CSE 291 (SP24)
Physical Simulations: Incremental Potential

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Dissipative System

- Dissipative system
- Stability of Euler integrators
- Incremental variational principle
- Adding dissipation
- Higher order method
- Optimization

Dissipative system

- Hamilton's least action principle always give us conservative forces.

$$\left(\int_0^T (K(\mathbf{q}, \dot{\mathbf{q}}) - V(\mathbf{q}))\, dt \right)^{\circ} = 0 \implies \boxed{\frac{d}{dt}\frac{\partial K}{\partial \dot{\mathbf{q}}}} \boxed{- \frac{\partial K}{\partial \mathbf{q}}} = \boxed{-\frac{\partial V}{\partial \mathbf{q}}}$$

change of momentum — fictitious force — conservative force

- D'Alembert principle is a generalization of least action that allows any force, but it is more like "just adding an additional term"

$$\left(\int_0^T (K(\mathbf{q}, \dot{\mathbf{q}}) - V(\mathbf{q}))\, dt \right)^{\circ} = \boxed{\int_0^T \langle \mathbf{f}(\mathbf{q}, \dot{\mathbf{q}}) | \mathring{\mathbf{q}} \rangle\, dt}$$

virtual work from any additional force

$$\implies \frac{d}{dt}\frac{\partial K}{\partial \dot{\mathbf{q}}} - \frac{\partial K}{\partial \mathbf{q}} = -\frac{\partial V}{\partial \mathbf{q}} + \mathbf{f}$$

Dissipative system

- Can't dissipative forces be written as derivative of a function?
- Rayleigh (1873) observed the following
  - Suppose we have some linear viscous force

$$m\ddot{\mathbf{q}} = \boxed{-\frac{\partial V}{\partial \mathbf{q}}} \boxed{-\mathbf{B}\dot{\mathbf{q}}}$$

conservative force

damping force linear in velocity

  - This (linear) damping is actually the variation of some (quadratic) function:

$$\mathbf{B}\dot{\mathbf{q}} = \frac{\partial}{\partial \dot{\mathbf{q}}} R(\dot{\mathbf{q}}) \qquad \boxed{R(\dot{\mathbf{q}}) = \frac{1}{2}\dot{\mathbf{q}}^\intercal \mathbf{B}\dot{\mathbf{q}}}$$

Rayleigh dissipation function

Rayleigh's Euler–Lagrange Equation

- Rayleigh: Given kinetic energy $K(\mathbf{q}, \dot{\mathbf{q}})$, potential energy $V(\mathbf{q})$, and a **dissipation function** $R(\mathbf{q}, \dot{\mathbf{q}})$
  - The equation of motion is given by the classical EL-eq with the derivative of dissipation but only with respect to velocity

$$\frac{d}{dt}\frac{\partial K}{\partial \dot{\mathbf{q}}} - \frac{\partial K}{\partial \mathbf{q}} = -\frac{\partial V}{\partial \mathbf{q}} - \frac{\partial R}{\partial \dot{\mathbf{q}}}$$

change of momentum | fictitious force | conservative force | dissipative force

Rayleigh's Euler–Lagrange Equation

$$\underbrace{\frac{d}{dt}\frac{\partial K}{\partial \dot{\mathbf{q}}}}_{\text{change of momentum}} \underbrace{- \frac{\partial K}{\partial \mathbf{q}}}_{\text{fictitious force}} = \underbrace{- \frac{\partial V}{\partial \mathbf{q}}}_{\text{conservative force}} \underbrace{- \frac{\partial R}{\partial \dot{\mathbf{q}}}}_{\text{dissipative force}}$$

- Related: Helmholtz's minimal dissipation principle, Onsager's maximal dissipation principle.
- Originally Rayleigh only considered quadratic R.
- After 1970's (Moreau) it's discovered that other non-quadratic R can recover nonlinear forces like Coulomb friction and plasticity.
- There is a natural time discretization: incremental potential (Kane, Marsden, Ortiz, West 1999)

Rayleigh's Euler–Lagrange Equation

$$\underbrace{\frac{d}{dt}\frac{\partial K}{\partial \dot{\mathbf{q}}}}_{\text{change of momentum}} \underbrace{- \frac{\partial K}{\partial \mathbf{q}}}_{\text{fictitious force}} = \underbrace{- \frac{\partial V}{\partial \mathbf{q}}}_{\text{conservative force}} \underbrace{- \frac{\partial R}{\partial \dot{\mathbf{q}}}}_{\text{dissipative force}}$$

- Conditions:

  $\dot{\mathbf{q}} \mapsto R(\mathbf{q}, \dot{\mathbf{q}})$ is convex, zero at $\dot{\mathbf{q}} = 0$, and otherwise nonnegative.

Energy dissipation

$$\underbrace{\frac{d}{dt}\frac{\partial K}{\partial \dot{\mathbf{q}}}}_{\text{change of momentum}} \underbrace{- \frac{\partial K}{\partial \mathbf{q}}}_{\text{fictitious force}} = \underbrace{-\frac{\partial V}{\partial \mathbf{q}}}_{\text{conservative force}} \underbrace{- \frac{\partial R}{\partial \dot{\mathbf{q}}}}_{\text{dissipative force}}$$

- Energy law (recall Noether's theorem for time independence)

$$\frac{d}{dt}\left(\frac{\partial K}{\partial \dot{\mathbf{q}}}\dot{\mathbf{q}} - K + V\right) = -\frac{\partial R}{\partial \dot{\mathbf{q}}}\dot{\mathbf{q}}$$

- If *K* and *R* are quadratic in $\dot{\mathbf{q}}$, then $\frac{\partial K}{\partial \dot{\mathbf{q}}}\dot{\mathbf{q}} = 2K \quad \frac{\partial R}{\partial \dot{\mathbf{q}}}\dot{\mathbf{q}} = 2R$

$$\frac{d}{dt}(K + V) = -2R$$

- To design dissipation, just model the rate of energy dissipation.

Interpret the equation in discrete setting

$$\frac{d}{dt}\frac{\partial K}{\partial \dot{\mathbf{q}}} - \frac{\partial K}{\partial \mathbf{q}} = -\frac{\partial V}{\partial \mathbf{q}} - \frac{\partial R}{\partial \dot{\mathbf{q}}}$$

change of momentum | fictitious force | conservative force | dissipative force

- In the discrete setting, let us first focus on the **backward Euler method**.
- For simplicity of exposition, we assume $K(\mathbf{q}, \dot{\mathbf{q}}) = \frac{1}{2}\dot{\mathbf{q}}^\intercal \mathbf{M}\dot{\mathbf{q}}$

  So the equation of motion is $\mathbf{M}\ddot{\mathbf{q}} = -\frac{\partial V}{\partial \mathbf{q}} - \frac{\partial R}{\partial \dot{\mathbf{q}}}$

Stability of Symplectic Euler and Backward Euler

- Dissipative system
- Stability of Euler integrators
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- Optimization

Back to F=ma

- Suppose the space of positions is given by $Q = \mathbb{R}^m$ where each point has coordinate $\mathbf{q} = (q_1, \ldots, q_m)^\intercal$
- Suppose the inertia is independent of $\mathbf{q}$

$$\text{KineticEnergy}(\dot{\mathbf{q}}) = \frac{1}{2}\dot{\mathbf{q}}^\intercal \mathbf{M} \dot{\mathbf{q}}$$

- Suppose we have a potential energy $U = U(q_1, \ldots, q_m)$
- Then the equation of motion is

$$(\mathbf{M}\ddot{\mathbf{q}})_i = -(dU)_i = -\frac{\partial U}{\partial q_i}$$

Symplectic & Backward Euler

- Discretize time $t^{(n)} = n\Delta t$. Call state at n-th time step $\mathbf{q}^{(n)}$
- Approximate 2nd time derivative

$$(\ddot{\mathbf{q}})^{(n)} \approx \frac{1}{\Delta t^2}\left(\mathbf{q}^{(n-1)} - 2\mathbf{q}^{(n)} + \mathbf{q}^{(n+1)}\right)$$

- Euler methods: Given $\mathbf{q}^{(n-1)}, \mathbf{q}^{(n)}$ solve for $\mathbf{q}^{(n+1)}$
  - Symplectic (explicit)

$$\frac{1}{\Delta t^2}\left(\mathbf{q}^{(n-1)} - 2\mathbf{q}^{(n)} + \mathbf{q}^{(n+1)}\right) = -\mathbf{M}^{-1}(dU)|_{\mathbf{q}^{(n)}}$$

  - Backward (implicit)

$$\frac{1}{\Delta t^2}\left(\mathbf{q}^{(n-1)} - 2\mathbf{q}^{(n)} + \mathbf{q}^{(n+1)}\right) = -\mathbf{M}^{-1}(dU)|_{\mathbf{q}^{(n+1)}}$$

Symplectic & Backward Euler

- Stability analysis on a test equation (A-stability)

$$\mathbf{M}^{-1} dU|_{\mathbf{q}} = \omega^2 \mathbf{q}$$

$$\ddot{q} + \omega^2 q = 0$$
$$q = a\cos(\omega t) + b\sin(\omega t)$$

  - Symplectic (explicit)

$$\frac{1}{\Delta t^2}\left(\mathbf{q}^{(n-1)} - 2\mathbf{q}^{(n)} + \mathbf{q}^{(n+1)}\right) = -\mathbf{M}^{-1}(dU)|_{\mathbf{q}^{(n)}}$$

  - Backward (implicit)

$$\frac{1}{\Delta t^2}\left(\mathbf{q}^{(n-1)} - 2\mathbf{q}^{(n)} + \mathbf{q}^{(n+1)}\right) = -\mathbf{M}^{-1}(dU)|_{\mathbf{q}^{(n+1)}}$$

Symplectic & Backward Euler

- Stability analysis on a test equation (A-stability)

$$\mathbf{M}^{-1} dU|_{\mathbf{q}} = \omega^2 \mathbf{q}$$

  - Symplectic (explicit)

$$q^{(n+1)} = -q^{(n-1)} + 2q^{(n)} - \Delta t^2 \omega^2 q^{(n)}$$

  - Backward (implicit)

$$q^{(n+1)} = -q^{(n-1)} + 2q^{(n)} - \Delta t^2 \omega^2 q^{(n+1)}$$

Symplectic & Backward Euler

- Stability analysis on a test equation (A-stability)

$$\mathbf{M}^{-1} dU|_{\mathbf{q}} = \omega^2 \mathbf{q}$$

  - Symplectic (explicit)

$$q^{(n+1)} = -q^{(n-1)} + (2 - \Delta t^2 \omega^2) q^{(n)}$$

  - Backward (implicit)

$$q^{(n+1)} = \frac{-q^{(n-1)} + 2q^{(n)}}{1 + \Delta t^2 \omega^2}$$

Symplectic & Backward Euler

- Symplectic (explicit) $q^{(n+1)} = -q^{(n-1)} + (2 - \Delta t^2 \omega^2) q^{(n)}$

$$\begin{bmatrix} q^{(n)} \\ q^{(n+1)} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 2 - \Delta t^2 \omega^2 \end{bmatrix} \begin{bmatrix} q^{(n-1)} \\ q^{(n)} \end{bmatrix}$$

- Backward (implicit) $q^{(n+1)} = \dfrac{-q^{(n-1)} + 2q^{(n)}}{1 + \Delta t^2 \omega^2}$

$$\begin{bmatrix} q^{(n)} \\ q^{(n+1)} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -\frac{1}{1+\Delta t^2 \omega^2} & \frac{2}{1+\Delta t^2 \omega^2} \end{bmatrix} \begin{bmatrix} q^{(n-1)} \\ q^{(n)} \end{bmatrix}$$

Symplectic & Backward Euler

- Symplectic (explicit) $\begin{bmatrix} q^{(n)} \\ q^{(n+1)} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 2 - \Delta t^2 \omega^2 \end{bmatrix} \begin{bmatrix} q^{(n-1)} \\ q^{(n)} \end{bmatrix}$
  - determinant = 1 (area preserving)
  - Both |eigenvalues|=1 when $\Delta t^2 \omega^2 < 4$ (conditional stability)

- Backward (implicit) $\begin{bmatrix} q^{(n)} \\ q^{(n+1)} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -\frac{1}{1+\Delta t^2 \omega^2} & \frac{2}{1+\Delta t^2 \omega^2} \end{bmatrix} \begin{bmatrix} q^{(n-1)} \\ q^{(n)} \end{bmatrix}$
  - determinant < 1 (shrinking)
  - All |eigenvalues|<1 for all $\Delta t^2 \omega^2$ (unconditionally stable)

Incremental Variation

- Dissipative system
- Stability of Euler integrators
- Incremental variational principle
- Adding dissipation
- Higher order method
- Optimization

Backward Euler

- Backward Euler

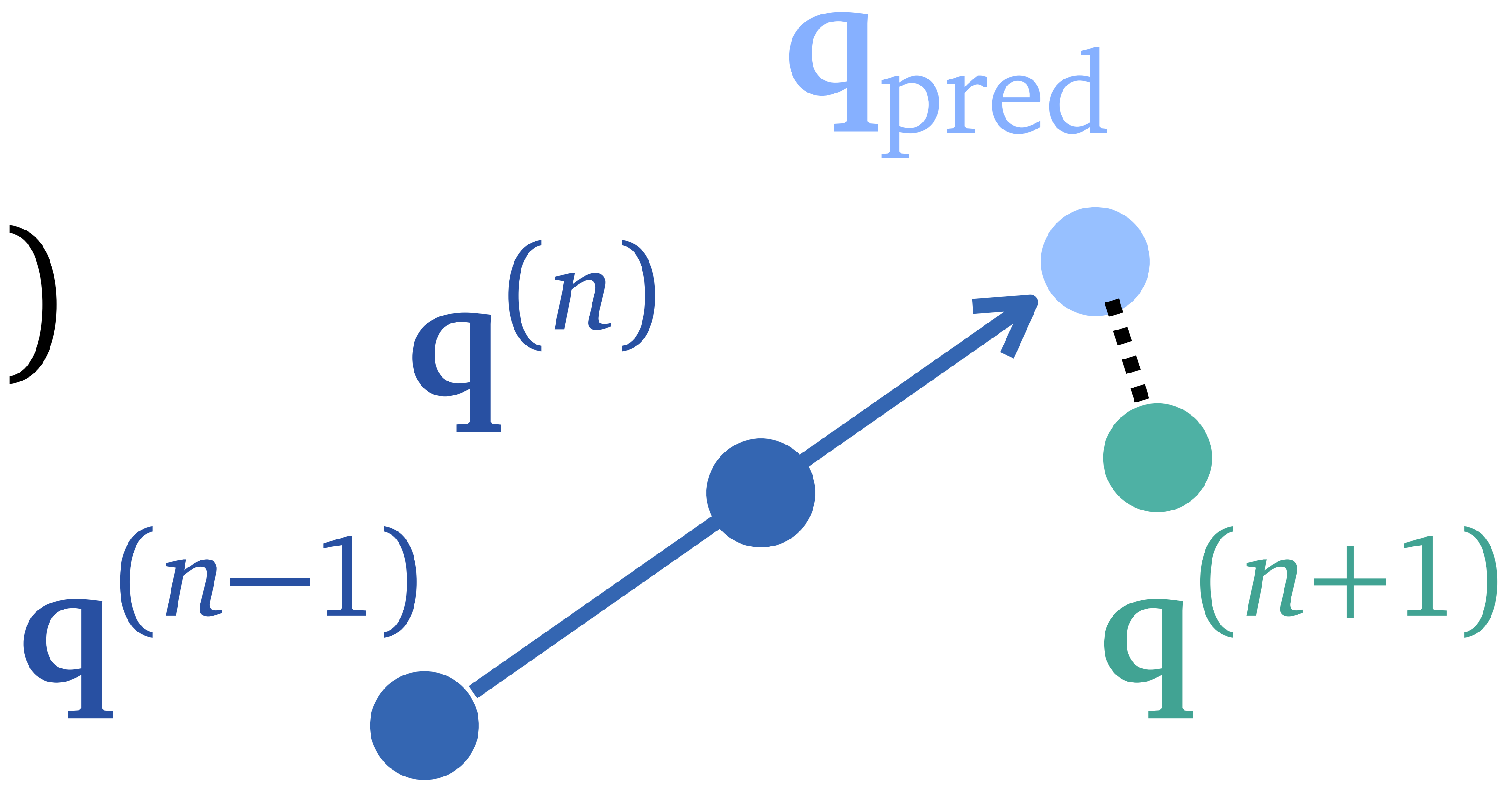
$$\frac{1}{\Delta t^2}\mathbf{M}\left(\mathbf{q}^{(n-1)} - 2\mathbf{q}^{(n)} + \mathbf{q}^{(n+1)}\right) = -(dU)|_{\mathbf{q}^{(n+1)}}$$

- Rearrange, with $\mathbf{q}_{\text{pred}} := 2\mathbf{q}^{(n)} - \mathbf{q}^{(n-1)}$

$$\frac{1}{\Delta t^2}\mathbf{M}\left(\mathbf{q}^{(n+1)} - \mathbf{q}_{\text{pred}}\right) + (dU)|_{\mathbf{q}^{(n+1)}} = 0$$

- This is actually an optimality condition

$$\mathbf{q}^{(n+1)} = \underset{\mathbf{q}\in\mathbb{R}^m}{\operatorname{argmin}} \frac{1}{2\Delta t^2}|\mathbf{q} - \mathbf{q}_{\text{pred}}|^2_{\mathbf{M}} + U(\mathbf{q})$$

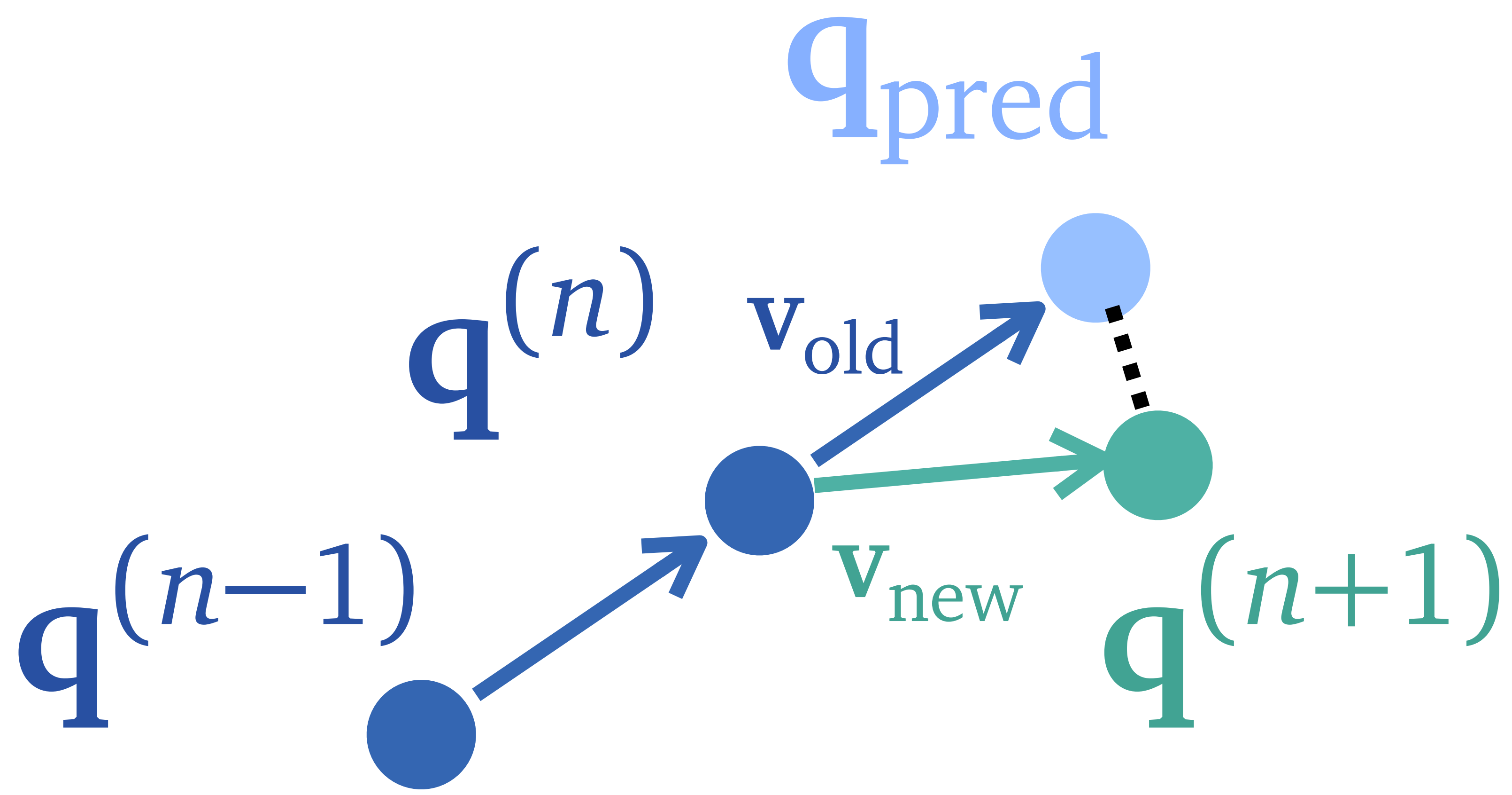


Backward Euler

$$\mathbf{q}^{(n+1)} = \underset{\mathbf{q}\in\mathbb{R}^m}{\operatorname{argmin}} \frac{1}{2\Delta t^2}|\mathbf{q}-\mathbf{q}_{\text{pred}}|^2_{\mathbf{M}} + U(\mathbf{q})$$

- In terms of velocity

$$\mathbf{v}_{\text{new}} = \frac{1}{\Delta t}(\mathbf{q}^{(n+1)} - \mathbf{q}^{(n)})$$
$$\mathbf{v}_{\text{old}} = \frac{1}{\Delta t}(\mathbf{q}^{(n)} - \mathbf{q}^{(n-1)})$$



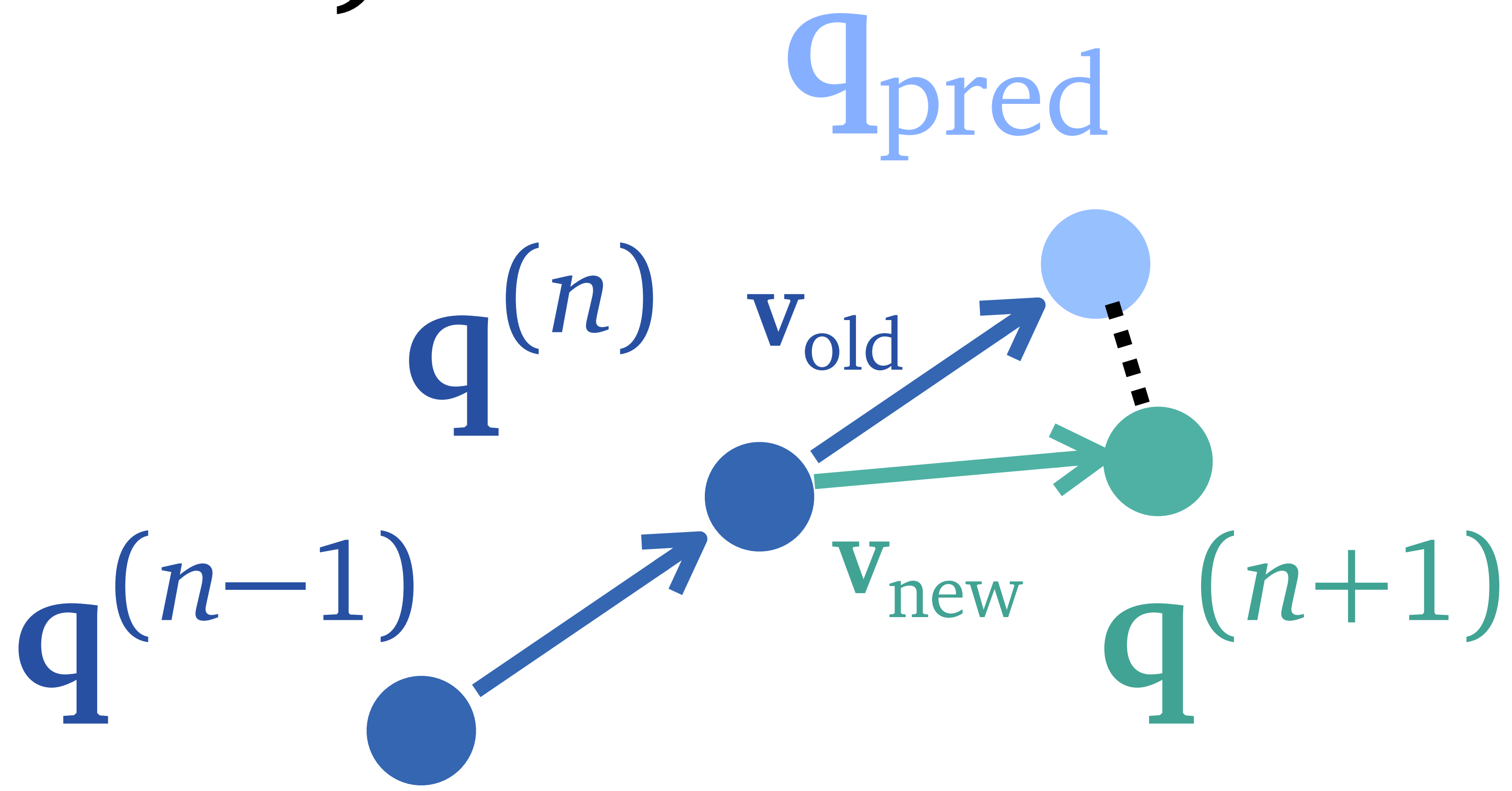
$$\mathbf{v}_{\text{new}} = \underset{\mathbf{v}\in\mathbb{R}^m}{\operatorname{argmin}} \frac{1}{2}|\mathbf{v}-\mathbf{v}_{\text{old}}|^2_{\mathbf{M}} + U(\mathbf{q}^{(n)} + \Delta t\mathbf{v})$$

Minimal incremental potential principle

- Physical system decides its new velocity by

$$\mathbf{v}_{\text{new}} = \operatorname*{argmin}_{\mathbf{v}\in\mathbb{R}^m} \frac{1}{2}|\mathbf{v}-\mathbf{v}_{\text{old}}|^2_{\mathbf{M}} + U(\mathbf{q}^{(n)} + \Delta t\mathbf{v})$$

  - Inertia:
    It doesn't want to be different from the old velocity (deviation measured by the inertia metric)

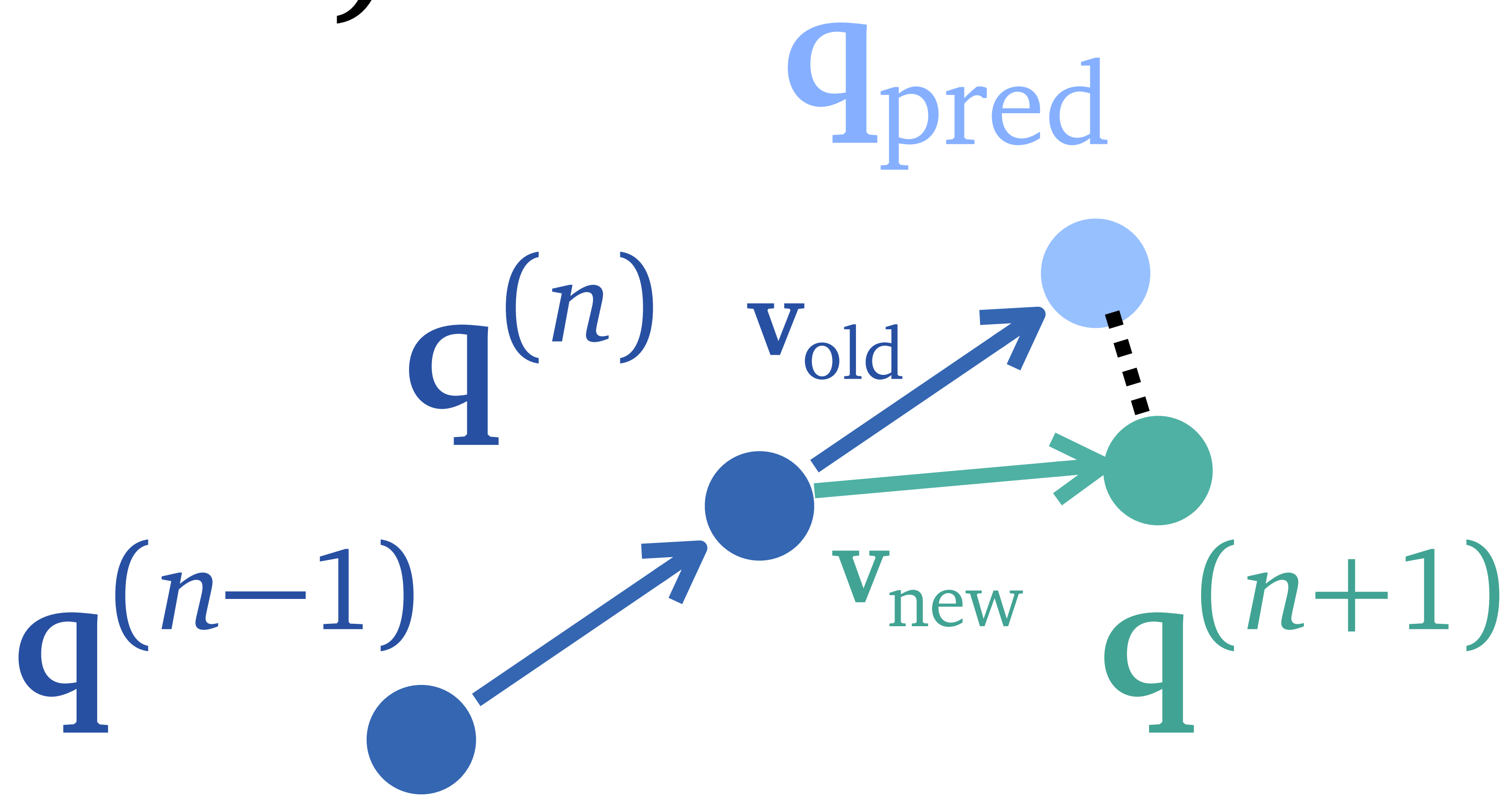


  - The new velocity is also penalized with potential energy of the resulting new position.

Minimal incremental potential principle

- Physical system decides its new velocity by

$$\mathbf{v}_{\text{new}} = \underset{\mathbf{v}\in\mathbb{R}^m}{\text{argmin}}\ \frac{1}{2}|\mathbf{v}-\mathbf{v}_{\text{old}}|^2_{\mathbf{M}} + U(\mathbf{q}^{(n)} + \Delta t\mathbf{v})$$

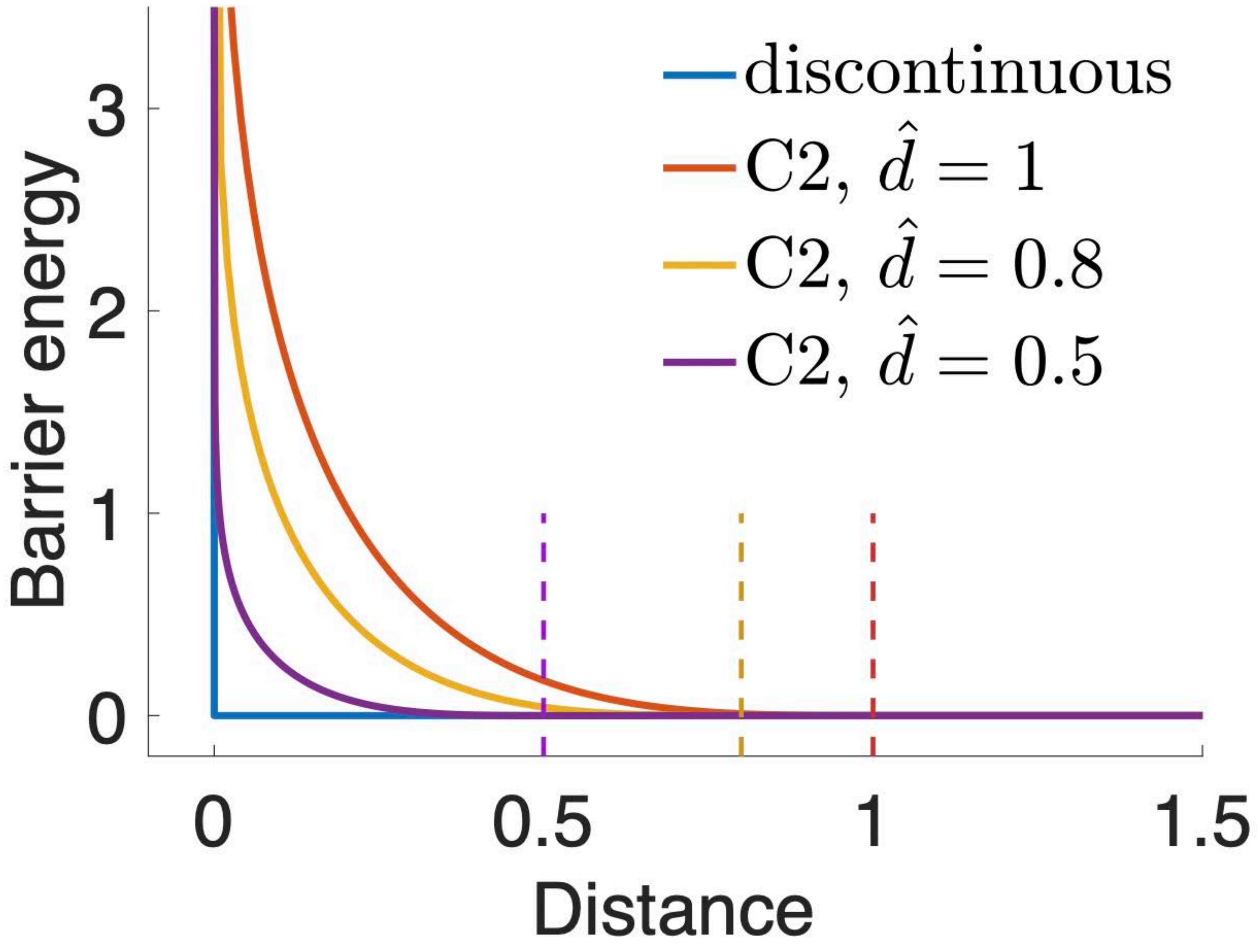


  - Every time step just requires a good numerical optimizer
  - Collision and contact:
    (Incremental potential contact 2020)
    Just build smooth barrier functions in potential and perform optimization properly

Minimal incremental potential principle

- Collision and contact:
  (Incremental potential contact 2020)
  Just build smooth barrier functions in potential and perform optimization properly

$$b(d, \hat{d}) = \begin{cases} -(d-\hat{d})^2 \ln\left(\frac{d}{\hat{d}}\right), & 0 < d < \hat{d} \\ 0 & d \geq \hat{d}. \end{cases}$$



Minimal incremental potential principle

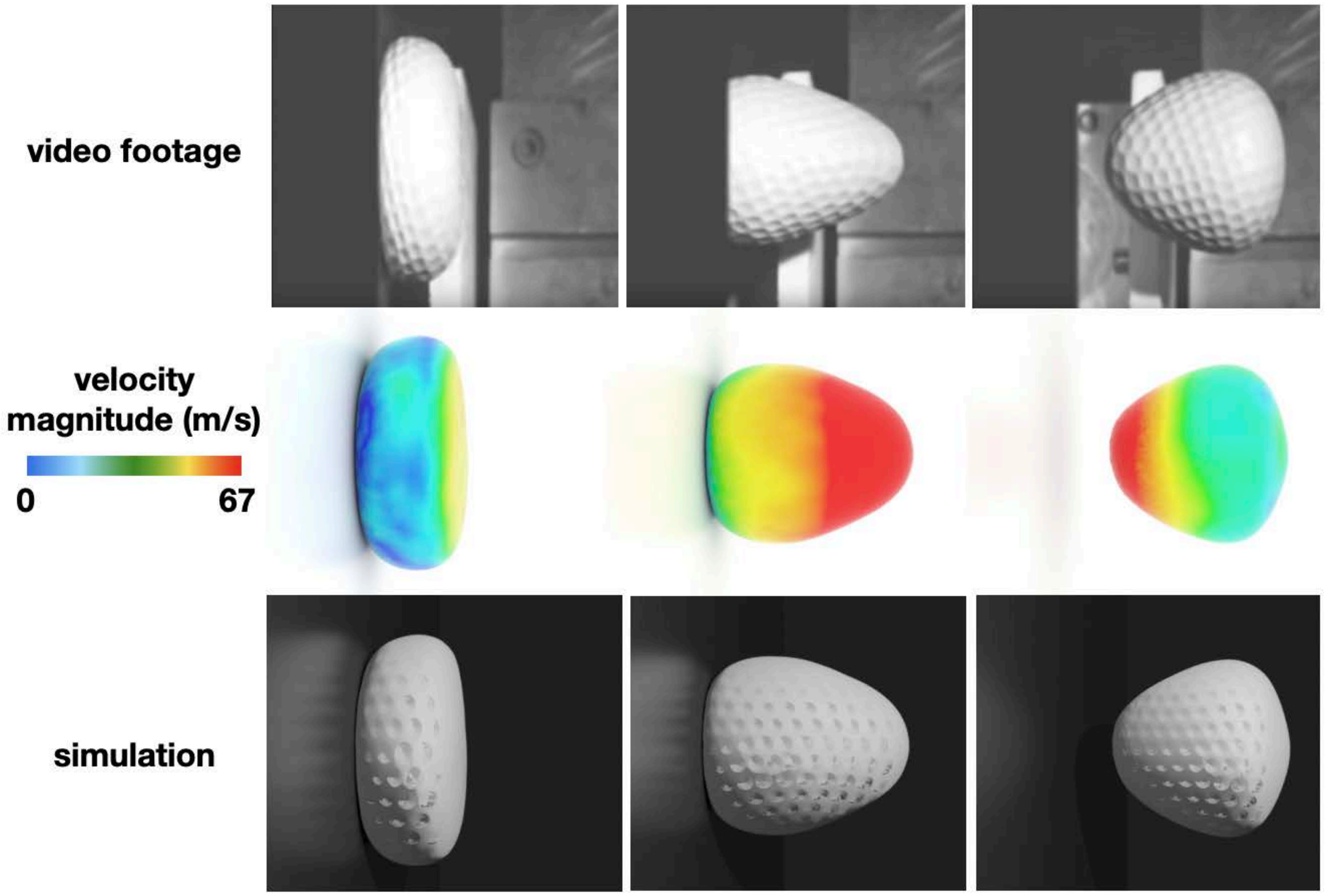


Fig. 19. **High-speed impact test.** Top: we show key frames from a high-speed video capture of a foam practice ball fired at a fixed plate. Matching reported material properties (0.04m diameter, $E = 10^7$Pa, $\nu = 0.45$, $\rho = 1150$kg/m^3) and firing speed ($v_0 = 67$m/s), we apply IPC to simulate the set-up with Newmark time stepping at $h = 2 \times 10^{-5}$s to capture the high-frequency behaviors. Middle and bottom: IPC-simulated frames at times corresponding to the video frames showing respectively, visualization of the simulated velocity magnitudes (middle) and geometry (bottom).

Dissipation in Incremental Variational Formulation

- Dissipative system
- Stability of Euler integrators
- Incremental variational principle
- Adding dissipation
- Higher order method
- Optimization

Dynamical system with dissipation

- Recall the backward Euler update on conservative system is

$$\mathbf{q}^{(n+1)} = \underset{\mathbf{q}\in\mathbb{R}^m}{\operatorname{argmin}} \frac{1}{2\Delta t^2}|\mathbf{q}-\mathbf{q}_{\text{pred}}|^2_{\mathbf{M}} + U(\mathbf{q})$$

$$\mathbf{q}_{\text{pred}} := 2\mathbf{q}^{(n)} - \mathbf{q}^{(n-1)}$$

- Add dissipation by adding a Rayleigh dissipation function

$$\mathbf{q}^{(n+1)} = \underset{\mathbf{q}\in\mathbb{R}^m}{\operatorname{argmin}} \frac{1}{2\Delta t^2}|\mathbf{q}-\mathbf{q}_{\text{pred}}|^2_{\mathbf{M}} + \boxed{U(\mathbf{q}) + \Delta t R(\mathbf{q}^{(n)}, \tfrac{\mathbf{q}-\mathbf{q}^{(k)}}{\Delta t})}$$

effective incremental potential

- Equivalently

$$\mathbf{v}_{\text{new}} = \underset{\mathbf{v}\in\mathbb{R}^m}{\operatorname{argmin}} \frac{1}{2}|\mathbf{v}-\mathbf{v}_{\text{old}}|^2_{\mathbf{M}} + \boxed{U(\mathbf{q}^{(n)} + \Delta t\mathbf{v}) + \Delta t\, R(\mathbf{q}^{(n)}, \mathbf{v})}$$

Dynamical system with dissipation

$$\mathbf{v}_{\text{new}} = \operatorname*{argmin}_{\mathbf{v}\in\mathbb{R}^m} \frac{1}{2}|\mathbf{v} - \mathbf{v}_{\text{old}}|^2_{\mathbf{M}} + U(\mathbf{q}^{(n)} + \Delta t\,\mathbf{v}) + \Delta t\, R(\mathbf{q}^{(n)}, \mathbf{v})$$

- Writing the system in F=ma:

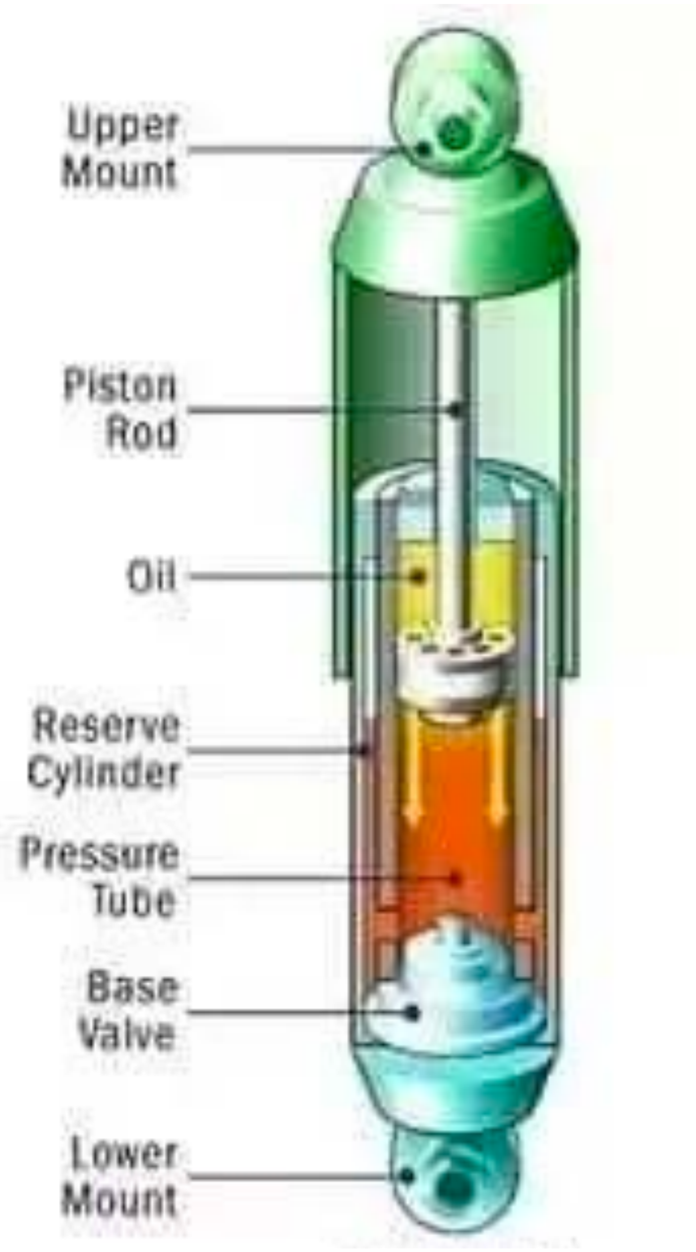
$$\mathbf{M}\frac{\mathbf{v}_{\text{new}} - \mathbf{v}_{\text{old}}}{\Delta t} = -\frac{\partial U}{\partial \mathbf{q}} - \frac{\partial R}{\partial \mathbf{v}}$$

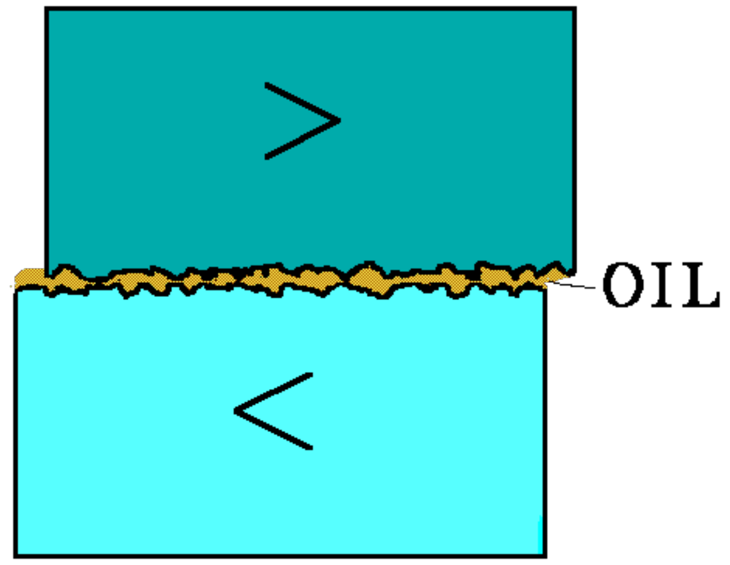
Dynamical system with dissipation

$$\mathbf{M}\frac{\mathbf{v}_{\text{new}} - \mathbf{v}_{\text{old}}}{\Delta t} = -\frac{\partial U}{\partial \mathbf{q}} - \frac{\partial R}{\partial \mathbf{v}}$$

- Example: Quadratic dissipation (lubricated friction, viscosity)

$$R(\mathbf{v}) = \frac{1}{2}\mathbf{v}^{\intercal}\mathbf{B}\mathbf{v}$$





Quasi-static system

- To study dissipative system, we often consider a quasi static regime
- Quasi-static: inertia is negligible.

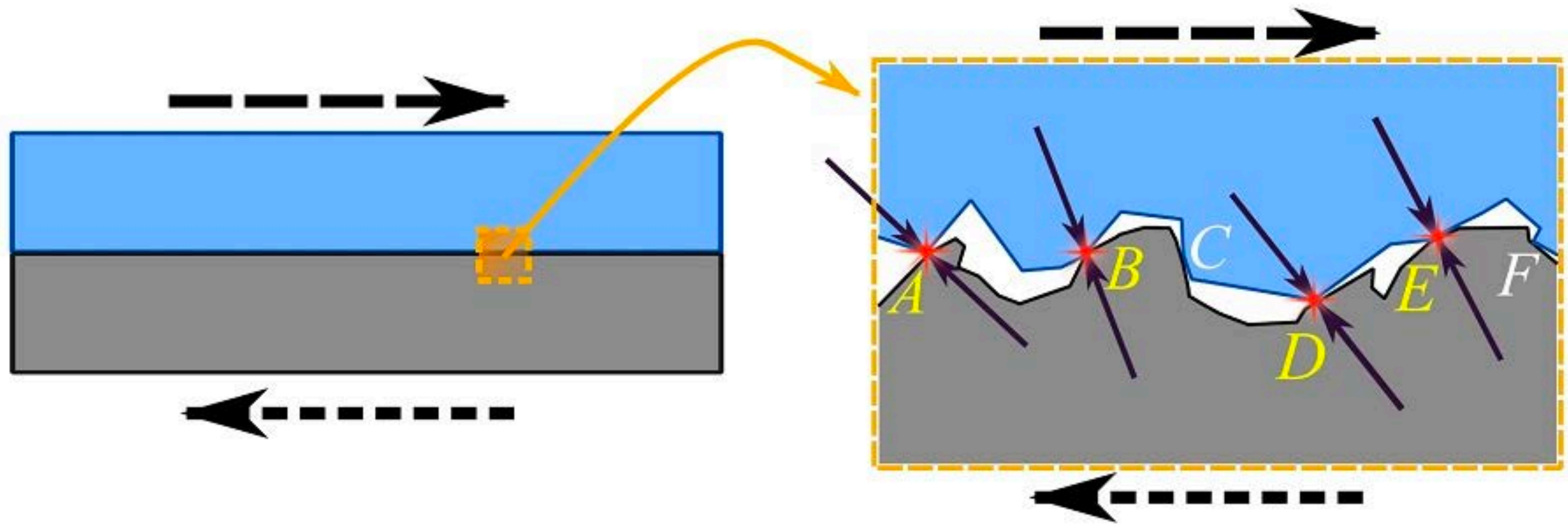
$$\mathbf{M}\frac{\mathbf{v}_{\text{new}} - \mathbf{v}_{\text{old}}}{\Delta t} = -\frac{\partial U}{\partial \mathbf{q}} - \frac{\partial R}{\partial \mathbf{v}}$$

- Dissipative force is in balance with potential force and external force:

$$\frac{\partial R}{\partial \mathbf{v}} = -\frac{\partial U}{\partial \mathbf{q}} + \mathbf{f}_{\text{ext}}$$

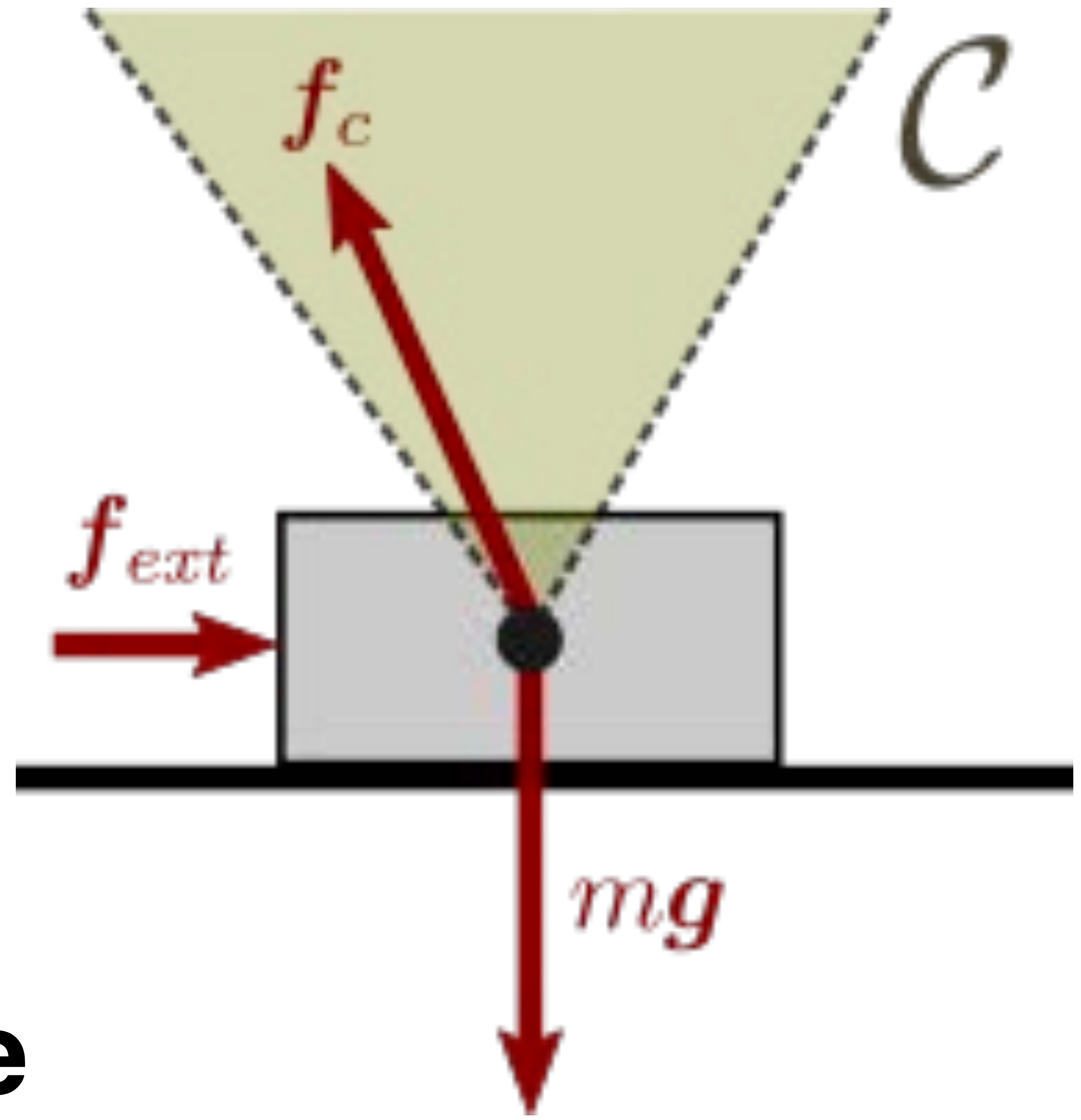
- For quadratic R, this determines a terminal velocity.
- Traditional way of studying general force: relation between **f**,**q**,**v**
- (Ir)reversible process: **f**_ext is (not) a function of **q**

Dry friction



Dry friction

- Law of friction:
  - **Amonton's 1st law:** Friction force is proportional to the normal force
  - **Amonton's 2nd law:** Friction force is independent of contact area
  - **Coulomb's law:** Once the motion starts, the friction force is independent of the sliding speed



- The force $\mathbf{f}_c$ at contact lies in a **friction cone** (in the dual space at contact)

Dry friction

- At each point of contact, we have an outward normal (covector) $\mathbf{n}$
- The relative velocity between contact should satisfy

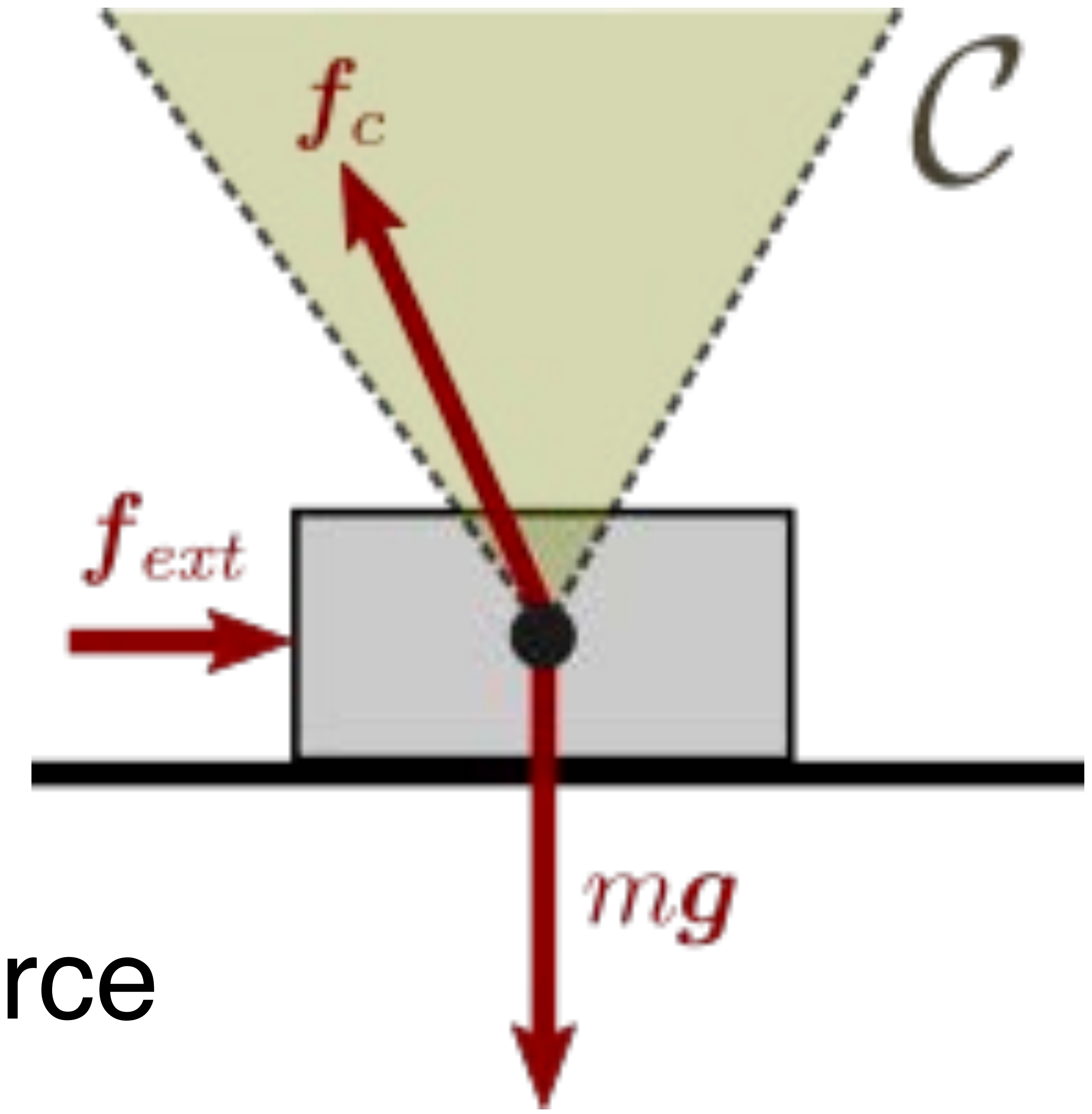
$$\langle \mathbf{n} | \mathbf{v} \rangle \geq 0$$

- The normal and tangential part of the contact force, and tangent velocity:

$$|\mathbf{f}^{\parallel}| \leq \mu \mathbf{f}^{\perp} \qquad |\mathbf{f}^{\parallel}| < \mu \mathbf{f}^{\perp} \Leftrightarrow \mathbf{v}^{\parallel} = 0$$

- When tangent velocity is nonzero, tangent force is in the same direction with it

$$\alpha \mathbf{f}^{\parallel} = \flat_{\mathbb{R}^3} \mathbf{v},\ \alpha \geq 0$$



Classical approach for contact

- Establish the points $\mathbf{p}_i$ of contact

parameters for motion $\qquad\qquad\qquad\qquad$ space of contact

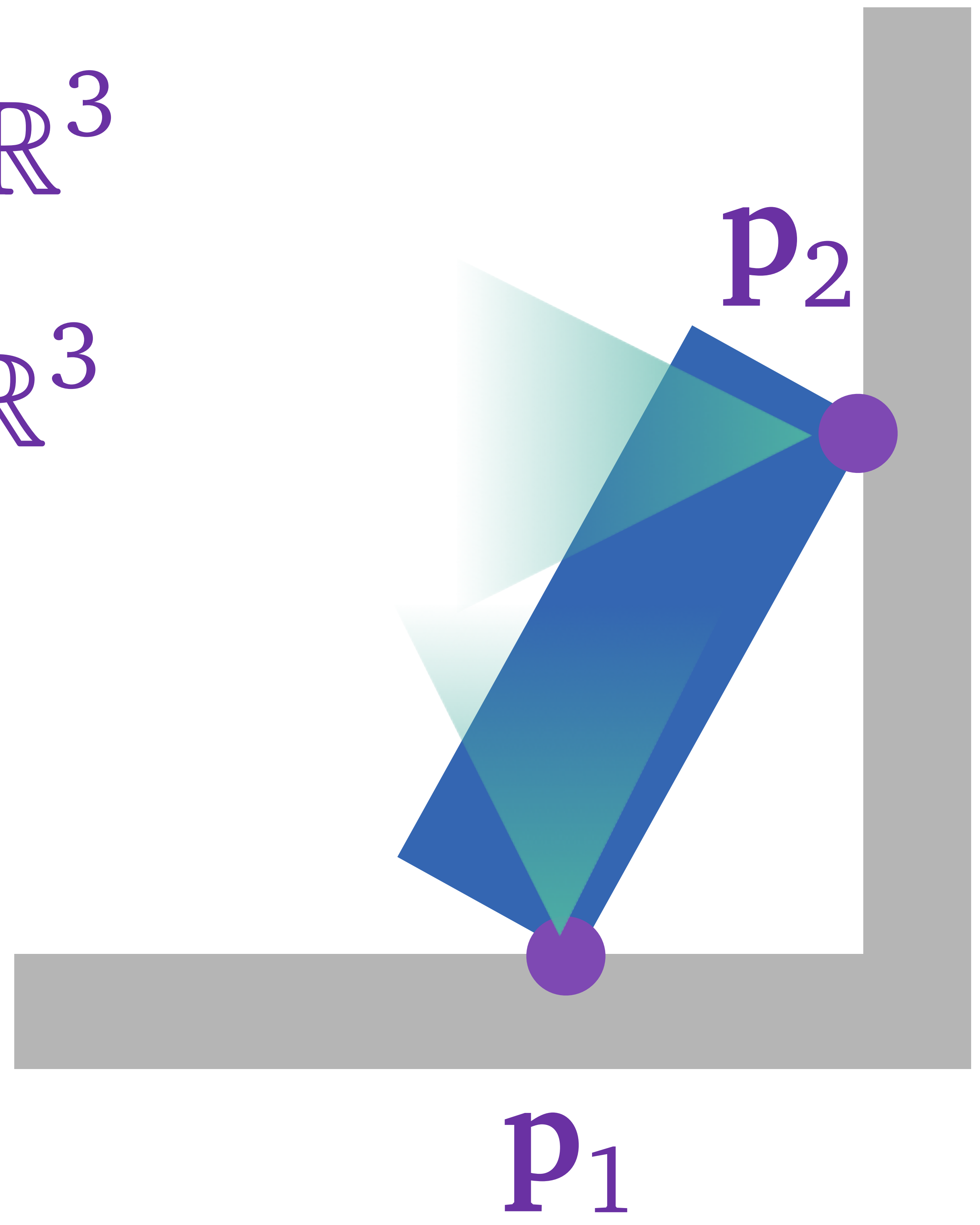
$$(\mathbf{c}, \mathbf{R}) \in Q \xrightarrow{\phi} (\mathbf{p}_1, \cdots, \mathbf{p}_k) \in \mathbb{R}^3 \times \cdots \times \mathbb{R}^3$$

$$(\dot{\mathbf{c}}, \dot{\mathbf{R}}) \in T_{(\mathbf{c},\mathbf{R})}Q \xrightarrow[d\phi]{} (\dot{\mathbf{p}}_1, \cdots, \dot{\mathbf{p}}_k) \in \mathbb{R}^3 \times \cdots \times \mathbb{R}^3$$

$$(\ddot{\mathbf{c}}, \ddot{\mathbf{R}}) \in T_{(\mathbf{c},\mathbf{R})}Q$$

$$\mathbf{M}^{-1} \uparrow$$

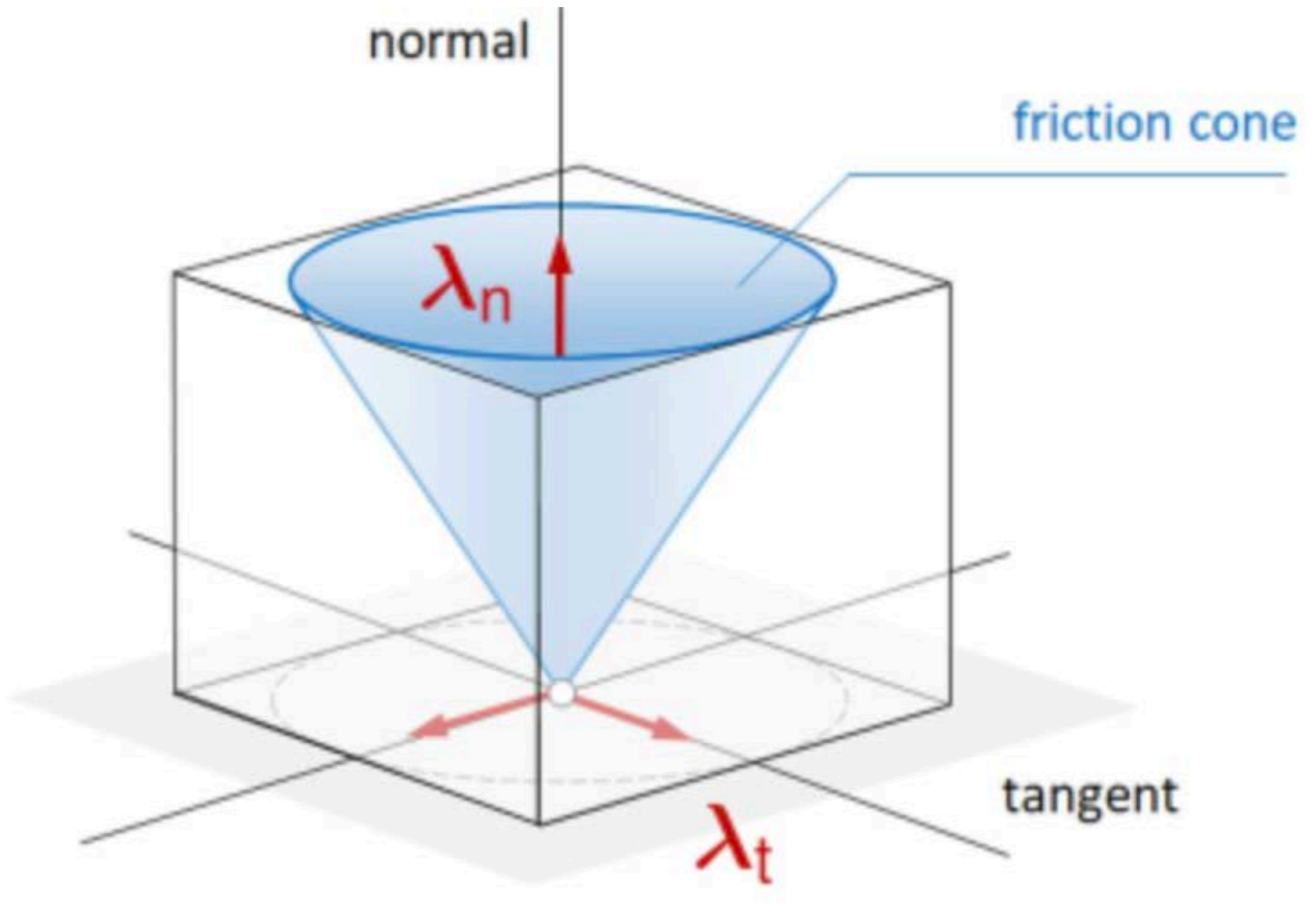
$$T^*_{(\mathbf{c},\mathbf{R})}Q \xleftarrow{d\phi^*} (\mathbf{f}_1, \ldots, \mathbf{f}_k) \in \mathcal{C}_1 \times \cdots \times \mathcal{C}_k \subset \mathbb{R}^{3*} \times \cdots \mathbb{R}^{3*}$$



- Solve for velocity and contact force together so that all contact conditions are satisfied.

Dry friction

- Siggraph 2022 course on contact and friction
  https://siggraphcontact.github.io/



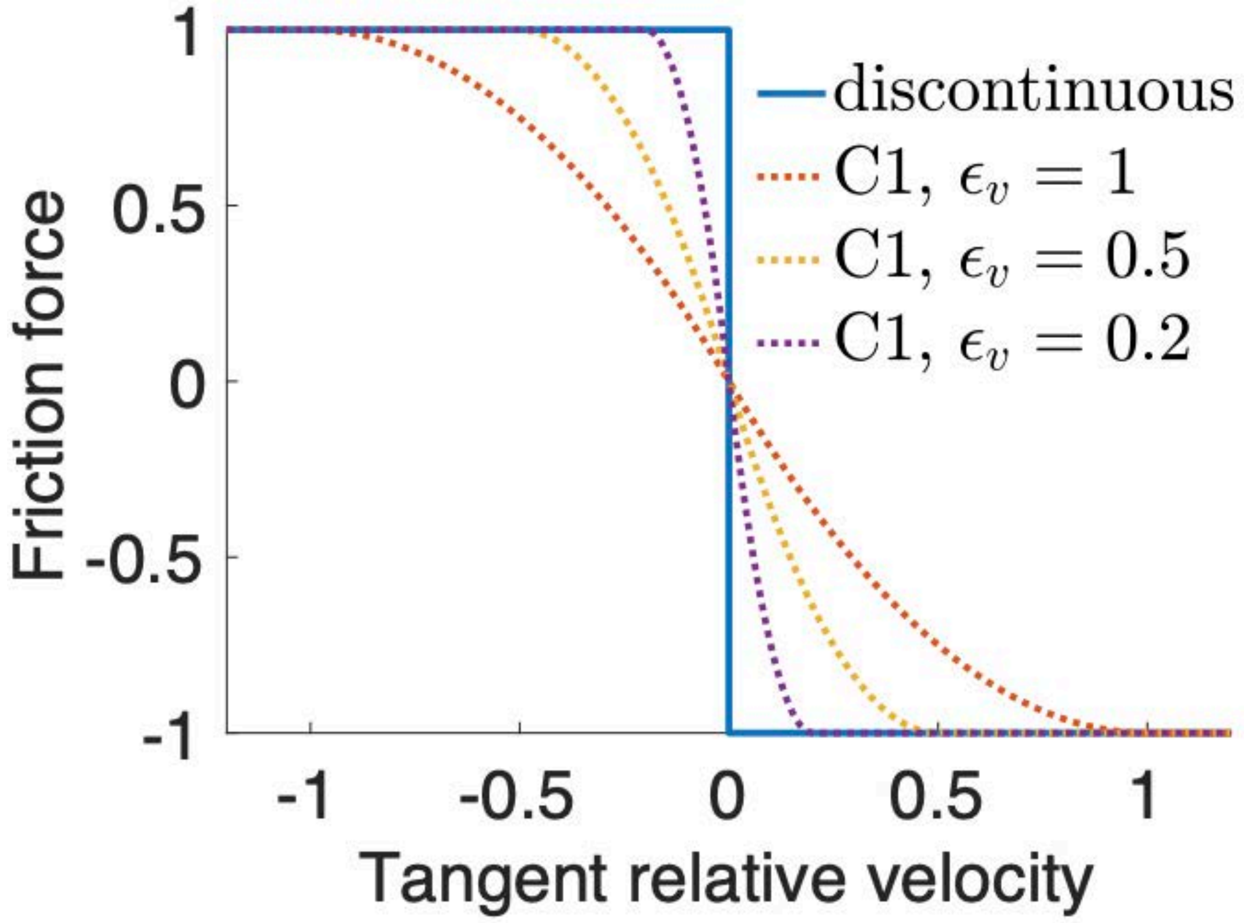
Dissipation function for dry friction

- Variational approach to dry friction

$$\mathbf{M}\frac{\mathbf{v}_{\text{new}} - \mathbf{v}_{\text{old}}}{\Delta t} = -\frac{\partial U}{\partial \mathbf{q}} - \frac{\partial R}{\partial \mathbf{v}}$$

$$R(\mathbf{v}) = \mu|\mathbf{v}|$$

- In incremental potential contact paper, it is also smoothed out



Higher Order Method

- Dissipative system
- Stability of Euler integrators
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Newmark algorithm

- Recall backward Euler method is equivalent to

$$\mathbf{q}^{(n+1)} = \underset{\mathbf{q} \in \mathbb{R}^m}{\operatorname{argmin}} \frac{1}{2\Delta t^2} |\mathbf{q} - \mathbf{q}_{\text{pred}}|^2_{\mathbf{M}} + U(\mathbf{q}) + \Delta t R(\mathbf{q}^{(n)}, \frac{\mathbf{q} - \mathbf{q}^{(k)}}{\Delta t})$$

where $\mathbf{q}_{\text{pred}} := 2\mathbf{q}^{(n)} - \mathbf{q}^{(n-1)}$

- Make a better prediction using acceleration information
- Source: Kane, Marsden, Ortiz, West 1999 "Variational Integrators and Newmark Algorithm for Conservative and Dissipative Systems."

Newmark algorithm

- Let incremental potential be

$$\tilde{U}^{(n)}(\mathbf{q}^{(n+1)}) = U(\mathbf{q}^{(n+1)}) + \Delta t\, R((1-s)\mathbf{q}^{(n)} + s\mathbf{q}^{(n+1)}, \frac{\mathbf{q}^{(n+1)} - \mathbf{q}^{n}}{\Delta t})$$

- The acceleration at current time can be read off from

$$\mathbf{a}^{(n)} = \mathbf{M}^{-1} \frac{\partial \tilde{U}^{(n-1)}(\mathbf{q}^{(n)})}{\partial \mathbf{q}^{(n)}}$$

- Velocity can be kept track of by

$$\mathbf{v}^{(n)} = \mathbf{v}^{(n-1)} + \Delta t \left((1-\gamma)\mathbf{a}^{(n-1)} + \gamma \mathbf{a}^{(n)} \right)$$

- The prediction of next time step

$$\mathbf{q}_{\text{pred}}^{(n+1)} := \mathbf{q}^{(n)} + \Delta t\, \mathbf{v}^{(n)} + \frac{\Delta t^2}{2}(1-2\beta)\mathbf{a}^{(n)}$$

- Solve $\mathbf{q}^{(n+1)} = \underset{\mathbf{q} \in \mathbb{R}^m}{\operatorname{argmin}} \frac{1}{2\Delta t^2} |\mathbf{q} - \mathbf{q}_{\text{pred}}|_{\mathbf{M}}^2 + \beta \tilde{U}^{(n)}(\mathbf{q})$

Numerical Optimization

- Dissipative system
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- Optimization

Optimization problem

- Using smooth barrier and dissipation function, every time step boils down to one unconstrained optimization problem

$$\underset{\mathbf{x}\in\mathbb{R}^m}{\text{minimize}}\ \mathcal{L}(\mathbf{x})$$

- Here $\mathbf{x}$ may be velocity or position

$$\mathbf{q}^{(n+1)} = \underset{\mathbf{q}\in\mathbb{R}^m}{\operatorname{argmin}}\ \frac{1}{2\Delta t^2}|\mathbf{q}-\mathbf{q}_{\text{pred}}|^2_{\mathbf{M}} + U(\mathbf{q})$$

$$\mathbf{v}_{\text{new}} = \underset{\mathbf{v}\in\mathbb{R}^m}{\operatorname{argmin}}\ \frac{1}{2}|\mathbf{v}-\mathbf{v}_{\text{old}}|^2_{\mathbf{M}} + U(\mathbf{q}^{(n)}+\Delta t\mathbf{v})$$

- Note that the initial guess (from the state of previous time frame) for optimization is usually very close to the optimizer.

Optimization problem

- Using smooth barrier and dissipation function, every time step boils down to one unconstrained optimization problem

$$\underset{\mathbf{x}\in\mathbb{R}^m}{\text{minimize}}\ \mathcal{L}(\mathbf{x})$$

- Use gradient descent using some metric $\flat = \mathbf{H}$

$$\mathbf{x}^{(n+1)} \leftarrow \mathbf{x}^{(n)} - \alpha\sharp(d\mathcal{L})_{\mathbf{x}^{(n)}} = \mathbf{x}^{(n)} - \alpha\mathbf{H}^{-1}\begin{bmatrix}\partial\mathcal{L}/\partial x_1 \\ \vdots \\ \partial\mathcal{L}/\partial x_m\end{bmatrix}$$

- We have to choose a good $\mathbf{H}$ and step size $\alpha > 0$

Optimization problem

$$\mathbf{x}^{(n+1)} \leftarrow \mathbf{x}^{(n)} - \alpha \sharp (d\mathcal{L})_{\mathbf{x}^{(n)}} = \mathbf{x}^{(n)} - \alpha \mathbf{H}^{-1} \begin{bmatrix} \partial \mathcal{L} / \partial x_1 \\ \vdots \\ \partial \mathcal{L} / \partial x_m \end{bmatrix}$$

- Classic gradient descent $\mathbf{H} = \mathbf{I}$
- Newton's method $\mathbf{H} = \mathrm{Hess}\,\mathcal{L}$
- Quasi-Newton's method (approximated Hessian)

Line search

$$\mathbf{x}^{(n+1)} \leftarrow \mathbf{x}^{(n)} - \alpha \sharp (d\mathcal{L})_{\mathbf{x}^{(n)}} = \mathbf{x}^{(n)} - \alpha \mathbf{H}^{-1} \begin{bmatrix} \partial \mathcal{L} / \partial x_1 \\ \vdots \\ \partial \mathcal{L} / \partial x_m \end{bmatrix}$$

- Use line search for choosing α
- Call $\mathbf{p} = \mathbf{H}^{-1} d\mathcal{L}$; backtracking line search:

Algorithm [edit]

This condition is from Armijo (1966). Starting with a maximum candidate step size value $\alpha_0 > 0$, using search control parameters $\tau \in (0,1)$ and $c \in (0,1)$, the backtracking line search algorithm can be expressed as follows:

1. Set $t = -c\,m$ and iteration counter $j = 0$.
2. Until the condition is satisfied that $f(\mathbf{x}) - f(\mathbf{x} + \alpha_j\,\mathbf{p}) \geq \alpha_j\,t$, repeatedly increment j and set $\alpha_j = \tau\,\alpha_{j-1}$.
3. Return α_j as the solution.

- Also make sure that this stepping doesn't pass through a barrier