Group Assignment 1

Computational Techniques for Molecular Modeling 2020-2021

CdF - 03/2021

Reading Assignment

- *Ryckaert, Ciccotti, Berendsen, Numerical integration of the Cartesian Equations of Motion of a System with Constraints: Molecular Dynamics of n-Alkanes, 1977*
- *HANS C. ANDERSEN, Rattle: A “Velocity Version” of the Shake Algorithm for Molecular Dynamics Calculations, 1983*
- *Ciccotti, Ryckaert, MOLECULAR DYNAMICS SIMULATION OF RIGID MOLECULES, 1986*
- Hairer, Lubich, Wanner, *Geometric Numerical Integration : Structure-Preserving Algorithms for Ordinary Differential Equations, (Springer, 2006)*
    - *Sections I.1, VI.1, VI.2, VI.3, VII.1*

Groups

- *Group 1*
  - *Manfred Nesti MATE*
  - *Luca Caivano MATE*
  - *A. Pegurri CHEM*
  - *C. Vitale CHEM*
  - *V. Paiola CHEM*
  - *A. Della Libera CHEM*
  - *B. Ursino MATE*
- *Group 2*
  - *M. Gabriel MATE*
  - *E. Capuano MATE*
  - *A. Pirozzi MATE*
  - *S. Pertesana CHEM*
  - *C. Canciani CHEM*
  - *F. Russo CHEM*

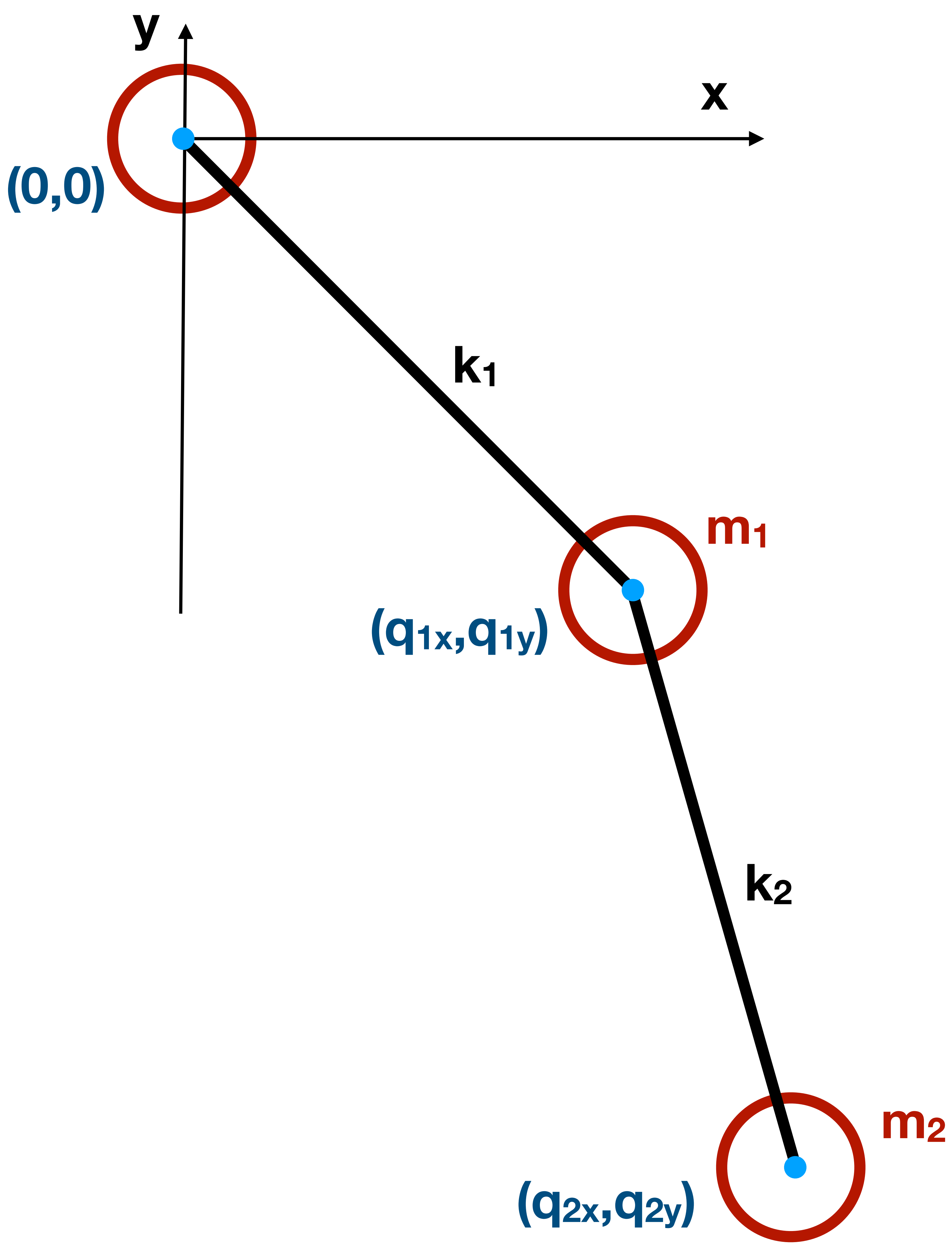
Reading Assignment Takes Away

- Lagrangian/*Hamiltonian formulation of mechanics*
- *Differential models on manifolds, incorporating constraints in the model*
- *Modeling constrained systems in Cartesian coordinates, constraint forces*
- *Consistent Symplectic Integrators for systems with rigid (holonomic) Constraints*
- *Störmer-Verlet method, "Velocity version" of Störmer-Verlet*
- *SHAKE algorithm*
- *RATTLE algorithm*

Programming Assignment 1

- Implement a simulator for the conservative double pendulum of Lecture 01
- Use a Symplectic Integrator
  - Group 1 : Position Verlet
  - Group 2 : Velocity Verlet
  - Group 3 ?
- Study accuracy of trajectories and total energy W.R.T. time step

Double Elastic Pendulum



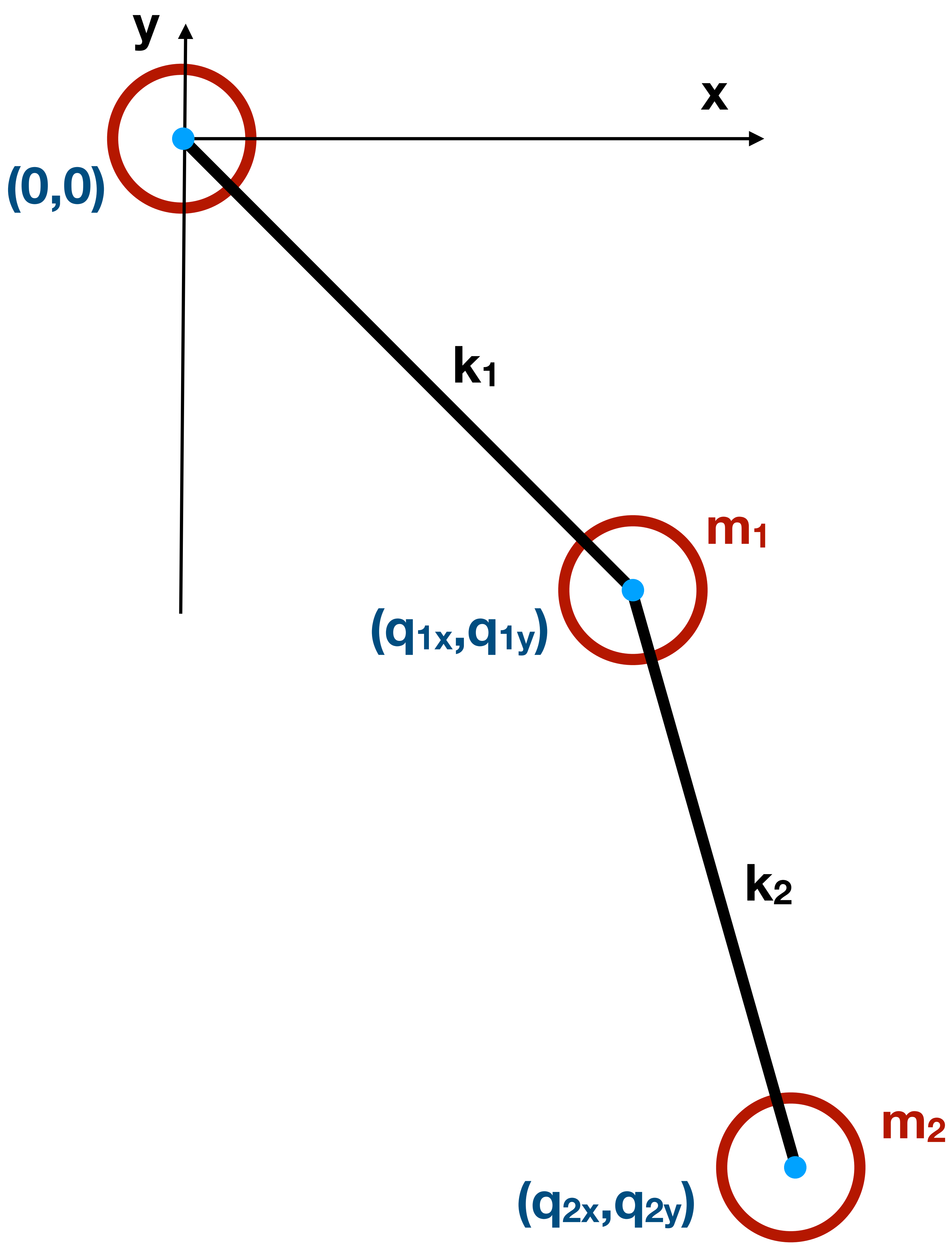
$$\mathbf{p}_i := m_i \dot{\mathbf{q}}_i$$

$$E = K(\mathbf{p}_1, \mathbf{p}_2) + T(\mathbf{q}_1, \mathbf{q}_2)$$

$$K(\mathbf{p}_1, \mathbf{p}_2) = \frac{\left|\mathbf{p}_1\right|^2}{2m_1} + \frac{\left|\mathbf{p}_2\right|^2}{2m_2}$$

$$\begin{aligned} T(\mathbf{q}_1, \mathbf{q}_2) = -m_1 \mathbf{g} \cdot \mathbf{q}_1 - m_2 \mathbf{g} \cdot \mathbf{q}_2 + \\ \frac{k_1}{2}\left(\left|\mathbf{q}_1\right| - l_1\right)^2 + \\ \frac{k_2}{2}\left(\left|\mathbf{q}_1 - \mathbf{q}_2\right| - l_2\right)^2 \end{aligned}$$

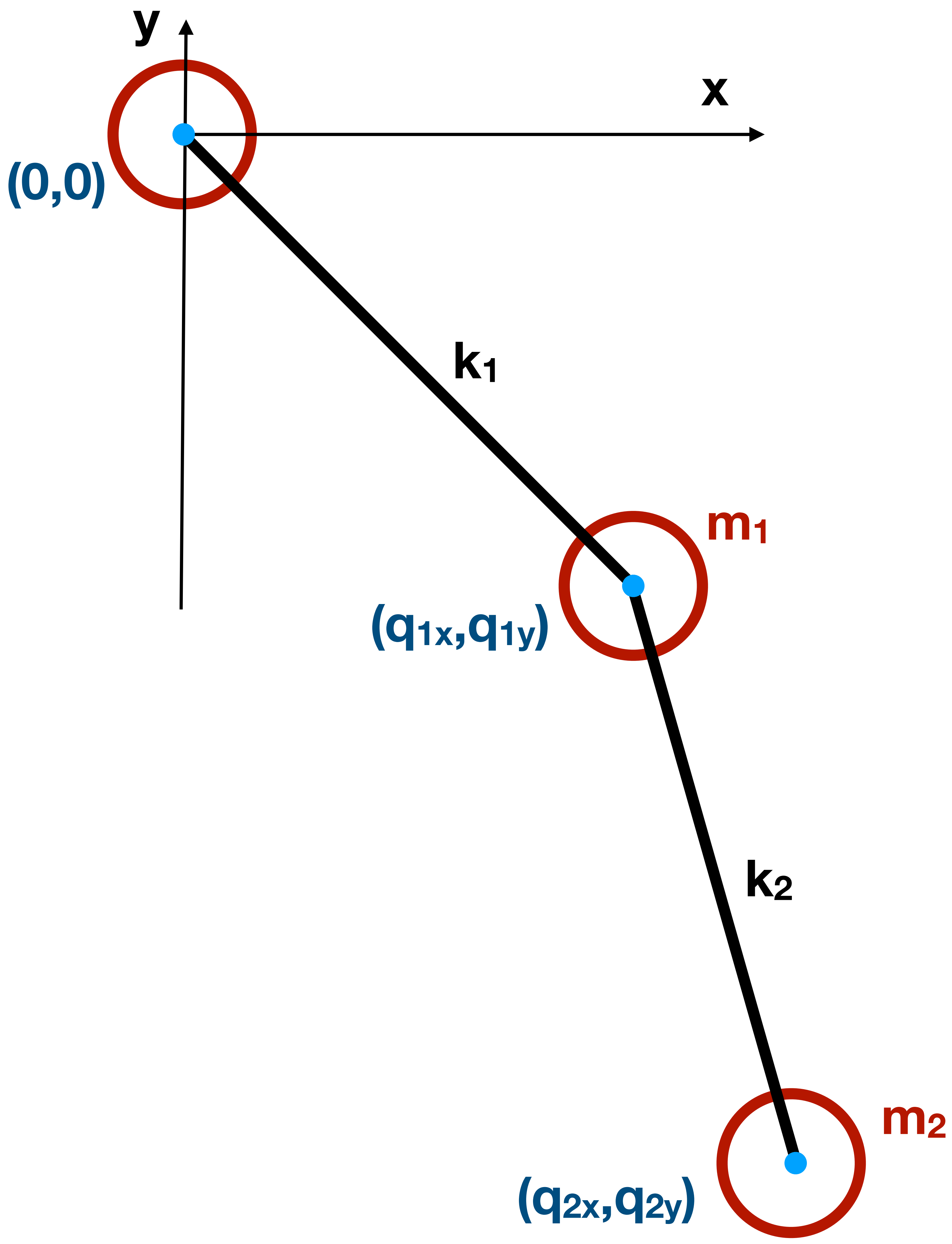
Double Elastic Pendulum



$$\dot{\mathbf{q}}_i = \frac{\partial K}{\partial \mathbf{p}_i}$$

$$\dot{\mathbf{p}}_i = -\frac{\partial T}{\partial \mathbf{q}_i}$$

Double Elastic Pendulum



$$\dot{\mathbf{p}}_i = -\frac{\partial\ T}{\partial\ \mathbf{q}_i}$$

$$\dot{\mathbf{q}}_i = \frac{\partial\ K}{\partial\ \mathbf{p}_i}$$

$$\frac{\partial T}{\partial q_{1,x}} = -m_1 g_x - k_1 q_{1,x}\left(\frac{l_1}{|q_1|} - 1\right) - k_2\left(q_{1,x} - q_{2,x}\right)\left(\frac{l_2}{|q_2 - q_1|} - 1\right)$$

$$\frac{\partial T}{\partial q_{1,y}} = -m_1 g_y - k_1 q_{1,y}\left(\frac{l_1}{|q_1|} - 1\right) - k_2\left(q_{1,y} - q_{2,y}\right)\left(\frac{l_2}{|q_2 - q_1|} - 1\right)$$

$$\frac{\partial T}{\partial q_{2,x}} = -m_2 g_x - k_2\left(q_{1,x} - q_{2,x}\right)\left(\frac{l_2}{|q_2 - q_1|} - 1\right)$$

$$\frac{\partial T}{\partial q_{2,y}} = -m_2 g_y - k_2\left(q_{1,y} - q_{2,y}\right)\left(\frac{l_2}{|q_2 - q_1|} - 1\right)$$

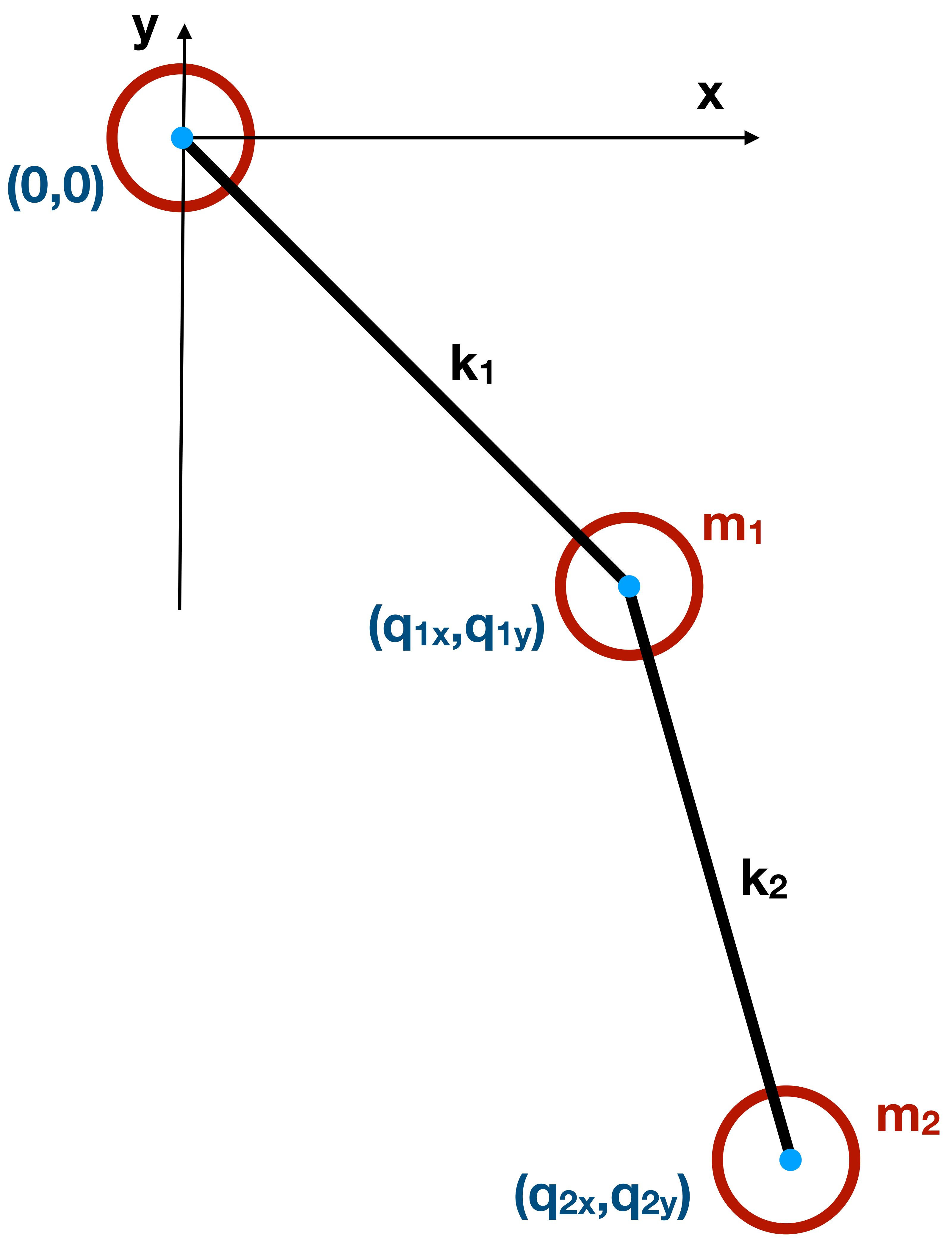
$$\frac{\partial K}{\partial p_{1,x}} = p_{1,x}/m_1$$

$$\frac{\partial K}{\partial p_{1,y}} = p_{1,y}/m_1$$

$$\frac{\partial K}{\partial p_{2,x}} = p_{2,x}/m_2$$

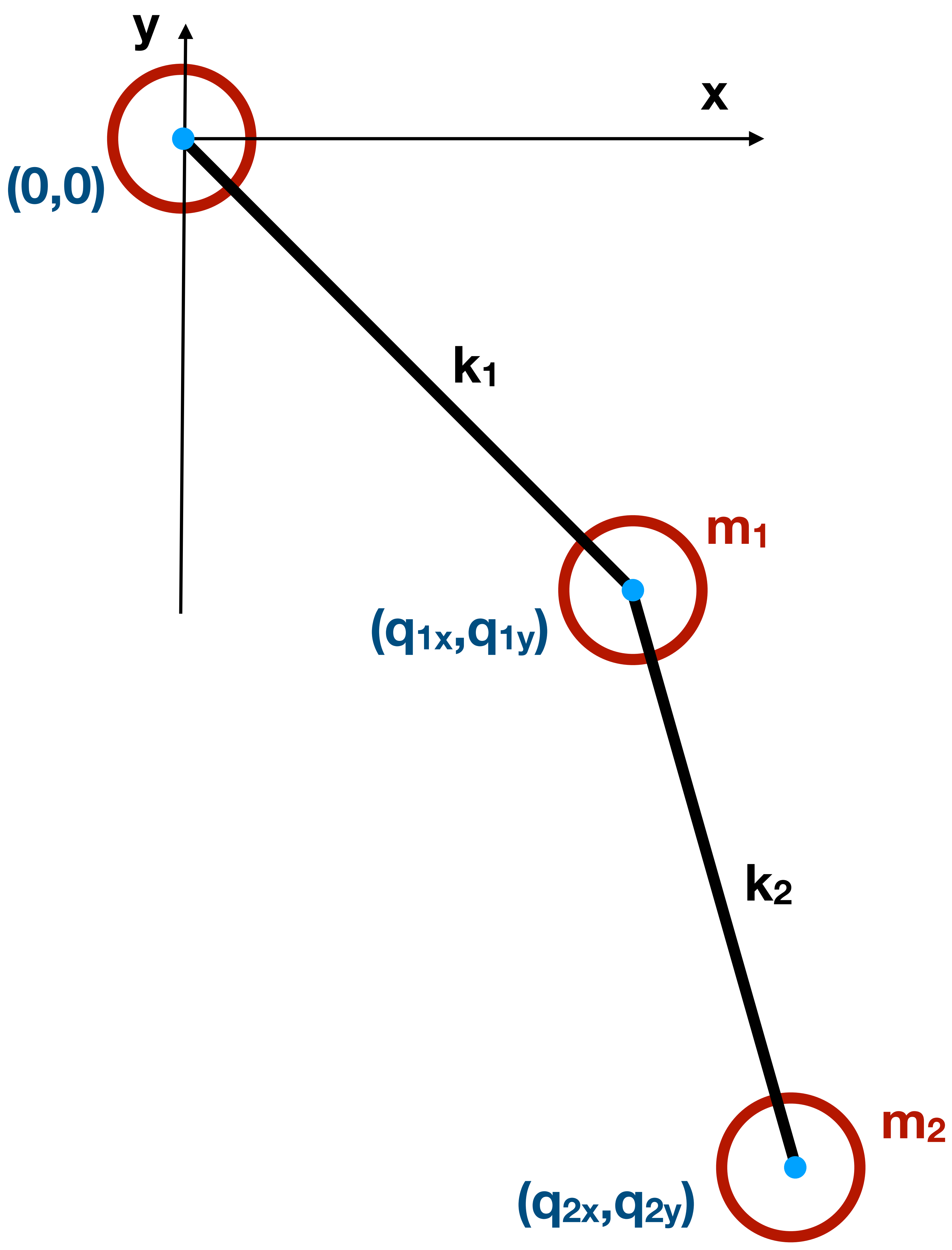
$$\frac{\partial K}{\partial p_{2,y}} = p_{3,y}/m_2$$

Double Elastic Pendulum




```
m1    = 1;
m2    = .2;
k1    = 100;
k2    = 100;
l1    = 1;
l2    = 1;
gx    = 0;
gy    = -9.81;
```

Double Elastic Pendulum with Friction



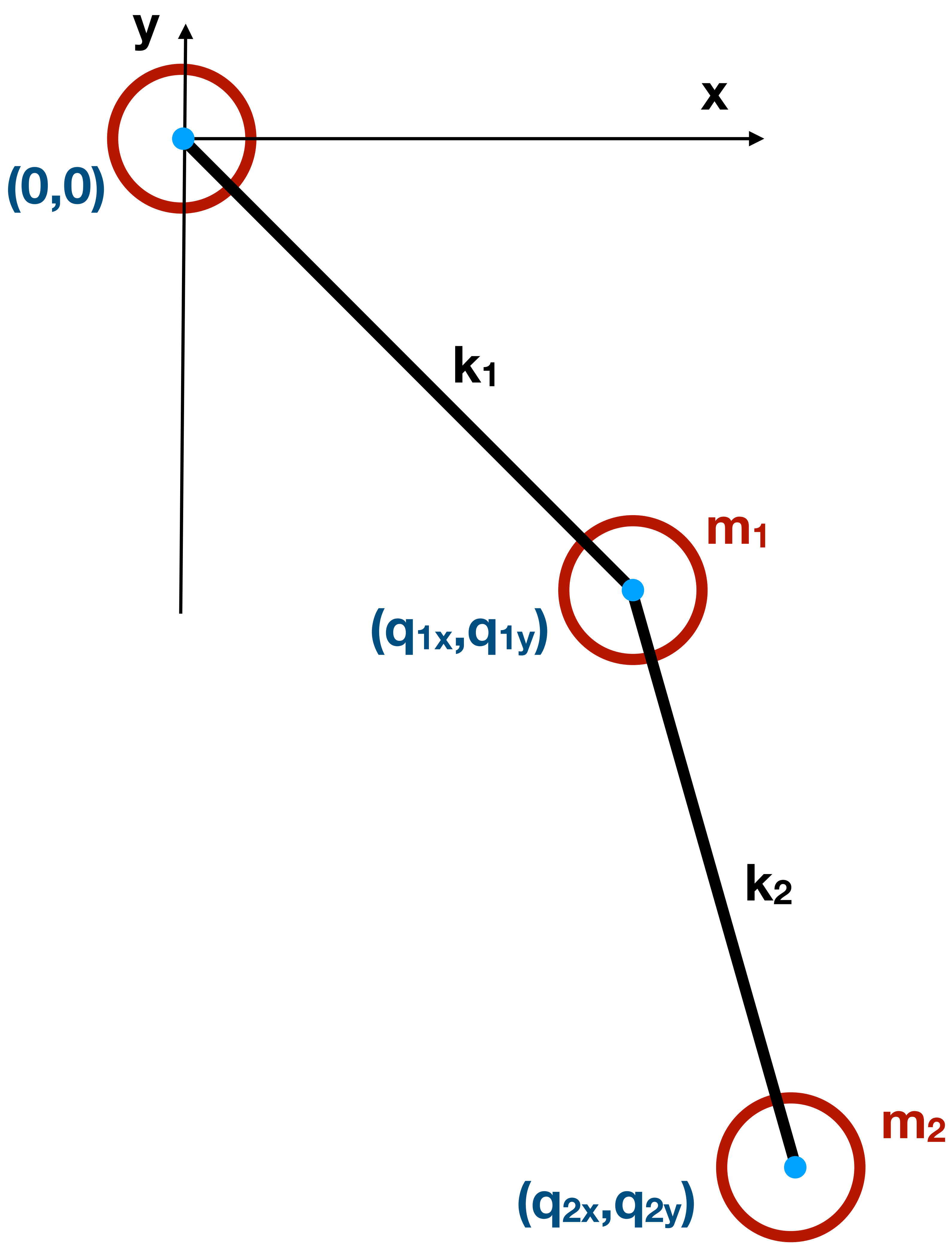
$$\mathbf{p}_i := m_i \dot{\mathbf{q}}_i$$

$$E = K(\mathbf{p}_1, \mathbf{p}_2) + T(\mathbf{q}_1, \mathbf{q}_2) + \theta S$$

$$K(\mathbf{p}_1, \mathbf{p}_2) = \frac{\left|\mathbf{p}_1\right|^2}{2m_1} + \frac{\left|\mathbf{p}_2\right|^2}{2m_2}$$

$$\begin{aligned} T(\mathbf{q}_1, \mathbf{q}_2) = -m_1 \mathbf{g} \cdot \mathbf{q}_1 - m_2 \mathbf{g} \cdot \mathbf{q}_2 + \\ \frac{k_1}{2}\left(\left|\mathbf{q}_1\right| - l_1\right)^2 + \\ \frac{k_2}{2}\left(\left|\mathbf{q}_1 - \mathbf{q}_2\right| - l_2\right)^2 \end{aligned}$$

Double Elastic Pendulum

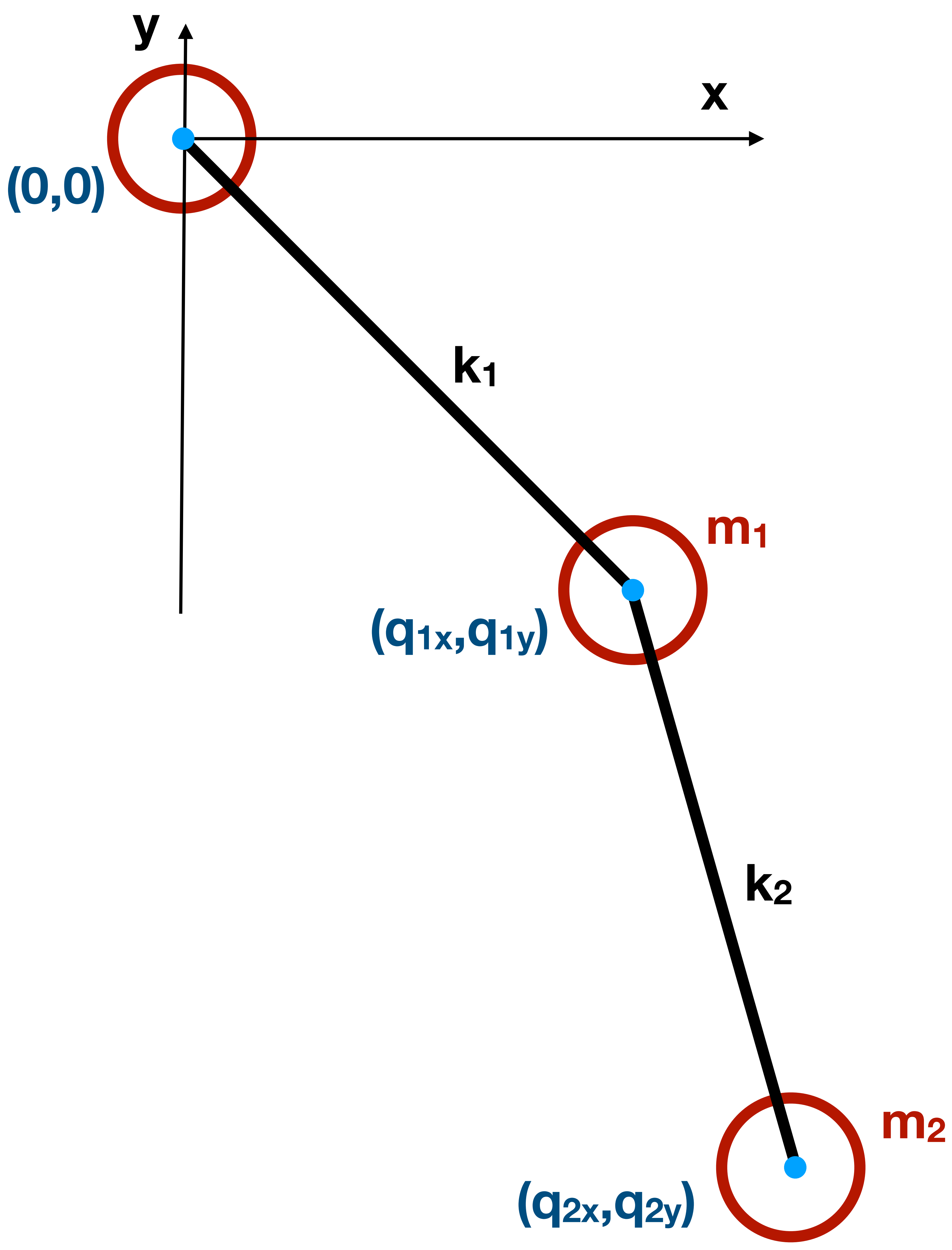


$$\dot{\mathbf{q}}_i = \frac{\partial K}{\partial \mathbf{p}_i}$$

$$\dot{\mathbf{p}}_i = -\frac{\partial T}{\partial \mathbf{q}_i} - \frac{\lambda}{m_i}\mathbf{p}_i$$

$$\dot{s} = \frac{\lambda}{\theta\, m_i^2} \left|\mathbf{p}_i\right|^2$$

Double Elastic Pendulum




```
m1    = 1;
m2    = .2;
k1    = 100;
k2    = 100;
l1    = 1;
l2    = 1;
gx    = 0;
gy    = -9.81;
fr    = .1;
th    = 300;
```

Programming Assignment 2

- Consider the model with very "stiff" springs $k_i \to \infty$
  - For large but finite k_i consider the effect of ingreasing "stiffness" on accuracy and conservation properties of the model
  - For infinite k_i (rigid links)
    - Reformulate the model so that the constraints are accounted for
    - Simulate in cartesian coordinates using SHAKE/RATTLE

Programming Assignment 3

- Apply the Verlet / Velocity-Verlet methods to the "Frozen Argon Crystal" example
  - Hairer, Lubich, Wanner, Sec. I.4

Tutorial : installing Octave from source

```
>> sudo yum install lzip qhull-devel pcre-devel gnuplot texinfo bison byacc flex  zlib-devel hdf5-devel fftw-devel glpk-devel libcurl-devel freetype-devel blas-devel lapack-devel gcc-c++ pcre-devel  qrupdate-devel suitesparse-devel arpack-devel ncurses-devel readline-devel  gperf mesa-libOSMesa-devel fontconfig-devel fltk-devel  gl2ps-devel java-1.8.0-openjdk-devel qt-devel qscintilla-devel  bzip2-devel atlas-devel libsndfile-devel portaudio-devel GraphicsMagick-c++-devel

>> wget ftp://ftp.gnu.org/gnu/octave/octave-5.1.0.tar.xz

>> tar xvJf octave-5.1.0.tar.xz

>> cd octave-5.1.0/

>> mkdir BUILD; cd BUILD

>>  ../configure --help

>> export JAVA_HOME=/usr/lib/jvm/java-1.8.0-openjdk/jre

>> ../configure --with-blas="-L/usr/lib64/atlas/ -latlas" --with-lapack="-L/usr/lib64/atlas/ -latlas" --prefix=/opt/octave/5.1.0

>>  make -j2

>> make check

>> sudo make install
```