

COMP LAB

G. Mallia

Timetable
Deadline

Aims
Systems

Vibrations

How

Simulation
types

Classical
simulation

How to write
a report

INTRODUCTION to the Computational Laboratory

Giuseppe Mallia

g.mallia@imperial.ac.uk

Imperial College London - Chemistry Department
Thomas Young Centre:
the London Centre for Theory and Simulation of Materials

AUTUM 2016/SPRING 2017

Outline

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1 TIMETABLE and DEADLINE

2 AIMS and SYSTEMS

3 VIBRATIONS

4 HOW

5 SIMULATION TYPES

6 CLASSICAL SIMULATION

7 HOW TO WRITE A REPORT

TIMETABLE and DEADLINE

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Session	Start Date	End Date	Report Deadline
1	10/10/2016	14 / 10 / 2016	21 / 10 / 2016
2	24/10/2016	28 / 10 / 2016	04 / 11 / 2016
3	07/11/2016	11 / 11 / 2016	18 / 11 / 2016
4	21/11/2016	25 / 11 / 2016	02 / 12 / 2016
5	05/12/2016	09 / 12 / 2016	16 / 12 / 2016
6	16/01/2017	20 / 01 / 2017	27 / 01 / 2017
7	30/01/2017	03 / 02 / 2017	10 / 02 / 2017
8	13/02/2017	17 / 02 / 2017	24 / 02 / 2017
9	27/02/2017	03 / 03 / 2017	10 / 03 / 2017
10	13/03/2017	17 / 03 / 2017	24 / 03 / 2017

TIMETABLE and DEADLINE

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■ Demonstrator

	Mon	Tue	Thur	Fri
2:00-3:00	☺	☺	☺	☺

DEADLINE:

when? **12:00pm on next Friday**

AIM:

The Thermal Expansion of MgO

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- to predict how the material expands when heated;
- to calculate the thermal expansion coefficient:

$$\alpha = \frac{1}{V_0} \left(\frac{\partial V}{\partial T} \right)_P$$

AIM:

The Thermal Expansion of MgO

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- to predict how the material expands when heated;

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$$\alpha = \frac{1}{V_0} \left(\frac{\partial V}{\partial T} \right)_P$$

- **QUASI-HARMONIC APPROXIMATION** (LD)

to compute vibrational energy levels of MgO;

to understand the **phonon dispersion** of a material and the vibrational density of state;

AIM:

The Thermal Expansion of MgO

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- to predict how the material expands when heated;
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$$\alpha = \frac{1}{V_0} \left(\frac{\partial V}{\partial T} \right)_P$$
- **QUASI-HARMONIC APPROXIMATION (LD)**
 - to compute vibrational energy levels of MgO;
 - to understand the **phonon dispersion** of a material and the vibrational density of state;
- **MOLECULAR DYNAMICS (MD)**
 - to simulate the vibrations as random motions of atoms inside a cell;

AIM:

The Thermal Expansion of MgO

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- to predict how the material expands when heated;
- to calculate the thermal expansion coefficient:
$$\alpha = \frac{1}{V_0} \left(\frac{\partial V}{\partial T} \right)_P$$
- **QUASI-HARMONIC APPROXIMATION (LD)**
 - to compute vibrational energy levels of MgO;
 - to understand the **phonon dispersion** of a material and the vibrational density of state;
- **MOLECULAR DYNAMICS (MD)**
 - to simulate the vibrations as random motions of atoms inside a cell;
- to compare QUASI-HARMONIC APPROXIMATION with MOLECULAR DYNAMICS results.

SYSTEMS: MgO crystal (fcc)

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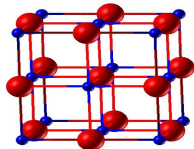
IDEAL, NON DEFECTIVE, PERIODIC SYSTEM IN 3D

■ CONVENTIONAL CELL

$$\mathbf{a}_c = \mathbf{b}_c = \mathbf{c}_c; \alpha_c, \beta_c, \gamma_c$$

N_c : number of atoms

V_c : volume



SYSTEMS: MgO crystal (fcc)

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IDEAL, NON DEFECTIVE, PERIODIC SYSTEM IN 3D

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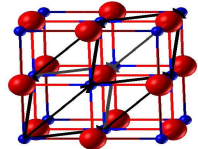
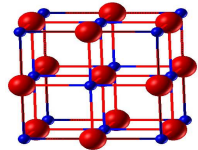
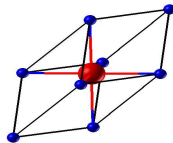
V_c : volume

■ PRIMITIVE CELL

$$\mathbf{a}_p = \mathbf{b}_p = \mathbf{c}_p; \alpha_p, \beta_p, \gamma_p$$

N_c : number of atoms

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SYSTEMS: MgO crystal (fcc)

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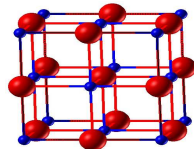
IDEAL, NON DEFECTIVE, PERIODIC SYSTEM IN 3D

■ CONVENTIONAL CELL

$$\mathbf{a}_c = \mathbf{b}_c = \mathbf{c}_c; \alpha_c, \beta_c, \gamma_c$$

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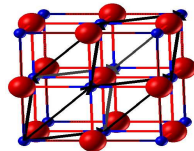
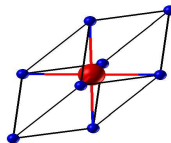


■ PRIMITIVE CELL

$$\mathbf{a}_p = \mathbf{b}_p = \mathbf{c}_p; \alpha_p, \beta_p, \gamma_p$$

N_c : number of atoms

V_p : volume



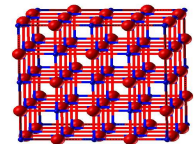
■ SUPERCELL

$$\mathbf{a}_s = \mathbf{b}_s = \mathbf{c}_s = 2 \times \mathbf{a}_c$$

$$\alpha_s, \beta_s, \gamma_s$$

N_s : number of atoms

V_s : volume



SYSTEMS II: lattice parameter of MgO

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What is the lattice parameter of MgO?

SYSTEMS II: lattice parameter of MgO

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What is the lattice parameter of MgO?

CONVENTIONAL CELL

$$\mathbf{a}_c = \mathbf{b}_c = \mathbf{c}_c; \alpha_c, \beta_c, \gamma_c$$

SYSTEMS II: lattice parameter of MgO

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What is the lattice parameter of MgO?

CONVENTIONAL CELL

$$\mathbf{a}_c = \mathbf{b}_c = \mathbf{c}_c; \alpha_c, \beta_c, \gamma_c$$

\mathbf{a}_c

SYSTEMS III

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Is it possible to move
from the CONVENTIONAL CELL
to the PRIMITIVE CELL?

SYSTEMS III

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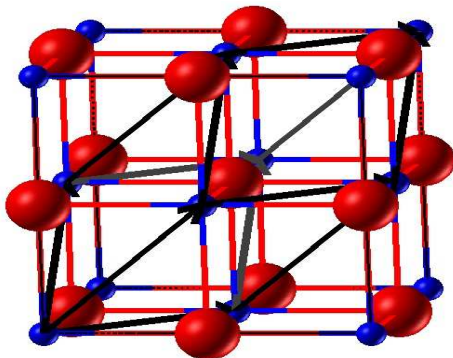
How

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Is it possible to move
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to the PRIMITIVE CELL?



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VIBRATIONS

VIBRATIONS: WHY ARE THEY IMPORTANT? ¹

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Atoms vibrate around their equilibrium positions.

- thermal properties: heat capacity, expansion
- phase transitions, including melting
- transport: thermal conductivity, sound
- electrical properties, e.g., superconductivity
- dielectric phenomena at low frequencies

¹From Prof N. M. Harrison's Lecture Notes: Vibrations in crystals

VIBRATIONS: FROM A FINITE SYSTEM TO AN INFINITE SYSTEM ¹

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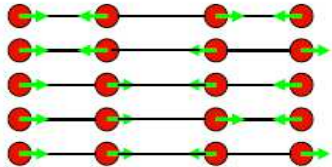
Simulation
types

Classical
simulation

How to write
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1 molecule



2 molecules



infinite crystal: continuum of vibrational modes

¹From Prof N. M. Harrison's Lecture Notes: Vibrations in crystals

VIBRATIONS: WAVELENGTH - WAVEVECTOR ¹

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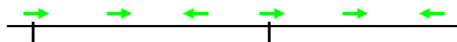
Classical
simulation

How to write
a report

$$\lambda = 2a, k = \pi/a$$



$$\lambda = 3a, k = 2\pi/3a$$



$$\lambda = \infty, k = 0$$



$$k = \frac{2\pi}{\lambda}$$

In this case, as k increases, the energy of vibration increases and the frequency too.

¹From Prof N. M. Harrison's Lecture Notes: Vibrations in crystals

VIBRATIONS: PHONON DISPERSION ¹

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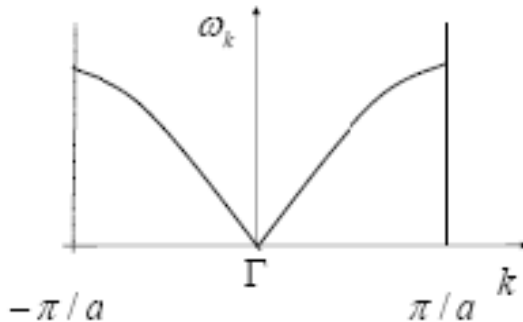
How

Simulation
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VIBRATIONAL FREQUENCY ω AS A FUNCTION OF k



¹From Prof N. M. Harrison's Lecture Notes: Vibrations in crystals

VIBRATIONS: PHONON DISPERSION ¹

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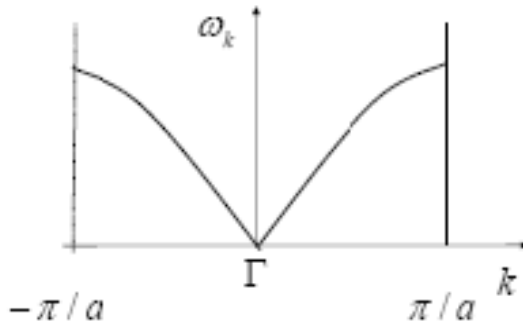
How

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VIBRATIONAL FREQUENCY ω AS A FUNCTION OF k



SIMILARLY, ELECTRONIC BAND STRUCTURE OF THE
HYDROGEN POLYMER

¹From Prof N. M. Harrison's Lecture Notes: Vibrations in crystals

VIBRATIONS: PHONON?

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How to write
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electron: WAVE or PARTICLE
radiation: WAVE or PARTICLE

VIBRATIONS: PHONON?

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How to write
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electron: WAVE or PARTICLE

radiation: WAVE or PARTICLE (**photon**)

VIBRATIONS: PHONON?

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How to write
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electron: WAVE or PARTICLE

radiation: WAVE or PARTICLE (**photon**)

vibration: WAVE or PARTICLE

VIBRATIONS: PHONON?

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How to write
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electron: WAVE or PARTICLE

radiation: WAVE or PARTICLE (**photon**)

vibration: WAVE or PARTICLE (**phonon**)

VIBRATIONS: 1D MONOATOMIC CHAIN (OR POLYMER) ¹

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INFINITE NUMBER OF VIBRATIONS → **BRANCH**

VIBRATIONS: 1D MONOATOMIC CHAIN (OR POLYMER) ¹

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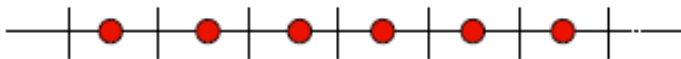
Vibrations

How

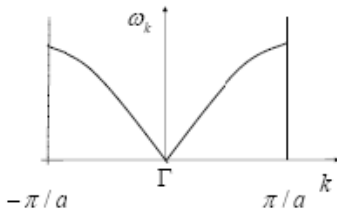
Simulation
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How to write
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INFINITE NUMBER OF VIBRATIONS → **BRANCH**



$$\omega_k = \sqrt{\frac{4J}{M}} |\sin(ka/2)|$$

VIBRATIONS: 1D MONOATOMIC CHAIN (OR POLYMER) ¹

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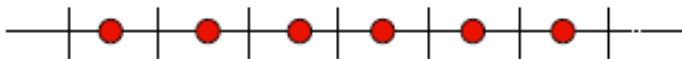
Vibrations

How

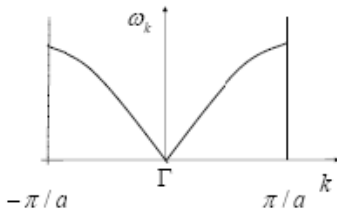
Simulation
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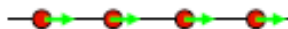


INFINITE NUMBER OF VIBRATIONS → **BRANCH**



$$\omega_k = \sqrt{\frac{4J}{M}} |\sin(ka/2)|$$

$$k = 0 (\Gamma \text{ point}): \omega_{k=0} = 0$$



$$k = \pi/a: \omega_{\pi/a} = \sqrt{\frac{4J}{M}}$$



$$k = \pi/2a: \omega_{\pi/2a} = \sqrt{\frac{2J}{M}}$$



VIBRATIONS: DIRECT AND RECIPROCAL SPACE

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1 PERIODIC DIRECTION IN THE
DIRECT SPACE!

\mathbf{a}

1 PERIODIC DIRECTION IN THE
RECIPROCAL SPACE!

$$\mathbf{a}^* = \frac{2\pi}{\mathbf{a}}$$

VIBRATIONS: 1D DIATOMIC CHAIN

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(SIMILARLY TO THE POLYMER WITH H_2 PER CELL)

FOLDING PROCESS!!!

VIBRATIONS: 1D HETERO DIATOMIC CHAIN ¹

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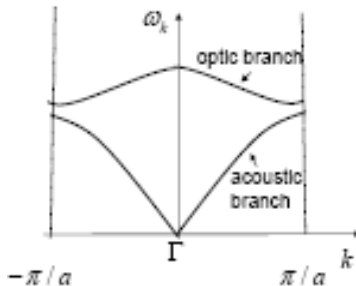
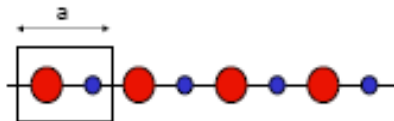
Vibrations

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¹From Prof N. M. Harrison's Lecture Notes: Vibrations in crystals

VIBRATIONS: OPTIC AND ACOUSTIC MODES

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OPTIC:

- 1) has a frequency that is in the vicinity of the optical region of the electromagnetic spectrum
- 2) the atomic motions associated are the same as the response to an oscillating electromagnetic field

ACOUSTIC:

- 1) has acoustic frequency

VIBRATIONS: LONGITUDINAL AND TRANSVERSE MODES ¹

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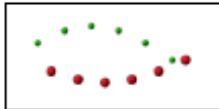
Longitudinal acoustic mode



Transverse acoustic mode



Transverse optic mode



¹From Prof N. M. Harrison's Lecture Notes: Vibrations in crystals

VIBRATIONS: 3D HETERO DIATOMIC CRYSTAL ¹

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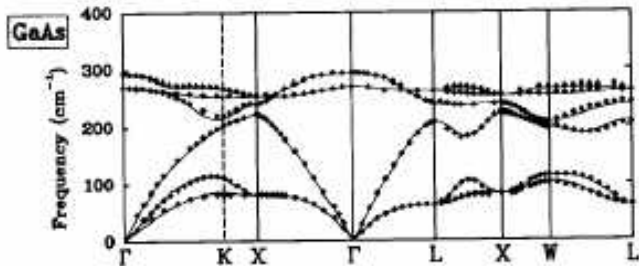
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Neutron data for GaAs

¹From Prof N. M. Harrison's Lecture Notes: Vibrations in crystals

HOW?

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COMPUTATIONAL EXPERIMENT / SIMULATION

- program
- input

Environment:
the choice of the Operating System → **linux**

Interface:
DLV = package for the visualisation of materials
structures and properties.

SIMULATION TYPES

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- CLASSICAL SIMULATION

Newton law → **GULP**

- QUANTUM-MECHANICAL SIMULATION

Schroedinger equation → **CRYSTAL**

Systems under investigation

Properties

Accuracy

Computational time

Resources

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CLASSICAL SIMULATION

INTERATOMIC POTENTIAL

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- coulombic interaction
- short term repulsive contribution
- Morse-like potential

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HELMHOLTZ FREE ENERGY

$$F = E_0 + \frac{1}{2} \sum_{k,j} \hbar \omega_{j,k} + k_B T \sum_{k,j} \ln[1 - \exp(-\hbar \omega_{j,k} / k_B T)]$$

¹From Prof N. M. Harrison's Lecture Notes: Vibrations in crystals

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HELMHOLTZ FREE ENERGY

$$F = E - TS$$

$$F = F(T, V)$$

MOLECULAR DYNAMICS ¹

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Initial configuration and initial velocities:
the initial configuration will be that of ideal MgO
the velocities will be random but scaled to produce
roughly the target temperature.

- Compute the forces on the atoms (F).
- Compute the accelerations $a = F/m$
- Update the velocities: $V_{\text{new}} = V_{\text{old}} + a * dt$
- Update the positions of the atoms: $R_{\text{new}} = R_{\text{old}} + V_{\text{new}} * dt$
- Repeat until average properties like E and T settle down
- Once settled measure some properties.

¹From Prof N. M. Harrison's Lecture Notes: Vibrations in crystals

GEOMETRY OPTIMIZATION I

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What does it mean?

GEOMETRY OPTIMIZATION I

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What does it mean?

Minimization of the energy as a function
of the atomic position
(x_i, y_i, z_i , with $i = 1, N$,
and N is the number of atoms)
and of the lattice parameters
(**a**,**b**,**c**, α , β , γ)

GEOMETRY OPTIMIZATION II

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How many variables for MgO ?

HOW TO WRITE A REPORT I

by Giulia C. De Fusco

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Introduction

- the system
- the methodology (theory in use)
- the aims of the exercise
- the tools in use (programs)

Body of the text

- write it like a scientific paper (well-articulated sentences, NOT a list of two-word answers)
- analyse *critically* obtained data and given answers
- round numerical answers to a specific number of decimal places (i.e. 4)
- add literature/web citations whenever a comparison with experimental data is required
- add explicitly every formula used one to obtain results
- check spelling

HOW TO WRITE A REPORT II

by Giulia C. De Fusco

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Pictures

- max 20
- reasonably sized (NOT one-page sized pictures, but still readable)
- white background (follow the instructions given on the website clicking on the link 'How to save a picture for your report')
- described in caption or in the text

Graphs

- add labels and units
- add a *critical* comment whenever required (NOT a merely descriptive comment)

HOW TO WRITE A REPORT III

by Giulia C. De Fusco

COMP LAB

G. Mallia

Timetable
Deadline

Aims
Systems

Vibrations

How

Simulation
types

Classical
simulation

How to write
a report

Tables

- add labels and units
- round numerical answers to a specific number of decimal places (i.e. 4)
- repeat heading if the table cannot fit in a single page

Conclusions

- give a general description of your calculations and your main findings
- outline the differences between the methods in use and the results obtained
- analyse critically these differences

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THANK YOU!!!