

Can we *really* predict the future?

BASIC IDEA

We give you the initial positions, velocities, and the interactions.

You predict everything! Really Everything?

PHILOSOPHICAL PROBLEMS

Is there free will?

Is there more than we can detect?

Emergence: some laws can only be discovered with 10^{23} particles.

PRACTICAL PROBLEMS

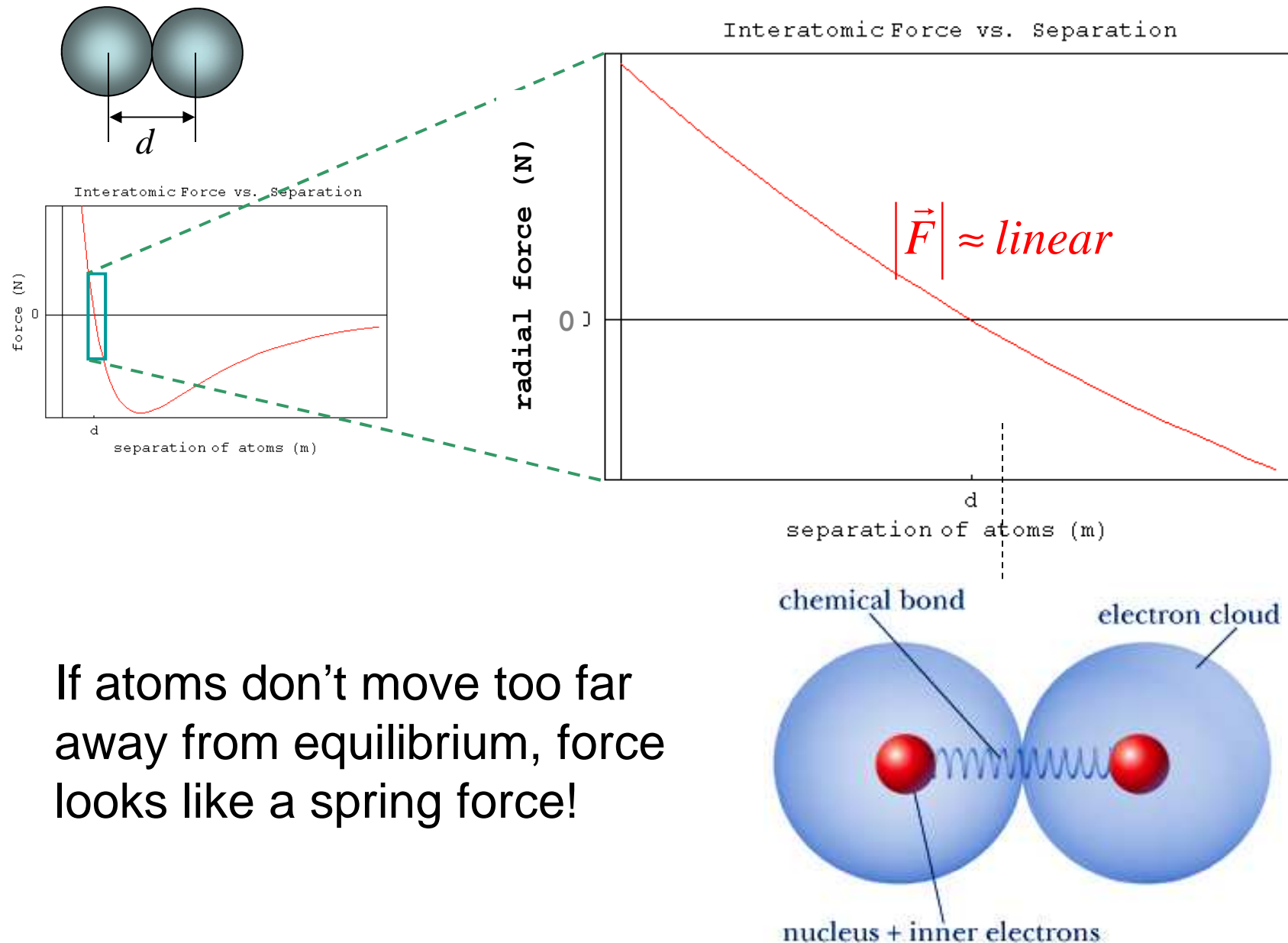
More than 10^{23} particles in a glass of water. Can't measure them all.

Sensitivity to initial conditions (chaos)

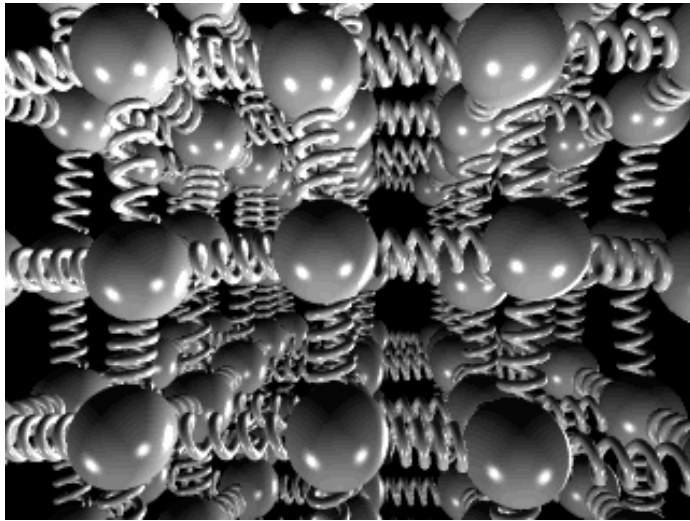
Quantum mechanics: *Probabilities* determine outcomes

Quantum mechanics: Heisenberg uncertainty principle

Model of solid: chemical bonds



A ball-spring model of a solid



Ball-spring model of a solid

To model need to know:

- spring length s
- spring stiffness
- mass of an atom

PERIODIC TABLE OF THE ELEMENTS

1																17		18	
1 H 1.008	2											13	14	15	16	1 H 1.008	2 He 4.003		
3 Li 6.941	4 Be 9.012	← Transition Metals →												5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
11 Na 22.99	12 Mg 24.30	3	4	5	6	7	8	9	10	11	12	13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95		
19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.87	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.61	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80		
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (97.91)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3		
55 Cs 132.9	56 Ba 137.3	71 Lu 175.0	72 Hf 178.5	73 Ta 180.9	74 W 183.8	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (209.0)	85 At (210.0)	86 Rn (222.0)		
87 Fr (223.0)	88 Ra (226.0)	103 Lr (262.1)	104 Rf (261.1)	105 Db (262.1)	106 Sg (263.1)	107 Bh (264.1)	108 Hs (265.1)	109 Mt (266.1)	110 (269.1)	111 (272.1)	112 (277.1)								

Lanthanides

57 La 138.9	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (144.9)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.2	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0
89 Ac (227.0)	90 Th 232.0	91 Pa 231.0	92 U 238.0	93 Np (237.0)	94 Pu (244.1)	95 Am (243.1)	96 Cm (247.1)	97 Bk (247.1)	98 Cf (251.1)	99 Es (252.1)	100 Fm (257.1)	101 Md (258.1)	102 No (259.1)

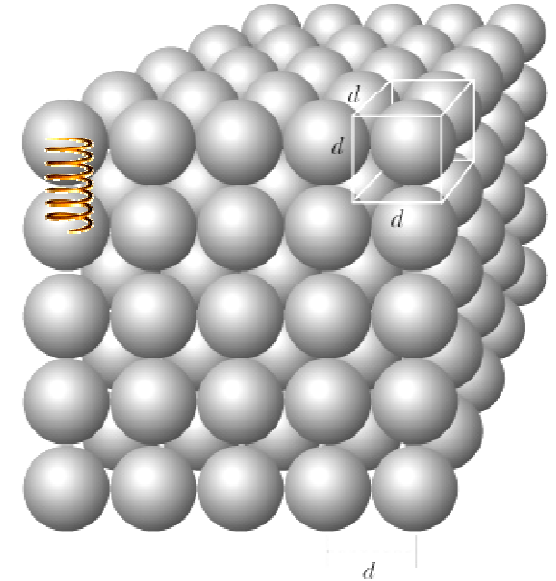
Actinides

Length of a bond: diameter of copper atom

	10	11	12
	28 Ni	29 Cu	30 Zn
	58.69	63.55	65.39
	46 Pd	47 Ag	48 Cd
	106.4	107.9	112.4

density $\rho = 8.94 \text{ g/cm}^3$:
molecular weight = 63.55 g/mole

N_A molecules



1. Number of atoms in one cm^3

$$N = \frac{8.94 \text{ g/cm}^3}{63.55 \text{ g/mole}} \cdot 6.022 \times 10^{23} \frac{\text{atoms}}{\text{mole}} = 8.47 \times 10^{22} \frac{\text{atoms}}{\text{cm}^3}$$

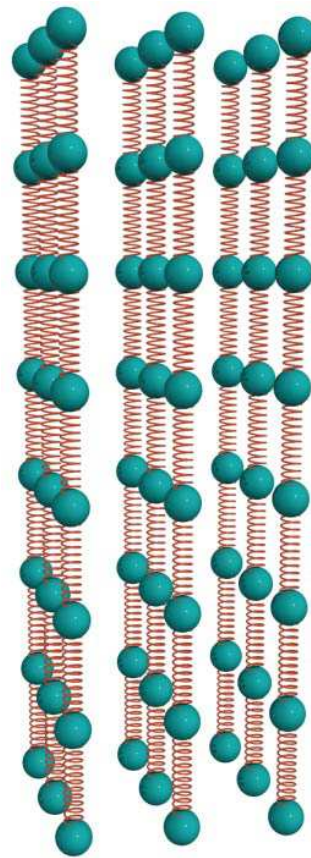
2. Volume per one atom:

$$V_{Cu} = \frac{1}{8.47 \times 10^{22} \text{ atoms/cm}^3} = 1.18 \times 10^{-23} \frac{\text{cm}^3}{\text{atom}}$$

3. Bond length:

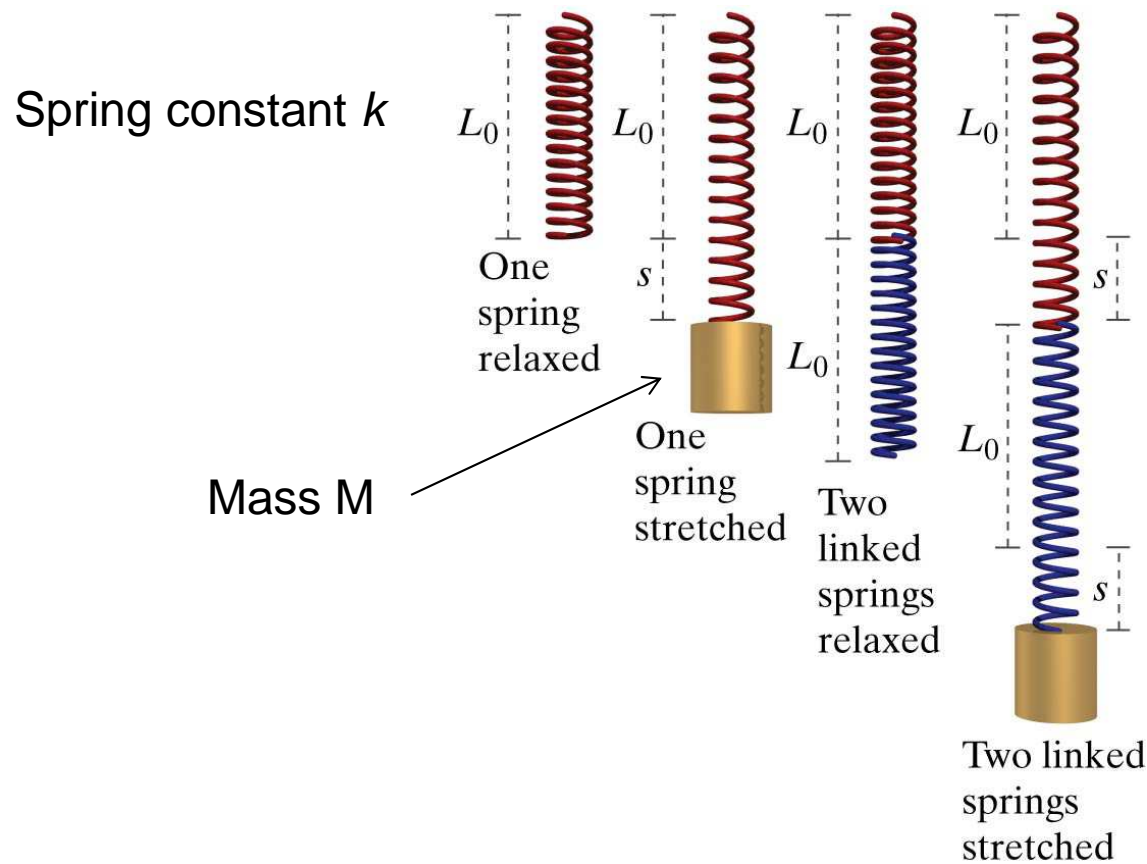
$$d_{Cu} = \sqrt[3]{1.18 \times 10^{-23} \text{ cm}^3} = 2.27 \times 10^{-8} \text{ cm} = 2.27 \times 10^{-10} \text{ m} = 2.27 \text{ \AA}$$

Ball-Spring Model of a Wire



How is the stiffness of the wire related to the stiffness of one of the short 7 springs (bonds)?

Two Springs in Series



Each spring must supply an upward force equal to Mg , thus, each stretches by s giving a total stretch of $2s$, or an effective spring constant of $k/2$.

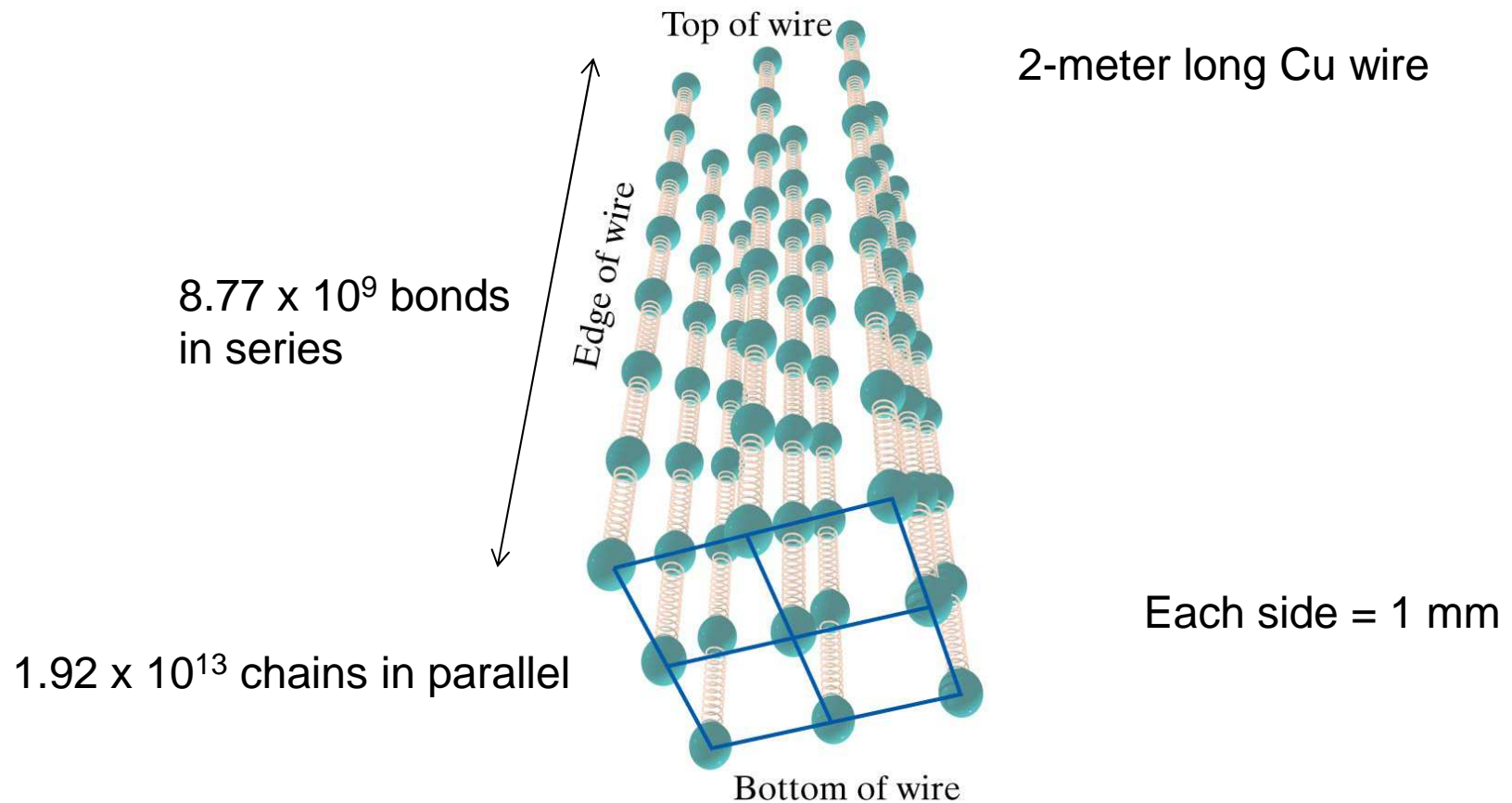
Two Springs in Parallel



Mass M

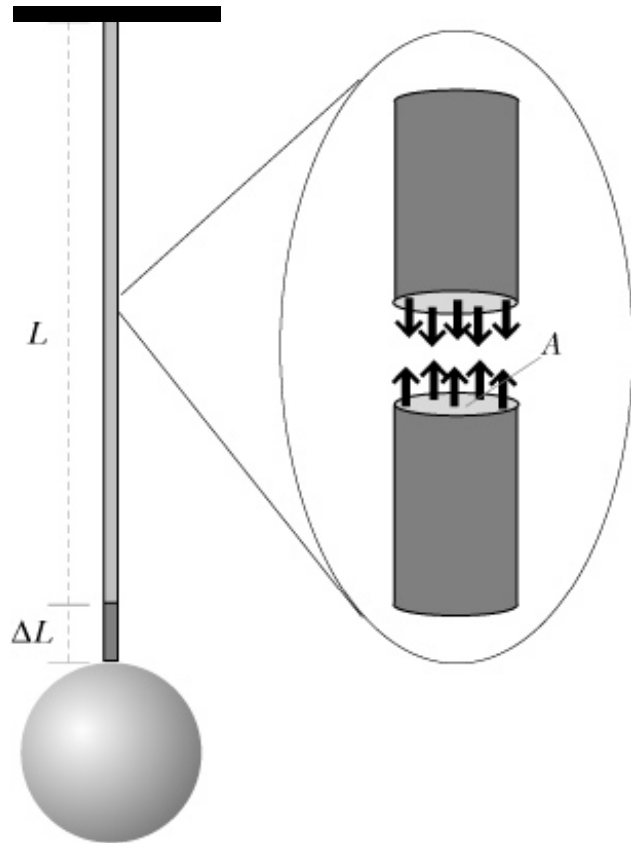
Each spring provides an upward force of $Mg/2$, so each stretches $s/2$, giving an effective spring constant of $2k$. 9

Stiffness of a Copper Wire



The stiffness of the wire is much greater than the effective spring stiffness between atoms due to the much greater number of chains in parallel than bonds in series.

Estimating interatomic “spring” stiffness



$$\text{strain} = \frac{\Delta L}{L}$$

$$\text{stress} = \frac{F_T}{A}$$

← tension

$$\text{stress} = Y \cdot \text{strain}$$

$$\frac{F_T}{A} = Y \frac{\Delta L}{L}$$

Y - Young's modulus
depends only on material



Thomas Young (1773-1829)

Compare:

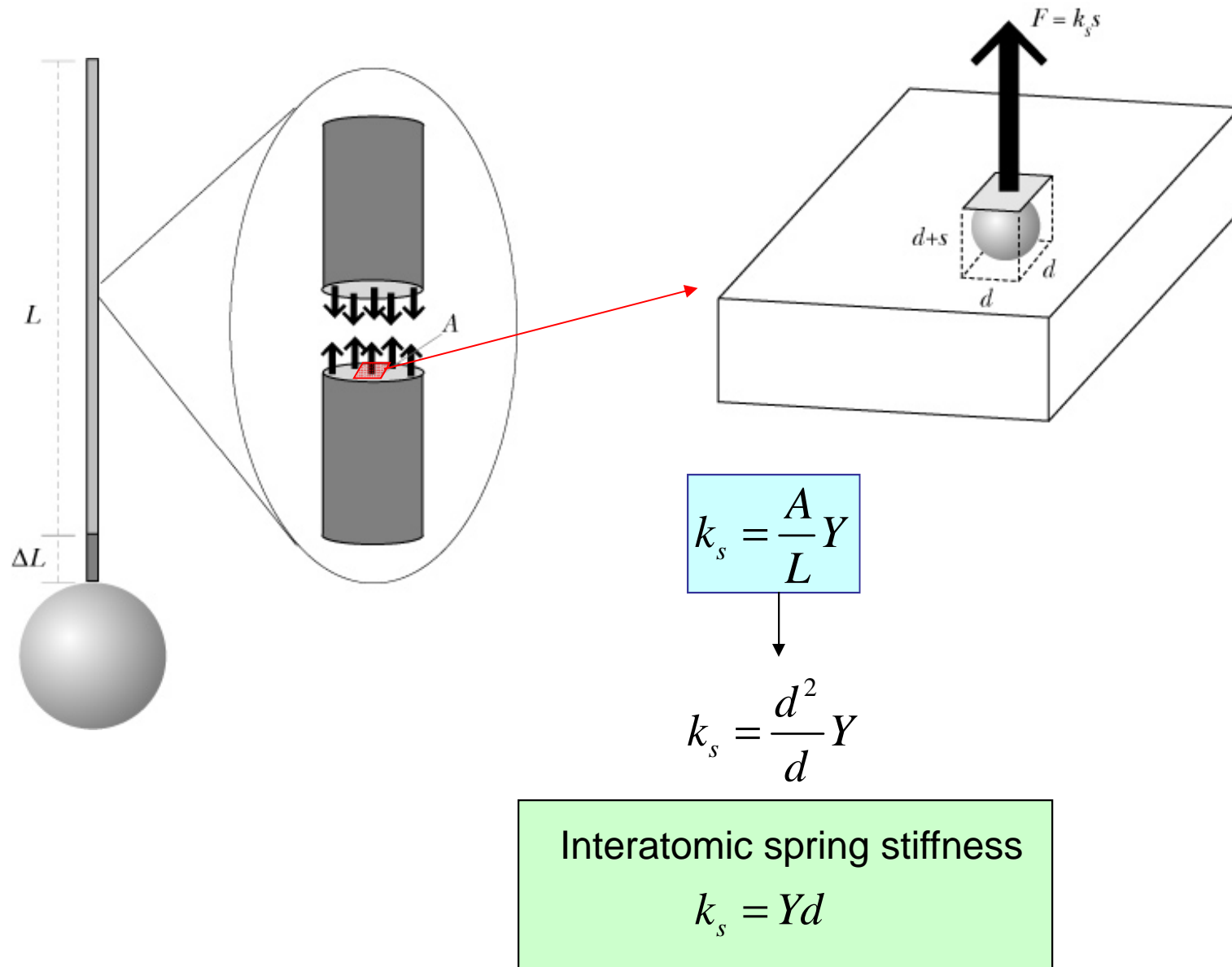
$$|\vec{F}_{spring}| = k_s |s|$$

$$\frac{|\vec{F}_{spring}|}{A} A = k_s \frac{|s|}{L} L$$

$$\frac{|\vec{F}_{spring}|}{A} = \frac{L}{A} k_s \frac{|s|}{L}$$

$$k_s = \frac{A}{L} Y$$

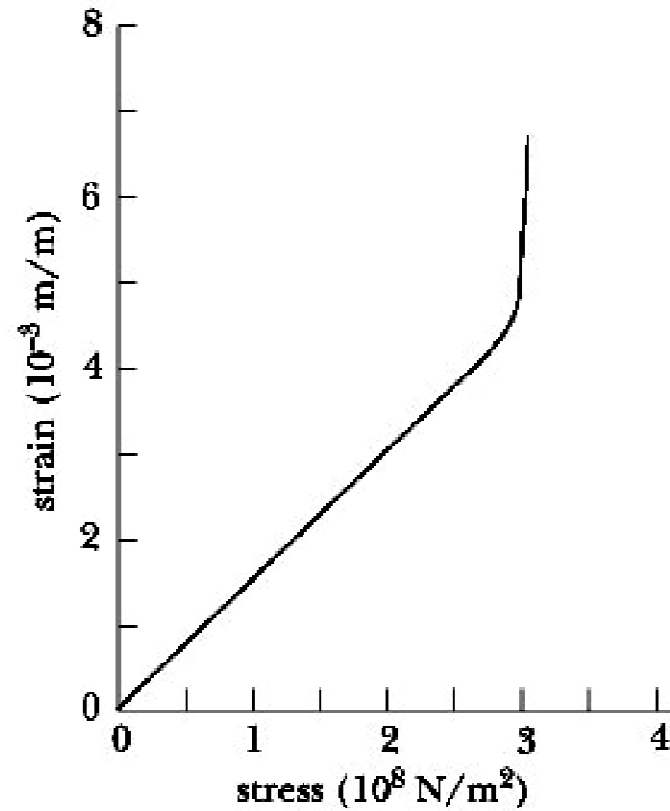
Effective interatomic spring stiffness



Limits of applicability of Young's modulus

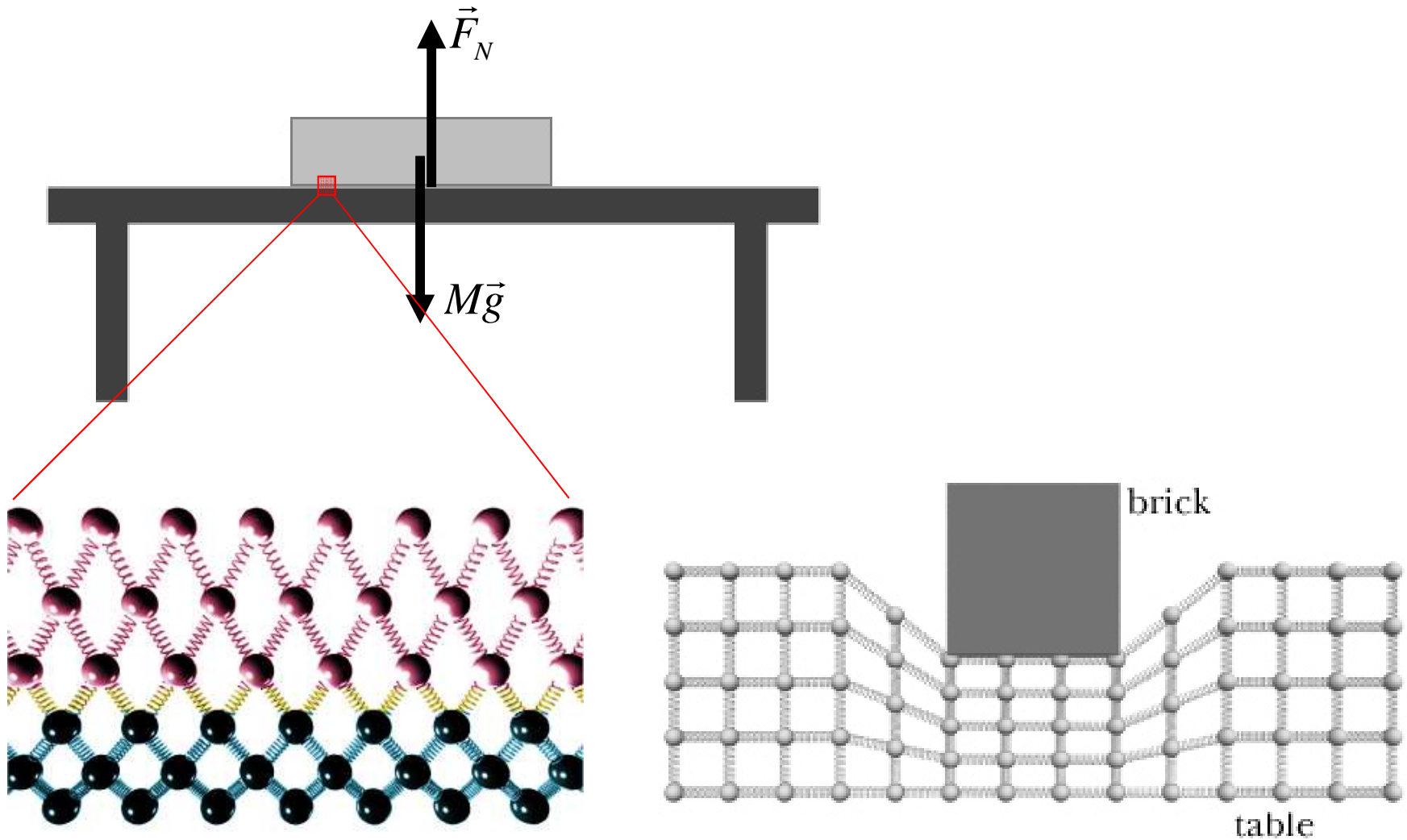
$$\text{stress} = Y \cdot \text{strain}$$

$$\frac{F_T}{A} = Y \frac{\Delta L}{L}$$

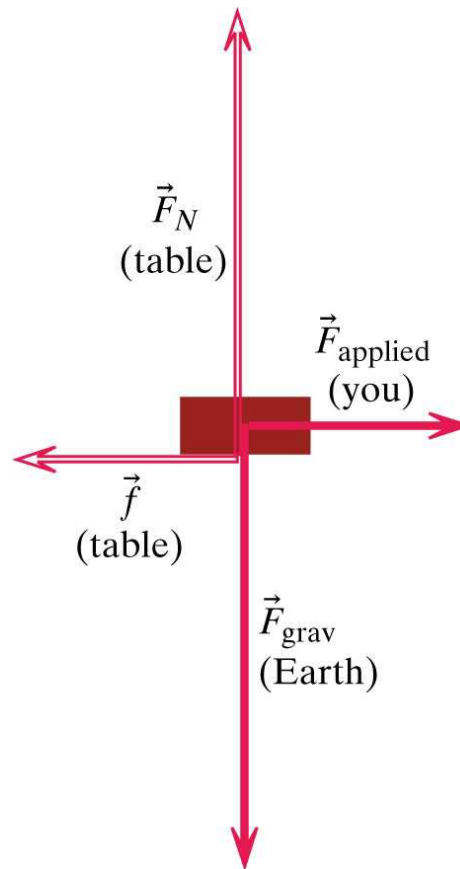


Aluminum alloy

Brick on a table: compression



Friction

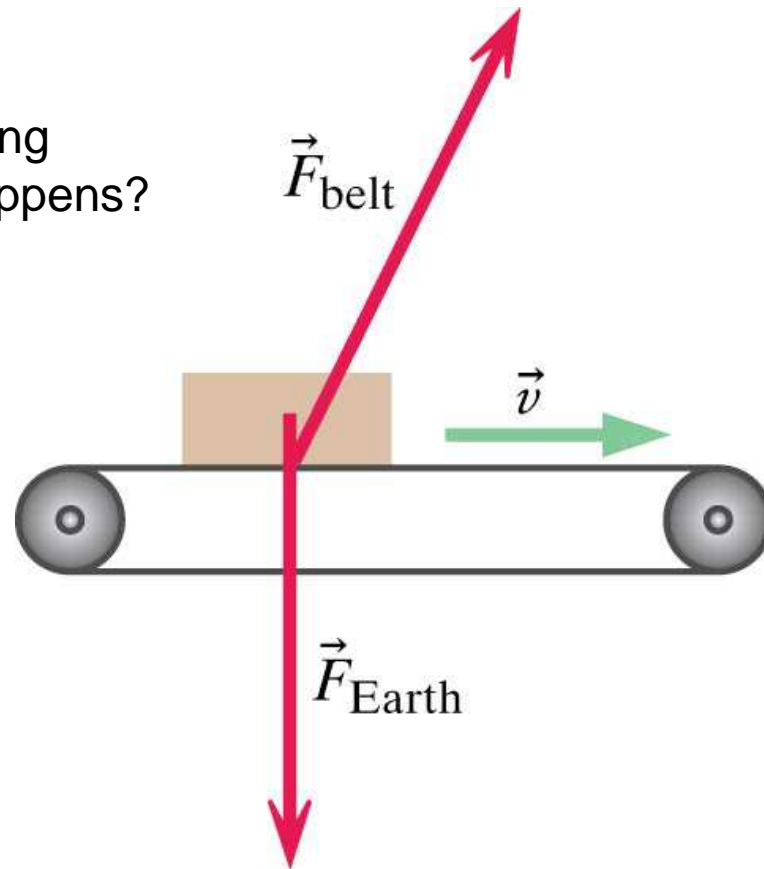


Exert a force so that the brick moves to the right at a constant speed.

What is the net force on the brick?

Friction Doesn't Always Oppose Motion

Box dropped onto moving conveyor belt. What happens?



How is it that a sprinter can accelerate?

Static Friction

- What happens when $F_{\text{applied}} < \mu_k F_N$?
- Block does not move due to static friction
- In general:

$$\mu_k \leq \mu_s$$