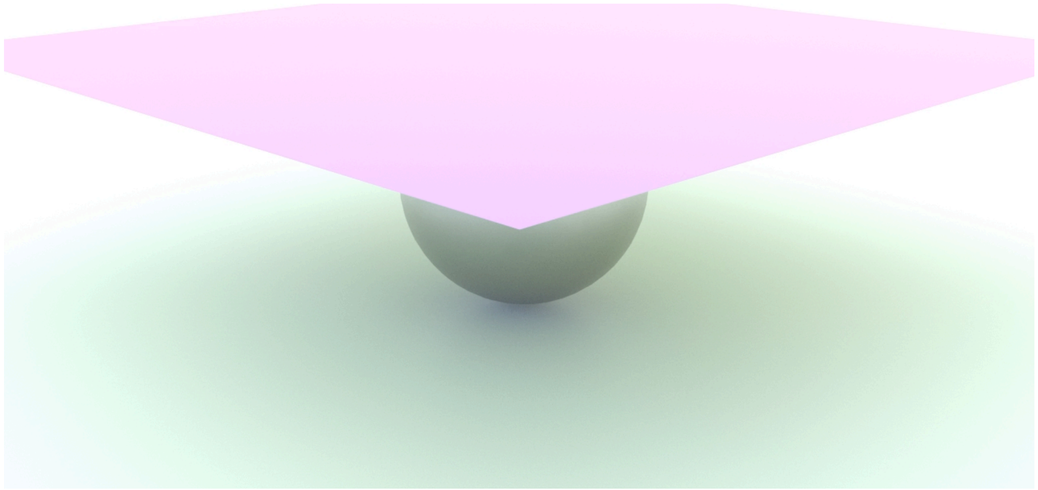
$$E(x) = \sum_e V_e \Psi(\mathbf{F}_e) + \frac{1}{2\Delta t^2}\|x - (x^n + \Delta t v^n)\|_M^2$$

$$\sum_e V_e \Psi_{\textbf{stretch}}(\mathbf{F}_e) + \sum_d w_d \Psi_{\textbf{bend}}(\theta_d)$$





Thin Objects

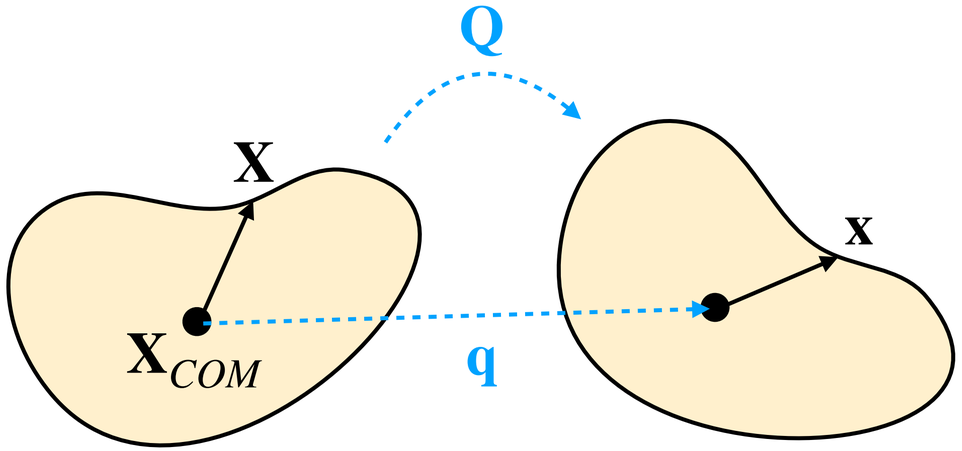


[Li et al. 2021]

Nearly Rigid Effects (Briefly)

If don't care about the tiny deformations,

Can simply track rotation\affine transformation $\mathbf{Q}$ and translation $\mathbf{q}$ per body!



$$\mathbf{x} = \mathbf{Q}(\mathbf{X} - \mathbf{X}_{COM}) + \mathbf{X}_{COM} + \mathbf{q}$$

Constant deformation gradient per body,

$$x^{n+1} = arg\min_{x} E(x)$$

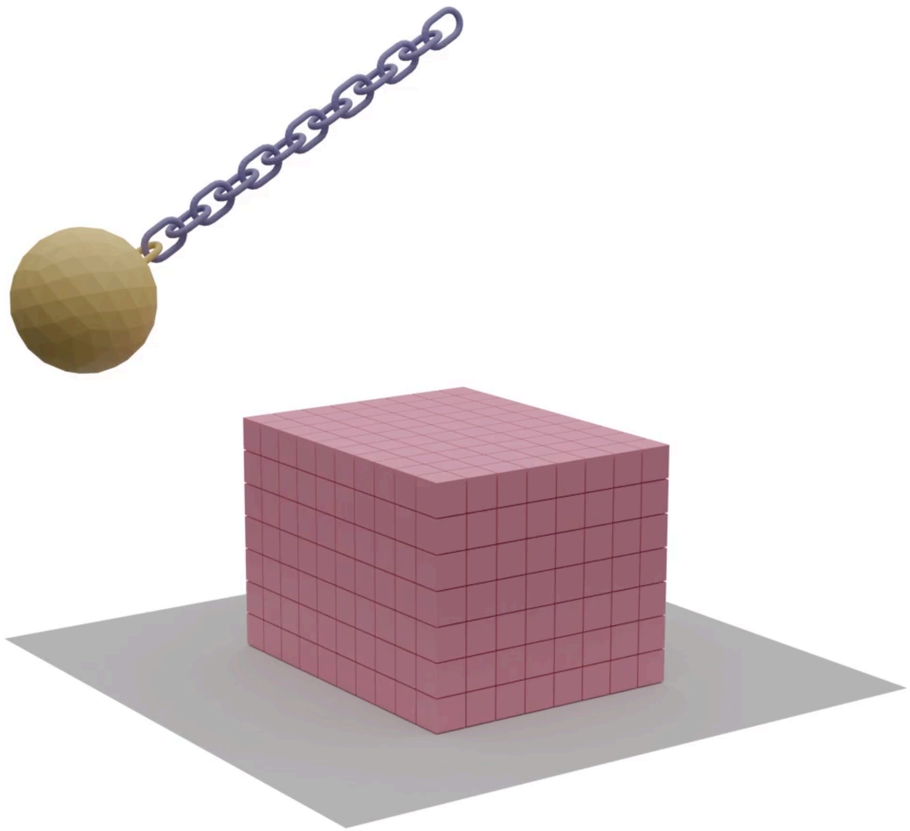
$$E(x) = \sum_{e} V_e \Psi(\mathbf{F}_e) + \frac{1}{2\Delta t^2}\|x - (x^n + \Delta t v^n)\|_M^2$$

Minimize in the subspace
(Let $x = \phi(Q, q)$)

$$Q^{n+1}, q^{n+1} = arg\min_{Q,q} E(\phi(Q, q))$$

$$E(\phi(Q, q)) = \sum_{e} V_e \Psi(\mathbf{F}_e(Q, q)) + \frac{1}{2\Delta t^2}\|\phi(Q, q) - (x^n + \Delta t v^n)\|_M^2$$

Nearly Rigid Objects



[Ferguson et al. 2021]

[Lan et al. 2022]

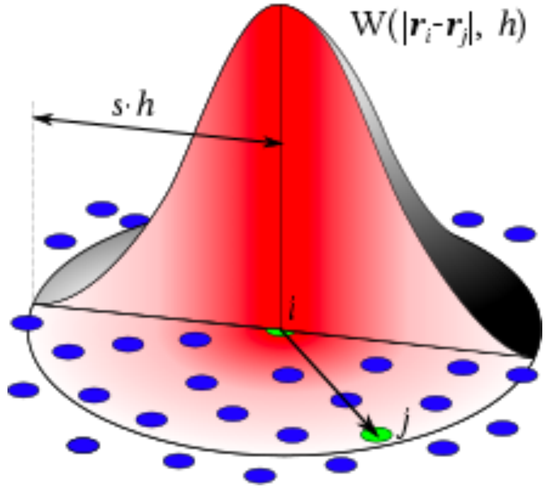
Fluids (Briefly)

$$x^{n+1} = arg\min_{x} E(x)$$

$$E(x) = \sum_{e} V_e \Psi(\mathbf{F}_e) + \frac{1}{2\Delta t^2}\|x - (x^n + \Delta t v^n)\|_M^2$$

$$\Psi(\mathbf{F}_e) = \mu(\det(\mathbf{F}_e) - 1)^2$$

No penalty on shearing,
only penalizes volume change



Use particles and neighbors to compute $\mathbf{F}$
via e.g. SPH, MLS

Fluids

[Xie et al. 2023]

Conclusion and Future Works

Optimization time integration

enables reliable and versatile physics-based simulation

$$x^{n+1} = arg\min_{x} E(x)$$

$$E(x) = \sum_{e} V_e \Psi(\mathbf{F}_e) + \frac{1}{2\Delta t^2}\|x - (x^n + \Delta t v^n)\|_M^2$$

Improving efficiency and scalability;

Incorporating path-dependent effects, e.g. damping, plasticity, friction, etc;

Application to inverse problems, e.g. computational design, robot learning, etc.

Topics Today

Part I: Fundamentals and The Big Picture (Minchen)

- Distortion Minimization
- Elastodynamics Simulation via Optimization Time Integration
- Case Study: Mass-Spring System
- More Topics on Optimization Time Integration

Part II: Advanced Topics (Eris)

- Constrained System
- Reduced-Order System
- Multilevel System
- Adaptive Simulation

Thank You!

Questions?

Image sources:

- https://r-wong253249-sp.blogspot.com/2013/11/pose-to-pose-and-frame-by-frame-research.html
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- https://drive.google.com/file/d/1oxeQ9L_DX_u_3nig-DMoW_GHZGO1Sva9/preview
- https://medium.com/@jaleeladejumo/gradient-descent-from-scratch-batch-gradient-descent-stochastic-gradient-descent-and-mini-batch-def681187473
- https://academic-accelerator.com/encyclopedia/spring-system
- https://en.wikipedia.org/wiki/Smoothed-particle_hydrodynamics
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- https://www-users.cse.umn.edu/~narain/files/admm-pd.pdf