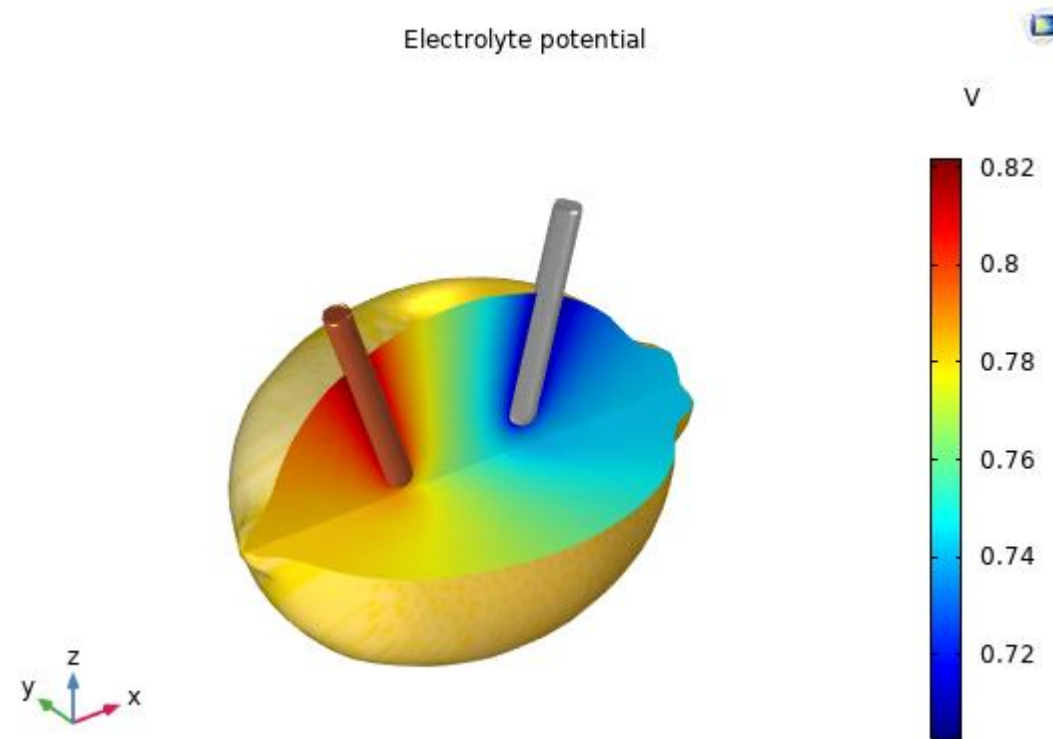
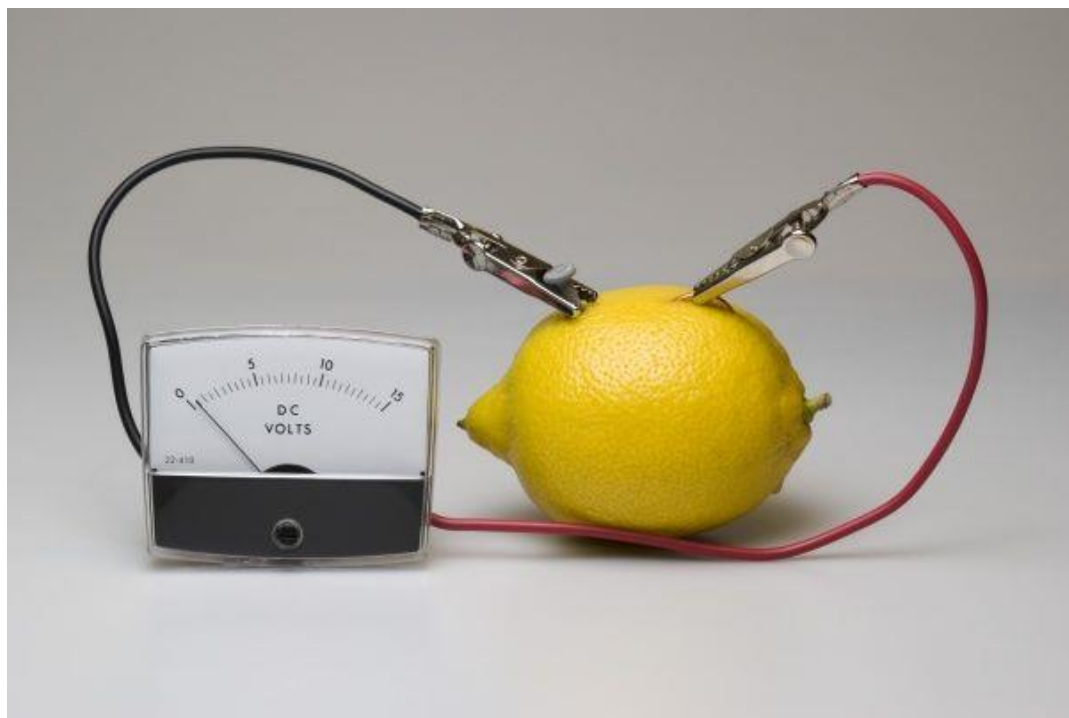
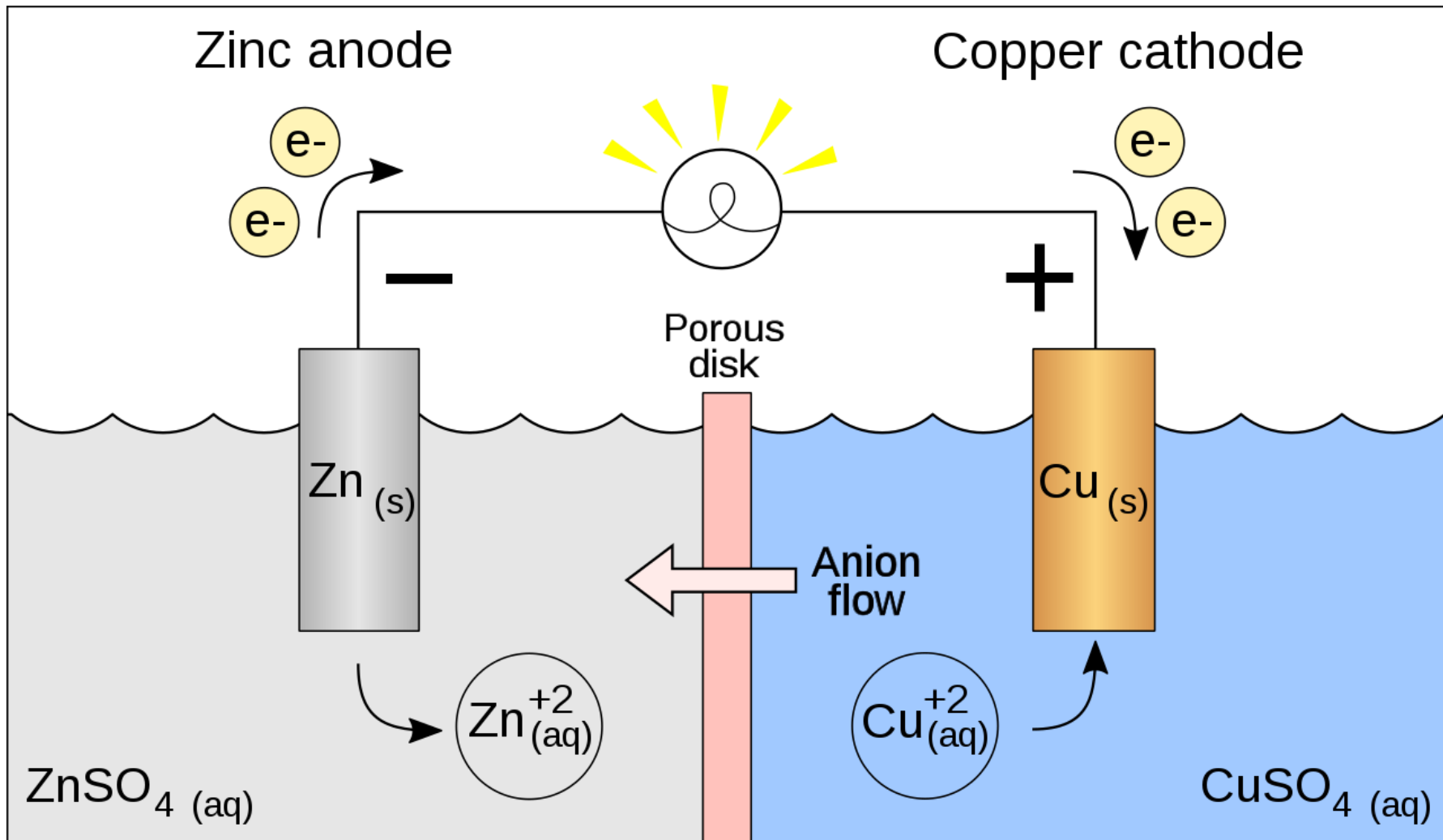


# Simulační výuková aplikace – baterie z citronu

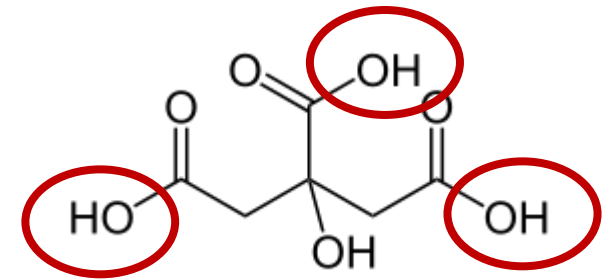
Jakub Koláček, Vysoké učení technické v Brně





# Charakteristika baterie z citronu (Zn-Cu)

- Složení elektrolytu (pH 2–3)
  - kyselina citronová 300 mM
  - **vodíkové ionty** **10 mM**
  - draselné ionty 35 mM
  - vápenné ionty 7 mM
  - **měďnaté ionty** **6 μM (stopové množství)**
  - zinečnaté ionty 9 μM (stopové množství)
- Elektrody
  - měďná elektroda
  - zinková elektroda

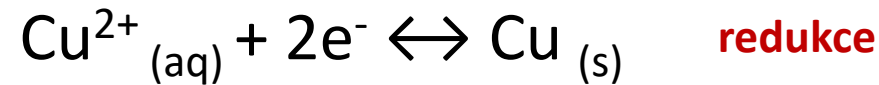


# Elektrody a elektrodový potenciál

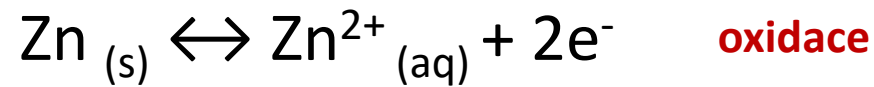
$$\Delta G = -nFE$$

 $E_{\text{STD}}$ 

-0,76 V

 $E_{\text{STD}}$ 

0,34 V

 $E_{\text{STD}}$ 

0,76 V

- Rozdíl redukčních elektrodových potenciálů = **napětí článku**
- Článek Cu – Zn má tedy standardní napětí 1,1 V

# Elektrody a elektrodový potenciál

$$\Delta G = -nFE$$



**vodné prostředí, další možné a předpokládané reakce**

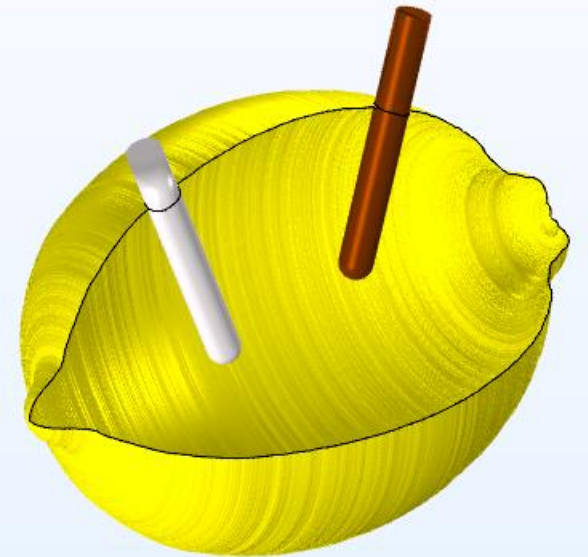
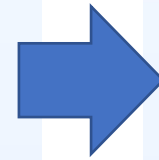
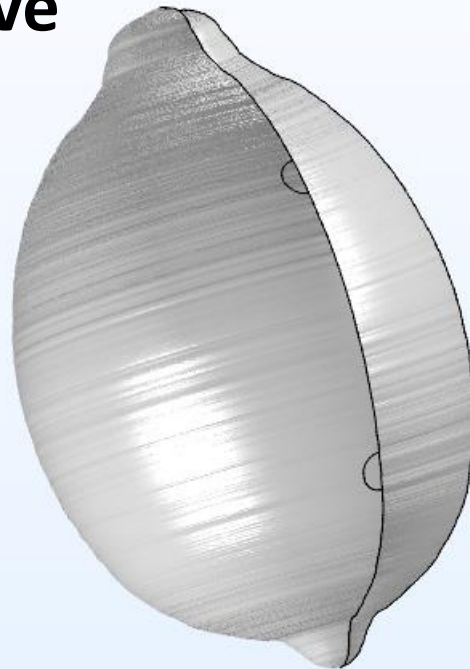
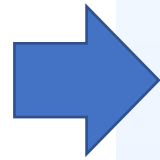
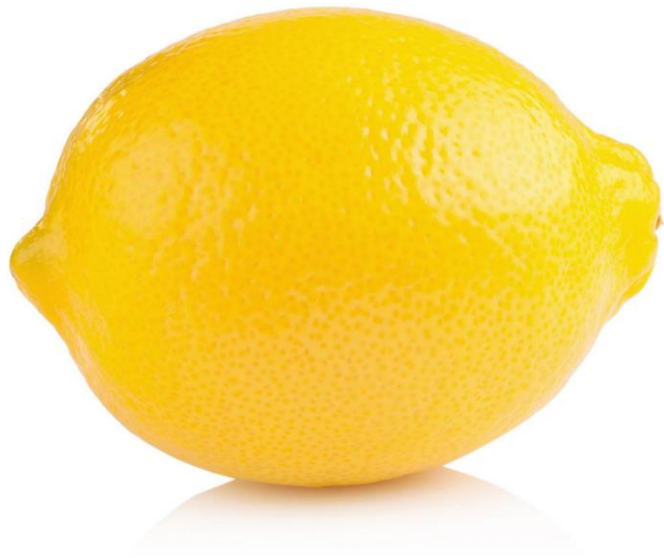


# Tvorba aplikace v COMSOL Multiphysics

- zjednodušení podmínek a zanedbání některých reakcí
  - konstantní pH elektrolytu, zanedbatelná koncentrace  $\text{Cu}^{2+}$
- tvorba modelu
- z modelu -> aplikace (Application Builder)
- publikace aplikace na COMSOL Server

# Geometrie modelu

**Image to Curve**



# Fyzika modelu

- Secondary Current Distribution
  - reakce na elektrodách
- Transport of Diluted Species
  - rozpouštění Zn elektrody

The image shows a screenshot of the COMSOL Multiphysics software interface, specifically the Model Builder and Settings panels for a Secondary Current Distribution node.

**Model Builder Panel:**

- Tree structure:
  - lemon\_battery\_newest2.mph (root)
    - Global Definitions
      - Parameters 1
      - Image (i2m\_im)
      - Default Model Inputs
      - Materials
      - Image to Curve 1
    - Component 1 (comp1)
      - Definitions
      - Geometry 1
      - Materials
      - Secondary Current Distribution (cd)**
        - Electrolyte 1
        - Insulation 1
        - Initial Values 1
        - Electrode Surface 1
          - Electrode Reaction 1
        - Electrode Surface 2
          - Electrode Reaction 1
        - Transport of Diluted Species (tds)
          - Transport Properties 1
          - No Flux 1
          - Initial Values 1
          - Electrode Surface Coupling 1
            - Reaction Coefficients 1
        - Events (ev)
        - Multiphysics
        - Mesh 1
      - Study 1
      - Study 2
      - Results



File Home Definitions Geometry Materials Physics Mesh Study Results Developer

Application Builder Component 1 Add Component Parameters Variables Functions Parameter Case Import Build All Add Material Secondary Current Distribution Add Physics Build Mesh Mesh 1 Compute Study 2 Add Study Electrolyte Potential Add Plot Group Windows Reset Desktop

### Model Builder

- lemon\_demo.mph (root)
  - Global Definitions
    - Parameters 1
    - Image (i2m\_im)
    - Default Model Inputs
    - Materials
    - Image to Curve 1
  - Component 1 (comp1)
    - Definitions
    - Geometry 1
    - Materials
    - Secondary Current Distribution (cd)
    - Transport of Diluted Species (tds)
    - Events (ev)
    - Multiphysics
    - Mesh 1
    - Study 1
    - Study 2
    - Results

### Settings

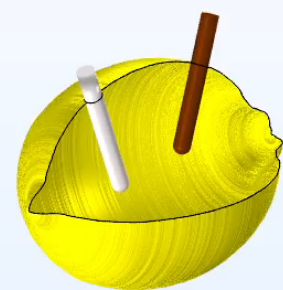
Materials

Label: Materials

Material Overview

| Material | Selection |
|----------|-----------|
|----------|-----------|

### Graphics



The Graphics window displays a 3D model of a yellow lemon. Two sticks are inserted into the lemon: a white one and a brown one. The lemon is rendered with a textured surface. The background is a light blue gradient.

Messages Progress Log

[May 26, 2022, 2:14 PM] Opened file: C:\Users\10930300\OneDrive - SYNLAB\Desktop\lemon\_demo.mph  
[May 26, 2022, 2:18 PM] Formed union of 3 solid objects.  
[May 26, 2022, 2:18 PM] Union has 5 domains, 38 boundaries, 64 edges, and 32 vertices.  
[May 26, 2022, 2:18 PM] Finalized geometry has 5 domains, 10 boundaries, 10 edges, and 6 vertices.

- `model.component("comp1").mesh("mesh1").run();`
- `model.param().set("c_H0", "10^-"+var_pH+"[mol/l]");`

- nastavení osy x v grafech

```
1  model.result(arg1).set("axislimits", false);
2  model.result(arg1).run();
3  app.form("main").formObject("graphics1").set("source", model.result(arg1));
4
5  model.result(arg1).set("axislimits", true);
6  model.result(arg1).set("xmin", 0.01);
7  model.result(arg1).set("xmax", model.result(arg1).getDouble("xmax"));
8  model.result(arg1).set("ymin", model.result(arg1).getDouble("ymin"));
9  model.result(arg1).set("ymax", model.result(arg1).getDouble("ymax"));
10 model.result(arg1).set("yminsec", model.result(arg1).getDouble("yminsec"));
11 model.result(arg1).set("ymaxsec", model.result(arg1).getDouble("ymaxsec"));
12 model.result(arg1).run();
13 app.form("main").formObject("graphics1").set("source", model.result(arg1));
14
15 model.result(arg1).set("axislimits", false);
16 model.result(arg1).run();
17 app.form("main").formObject("graphics1").set("source", model.result(arg1));
18
19 model.result(arg1).set("axislimits", true);
20 model.result(arg1).set("xmin", 0.01);
21 model.result(arg1).set("xmax", model.result(arg1).getDouble("xmax"));
22 model.result(arg1).set("ymin", model.result(arg1).getDouble("ymin"));
23 model.result(arg1).set("ymax", model.result(arg1).getDouble("ymax"));
24 model.result(arg1).set("yminsec", model.result(arg1).getDouble("yminsec"));
25 model.result(arg1).set("ymaxsec", model.result(arg1).getDouble("ymaxsec"));
26 model.result(arg1).run();
27 app.form("main").formObject("graphics1").set("source", model.result(arg1));
```

File Home Form

Form Objects: Input Field, Text Label, Button, Data Display, Check Box, Graphics, More Objects

Layout: Grid, Sketch

Sketch: Show Grid Lines, Arrange

Grid: Row Settings, Column Settings, Merge Cells, Split Cell, Extract Subform

Test: Test Application, Apply Changes, Preview Form, Test in Web Browser

### Application Builder

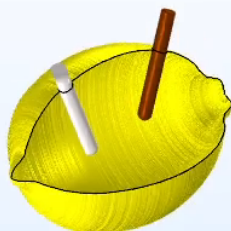
- lemon\_battery\_newest2.mph (root)
  - Inputs
  - Themes
  - Main Window
  - Forms
    - main
      - Forms
        - topMenu
        - designCommands
        - designSettings
        - designInput
        - physicsCommands
        - physicsSettings
        - physicsInputCurrent
        - physicsInputPH
        - simulateCommands
        - simulateSettings
        - simulateInput
        - resultsCommands
        - resultsSettings
        - exportCommands
        - exportSettings
        - exportInput
      - Declarations
      - Methods
    - calc\_main
    - Events
    - Declarations
    - Methods
    - Libraries

### Lemon Battery

Design Physics Simulate Graphs Animations Calculator

Load Defaults Plot Geometry Plot Mesh

Electrode Surface Mesh: Fine



About

### Settings

Form

Name: designInput

Title:

Icon: Default

Size

Initial size: Automatic

Margins

Horizontal: 0

Vertical: 0

Dialog Settings

Store changes: On request

Resizable

Grid Layout for Contained Form Objects

| Column | Width | Size |
|--------|-------|------|
| 1      | Fit   | N/A  |
| 2      | Fit   | N/A  |

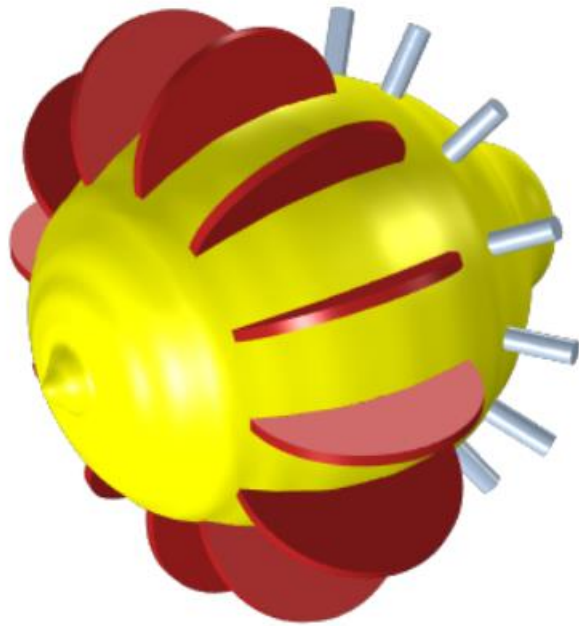
| Row | Height | Size |
|-----|--------|------|
| 1   | Fit    | N/A  |

Inherit columns: None

Cell margins

Horizontal: 5

# Optimalizace baterie





2018, Mark Rober

<https://www.youtube.com/watch?v=a1D-fZP8qJk>

Děkuji za pozornost