# Class 1: Lagrange mechanics and first steps into numerical integration

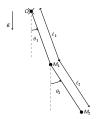
Florence Bertails-Descoubes <sup>1</sup>, Thibaut Métivet <sup>2</sup>, Jean Jouve <sup>3</sup>



2023, October 3 - Ensimag

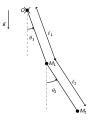
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<sup>1</sup> florence.descoubes@inria.fr <sup>2</sup> thibaut.metivet@inria.fr <sup>3</sup> jean.jouve@inria.fr



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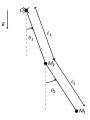
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# Questions

- How to formulate the equations of motion of this object?
- $\bullet$  How to solve these equations in a "safe" way ?



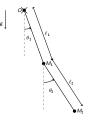


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Goal of this lecture: understand there are many possible choices and learn best practices



### Questions

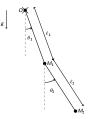
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#### Outline of the class

- I. Lagrange mechanics: how to formulate the equations of motion
- II. Finite differences: how to solve the equations of motion



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NB: Once these concepts are known, more complex systems can be considered



# Keywords and bibliography

#### Part I: Lagrange mechanics

• Analytical Mechanics

Landau and Lifshitz, Mechanics Vol 1; J. Ferreira, Mécanique analytique

• Calculus of Variations

J.-P. Bourguignon, Calcul variationnel ("Variational calculus")

# Part II: Finite differences

- Numerical Analysis
  - G. Allaire, Analyse numérique et optimisation ("Numerical analysis and optimization")

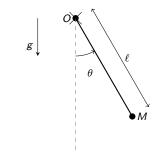
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- Energy conservation properties
  - E. Hairer et al., Geometric numerical integration

# Part I: Lagrange mechanics

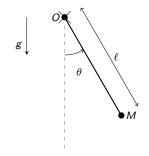
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# The simple pendulum



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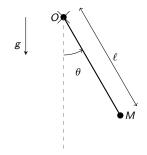


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#### Exercise

• Write the equations of motion of the simple pendulum...

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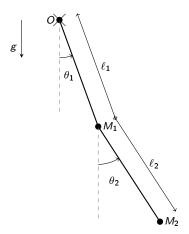


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### Exercise

- Write the equations of motion of the simple pendulum...
- ...using Newton's second law

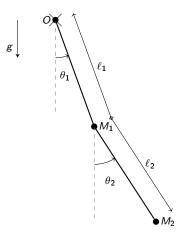
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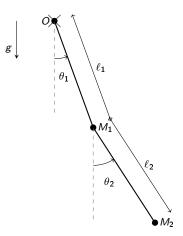
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Generalized coordinates, denoted  $q_i$ , are *n* independent variables (functions of time) which allow to characterize the configuration of a system possessing *n* degrees of freedom. The generalized velocities of the system are defined by  $\frac{d}{dt}q_i = \dot{q}_i$ .

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*Example:* For the simple pendulum, the position of the mass M can be computed as  $OM = \ell e_r$  and its velocity  $v_M$  as  $v_M = \ell \dot{\theta} e_{\theta}$  (in the basis  $(e_r, e_{\theta})$  defined by  $\theta$ ).

#### Equations of motion

At instant t, having both the  $q_i(t)$  and the  $\dot{q}_i(t)$  is necessary, and also sufficient, to determine the accelerations  $\ddot{q}_i(t)$  of the system at t, and thus predict the trajectory  $q_i(t_+)$  forward in time,  $t_+ > t$ .

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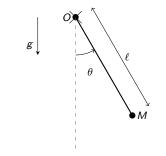
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- Principle of virtual work (see next exercise)
- Principle of least action: more general settings, beyond Newtonian dynamics!

 $\rightarrow$  Both principles lead to the so-called Euler-Lagrange equations which take a specific form in Newtonian dynamics

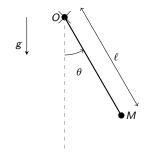
# Back to the simple pendulum



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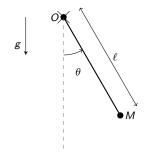


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### Exercise

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### Exercise

- Write the equations of motion of the simple pendulum...
- $\bullet$  ...using the principle of virtual work

Let  $q = \{q_0, \ldots, q_i, \ldots, q_{n-1}\}$  and  $\dot{q} = \frac{\mathrm{d}}{\mathrm{d}t}q$ .

We consider a system subject to holonomic constraints (the  $q_i$  are independent) and conservative forces. Let T be the kinetic energy of the system, and U its potential energy.

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#### Principle of least action (Hamilton principle)

The actual trajectory q(t) followed by the system between two instants a and b > a should be such that the action of the system,

$$S(q, \dot{q}) = \int_{a}^{b} \underbrace{\mathcal{L}(q(t), \dot{q}(t), t)}_{T-U} \mathrm{d}t,$$

is minimal.

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$$\mathcal{L}: \left| \begin{array}{ccc} \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R} & \longrightarrow & \mathbb{R} \\ (x, u, t) & \longmapsto & \mathcal{L}(x, u, t) \end{array} \right|$$

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*Remark:* S is a *functional*, as it takes as arguments the two functions q and  $\dot{q}$ .

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# Euler-Lagrange equations

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#### Theorem

A necessary condition for the action S to be minimal is that q satisfies for all  $t \in [a, b]$  the so-called Euler-Lagrange equations,

$$\forall i = 0..n, \quad \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}_i} - \frac{\partial \mathcal{L}}{\partial \mathbf{q}_i} = 0.$$

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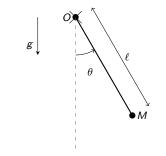
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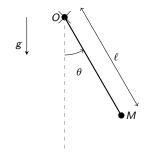
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*Remark:* This is a variational principle (minimum condition on a functional). It can be applied beyond dynamics, for instance to find object shapes with minimal weight, or to compute shapes at static equilibrium.



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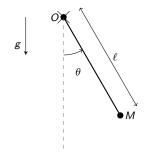
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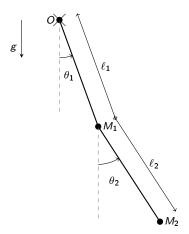


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#### Exercise

- Write the equations of motion of the simple pendulum...
- ...using the Euler-Lagrange formalism

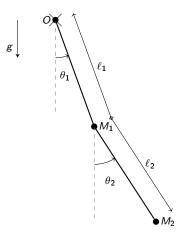
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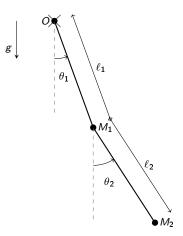
# The double pendulum



# Exercise

• Write the equations of motion of the double pendulum...

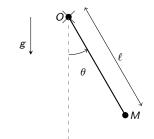
# The double pendulum



## Exercise

- Write the equations of motion of the double pendulum...
- ...using the Euler-Lagrange formalism

# Part II: Finite differences

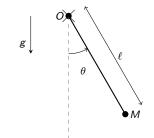


Computing the dynamics

$$\ddot{ heta}+rac{g}{\ell}\sin heta=0$$
 with  $heta(0)= heta_0$  and  $\dot{ heta}(0)=\lambda_0$ 

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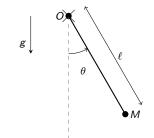
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- Nonlinear equation, no explicit solution
- $\bullet \rightarrow$  Recourse to numerical integration

# Cauchy problem

We consider the following first-order differential equation with initial value,

$$\begin{cases} \dot{x} = f(x(t), t) & t \in [a, b] \\ x(a) = x_0 \end{cases}$$

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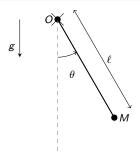
where f is a continuous function from  $\mathbb{R}^p \times \mathbb{R}$  to  $\mathbb{R}^p$ ,  $p \ge 1$ . Such a problem belongs to the class of Cauchy problems. The unknown of the problem is the function x from  $\mathbb{R}$  to  $\mathbb{R}^p$ .

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# Cauchy problem

#### Exercise

Show that the simple pendulum equation of motion enters the formalism above.



Equation of motion (reminder)

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#### Exercise

- Show that a Lipschitz continuous function is necessarily continuous.
- Is the opposite true?

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If f is locally Lipschitz continuous with respect to its first (state) variable x(t), then there exists a unique solution  $\bar{x}$  to the Cauchy problem, and  $\bar{x}$  is  $C^1$  continuous.

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 $\rightarrow$  The greater *m*, the faster the method converges to the exact solution.

## Single-step numerical scheme

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A single-step numerical scheme is defined as the recurrence

 $x_0$  given  $x_{k+1} = x_k + h\Phi(x_k, h, t_k)$ 

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*Remark:* Convergence is generally hard to prove directly. Instead, one usually prefers to prove consistency + stability w.r.t. errors instead.

Recall that  $x_{k+1} = x_k + h\Phi(x_k, h, t_k)$ , i.e.  $\frac{x_{k+1} - x_k}{h} - \Phi(x_k, t_k, h) = 0$ .



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Remark:

• "Consistent" means that the scheme "converges" to the original Cauchy problem when  $h \rightarrow 0$ . If the scheme is not consistent, it means that we are trying to find an approximate solution to another problem!

 $\rightarrow$  Consistency is necessary to have convergence (but not sufficient...).

• The order of convergence is directly related to the order of consistency of a numerical scheme.

### Exercise

Show that Explicit Euler is a consistent scheme of first order.

Reminder: Explicit Euler:

$$\mathbf{x_{k+1}} = \mathbf{x_k} + hf(\mathbf{x_k}, \mathbf{t_k})$$

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### Definition

The numerical scheme is stable with respect to errors if there exists a constant M > 0and a constant  $\bar{\varepsilon} > 0$  (both independent of h) such that

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Remark:

- Means that a perturbation on the initial condition and on the increment Φ only yields a bounded perturbation on the numerical scheme, and so the scheme does not amplify errors.
- Easy criterion: stability w.r.t. errors is guaranteed when  $\Phi$  satisfies some regularity properties: typically, when  $\Phi$  is Lipschitz continuous w.r.t. x.

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# Convergence

## Theorem

*Convergence* = *consistency* + *stability* 

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### Exercise

Show that Explicit Euler is a convergent scheme.

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### Exercise

Derive the Explicit Euler scheme for the simple scalar Cauchy problem

$$x(a) = x_0$$
  $\dot{x}(t) = -\lambda x(t)$   $\forall t \in [a, b]$  with  $\lambda > 0$ .

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$$||x_k|| \leq R \quad \forall k = 0, \cdots, N \quad \text{and } \forall h \in [0, h^*[.$$

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 $\rightarrow$  To keep in mind: stability w.r.t. errors is useful for proving convergence. Stability as defined above is useful when considering integration of systems on moderate or large time intervals, or when using a large timestep (which is often useful in practice!).

## Explicit vs. Implicit Euler

### Exercise 1

Consider the linearized pendulum problem (valid for small angle  $\theta$ ),

$$\ddot{ heta}+rac{{m {\cal g}}}{\ell} heta=0\qquad$$
 with  $heta(0)= heta_0$  and  $\dot{ heta}(0)=\lambda_0,$ 

and express the condition on the time step h for Explicit Euler to be stable.

# Explicit vs. Implicit Euler

Exercise 2

Same question for Implicit Euler.

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Implicit Euler is inconditionally stable.

### In a nutshell

• A short tour on the important notions and properties of finite difference schemes

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• References: G. Allaire, Analyse numérique et optimisation ("Numerical analysis and optimization"), E. Hairer et al., Geometric numerical integration.