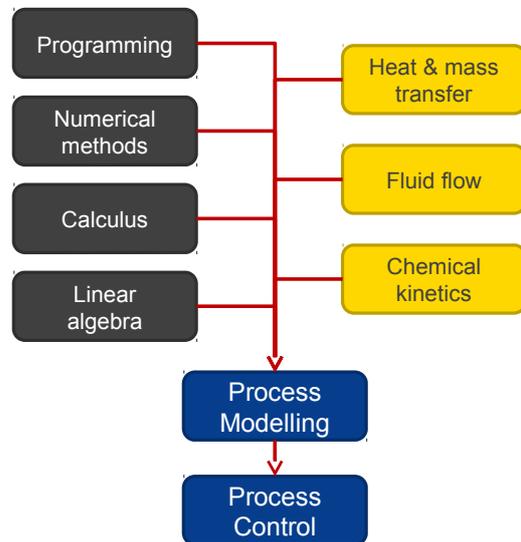


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Process modelling

- senior level course, core (CEIC3000)
- reliant on *lots of prerequisite knowledge* maths, computing, chemical engineering
- students should be able to ...
 - *build a model of a process*
 - » heat flow, material flow, chemistry
 - *analyse the model*
 - » analytical maths with DEs
 - » numerical solutions of DEs
 - » qualitative analysis of system



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Notebook computing

Jupyter notebooks: literate computing

- **code plus**
 - » context, output, analysis
- **no barrier to entry**
 - » runs on cloud via web browser
- lots of languages
 - » **Python, Octave, R, Julia...**



cocalc.com @co_calc
Jupyter notebooks + more
freemium: free to use, US\$7/mo for upgrades

problem statement →

- rich text (Markdown)
- graphics, equations, links, videos

solution →

- rationale, approach, description

code (input) →

- Python with numpy, matplotlib

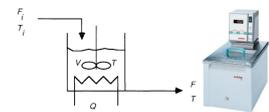
descriptive →

- “why?” not just what

results (output) →

- text, plots, ...

Q2: heater circulator
A perfectly mixed, stirred-tank heater has a single feed stream and a single output stream, as shown.



Jupyter-NEC 4: bench-top heater circulator
This model is suitable for a lab-scale water bath (heater circulator) that is used to control the temperature of a reaction. $Q(t)$ is either fully on or off in square waves and T_1 , V , F_1 , and F_2 are constants. Illustrate the typical behavior of $T(t)$. Select reasonable numbers for each of the unknown parameters for a lab-scale heater circulator.

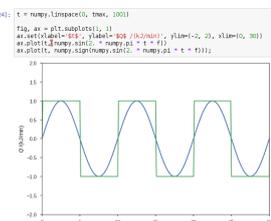
(b) Implementation
We need to find appropriate values for the parameters in the model. Many are pretty easy to find in the [literature](#), but the material capacity $\rho V C_p$ can be reasonably estimate. When it comes to making a square wave, the `sign()` function can be quite handy. ([Documentation of sign\(\)\)](#)

```

In [223]: # Parameters for the model; keep track of units!
Q0 = 200000 # 0 value when on / Watts
Q1 = 1.0 # inlet fluid heat capacity J/Kg
F1 = 10.0 # inlet temperature K
F2 = 25.0 # inlet flow rate L/min
rho = 1000 # bulk density g/cc

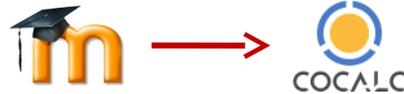
In [224]: # Initial flow at time t; Jupyter ***
def Q(t):
    return Q0 * (1.0 + numpy.sign(numpy.sin(2. * numpy.pi * t * F1)) / 2.0
def T(t):
    """Time derivative of the bath temperature; K/min ***
    returns T1, V, V1, T1 = T2(t), F1, F2 = F2
    """
    return Q(t) / (rho * V * Cp)

Plot Q(t) over a suitable range of t to make sure it is correct.
In [241]: t = numpy.linspace(0, 2000, 1000)
T10, V = get_parameters()
T1, V1 = get_parameters()
T2 = T1 + 10
T = plot(t, numpy.sign(numpy.sin(2. * numpy.pi * t * F1))
In [242]: T = numpy.linspace(0, 2000, 1000)
T10, V = get_parameters()
T1, V1 = get_parameters()
T2 = T1 + 10
T = plot(t, numpy.sign(numpy.sin(2. * numpy.pi * t * F1))
  
```



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Scaffolding



Template for the solution for each tutorial and assignment question

- **Question** details *plus*
 - » hints, partial code
- **Solutions** including
 - » complete code
 - » tips, discussion, extensions
- Sustainable
 - » template with metadata
 - + processing scripts
 - = question + solution notebooks

Question stage

- Tutorial 12 102.1KB PDF document
- Tutorial 12 (Python)
- Tutorial 12 (Octave/Matlab)

Q3: Chemical reaction with Hopf bifurc

The sequence of five chemical reactions has produced the following system of equations:

$$\frac{d\vec{x}}{dt} = \begin{bmatrix} k_1 C_A C_X - k_4 C_X - k_2 C_X C_Y \\ -k_3 C_Y + k_5 C_Z \\ k_4 C_X - k_5 C_Z \end{bmatrix}$$

Most of our analysis is analytical, but we want to plot some phase diagrams to demonstrate the Hopf bifurcation at $C_A = (k_3 + k_4 + k_5)/k_2$.

```
In [ ]: def dxdt(x, t):
        return [ k1 * CA * CX - k4 * CX - k2 * CX * CY,
                -k3 * CY + k5 * CZ,
                k4 * CX - k5 * CZ ]
```

Solution stage

- Tutorial 12 102.1KB PDF document
- Tutorial 12 (Python) solutions
- Tutorial 12 (Octave/Matlab) solutions
- Tutorial 12 solutions 796.1KB PDF document

Q3: Chemical reaction with Hopf bifurc

The sequence of five chemical reactions has produced the following system of equations:

$$\frac{d\vec{x}}{dt} = \begin{bmatrix} k_1 C_A C_X - k_4 C_X - k_2 C_X C_Y \\ -k_3 C_Y + k_5 C_Z \\ k_4 C_X - k_5 C_Z \end{bmatrix}$$

Most of our analysis is analytical, but we want to plot some phase diagrams to demonstrate the Hopf bifurcation at $C_A = (k_3 + k_4 + k_5)/k_2$.

```
In [10]: def dxdt(x, t):
          [ k1 * CA + x[0] - k4 * x[0] - k2 * x[0] * x[1],
            -k3 * x[1] + k5 * x[2],
            k4 * x[0] - k5 * x[2] ]
```

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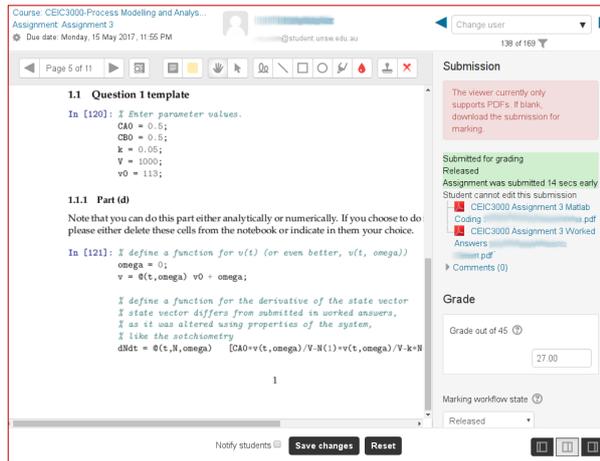
Templates for assignments

For the student

- » template gives hints, guidance
- » Jupyter: File → Download → PDF

For the marker

- » compatible with Moodle PDF grader
- » fully electronic workflow for grading
- » easy to make verbose, insightful comments, annotations
- » faster to mark



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Evaluation: Where next?

Students say: best features of this course...

- good guidance provided for computation work in templates
- Sage Math Cloud (now called CoCalc)
- lots of help in tutorial questions
- use of computational tools
- cooperative learning between theory, hand solving and computer solving
- strong links between maths and applications in practice
- developed mathematical thinking required to apply maths to the world
- challenging but at an appropriate level

We saw:

- more 'aha' moments in tutorials
- more assignments are own work not copied code

Next steps:

- Remove PDFs of tutorial sheets and assignments completely
 - » everything via Jupyter
- Further experimentation:
 - » CoCalc's "Course" tools
 - » notebook grading tools (nbgrader)

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