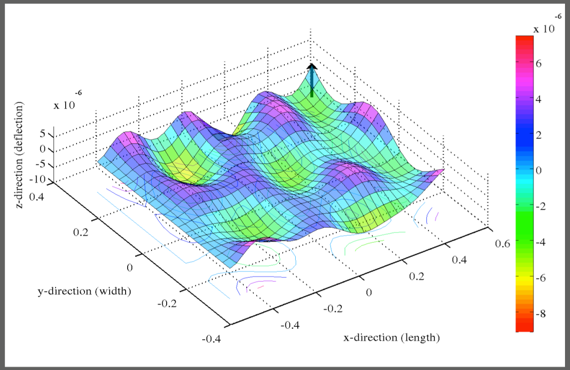
Research directions in computational mechanics across length-scales

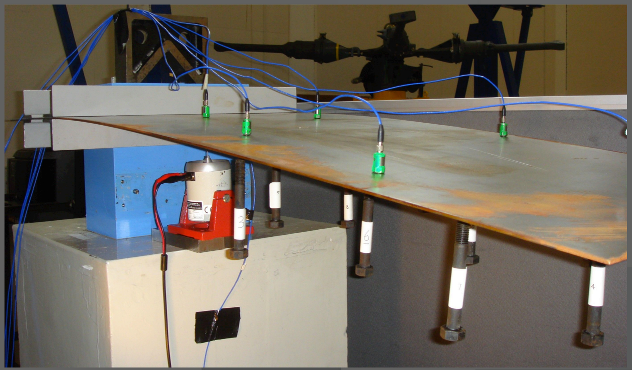
Swansea University
Prifysgol Abertawe

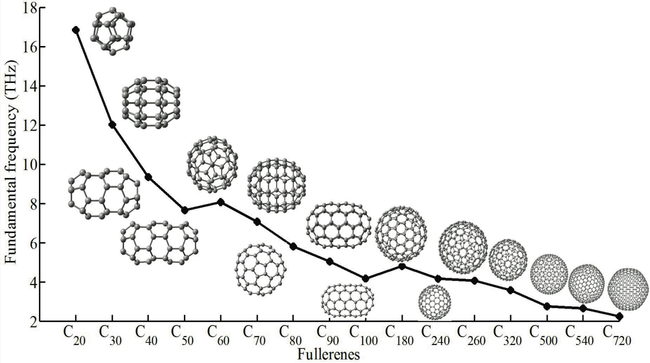
Universidade Federal de Uberlândia
15 February 2013

Sondipon Adhikari

Twitter: @ProfAdhikari, http://engweb.swan.ac.uk/~adhikaris/







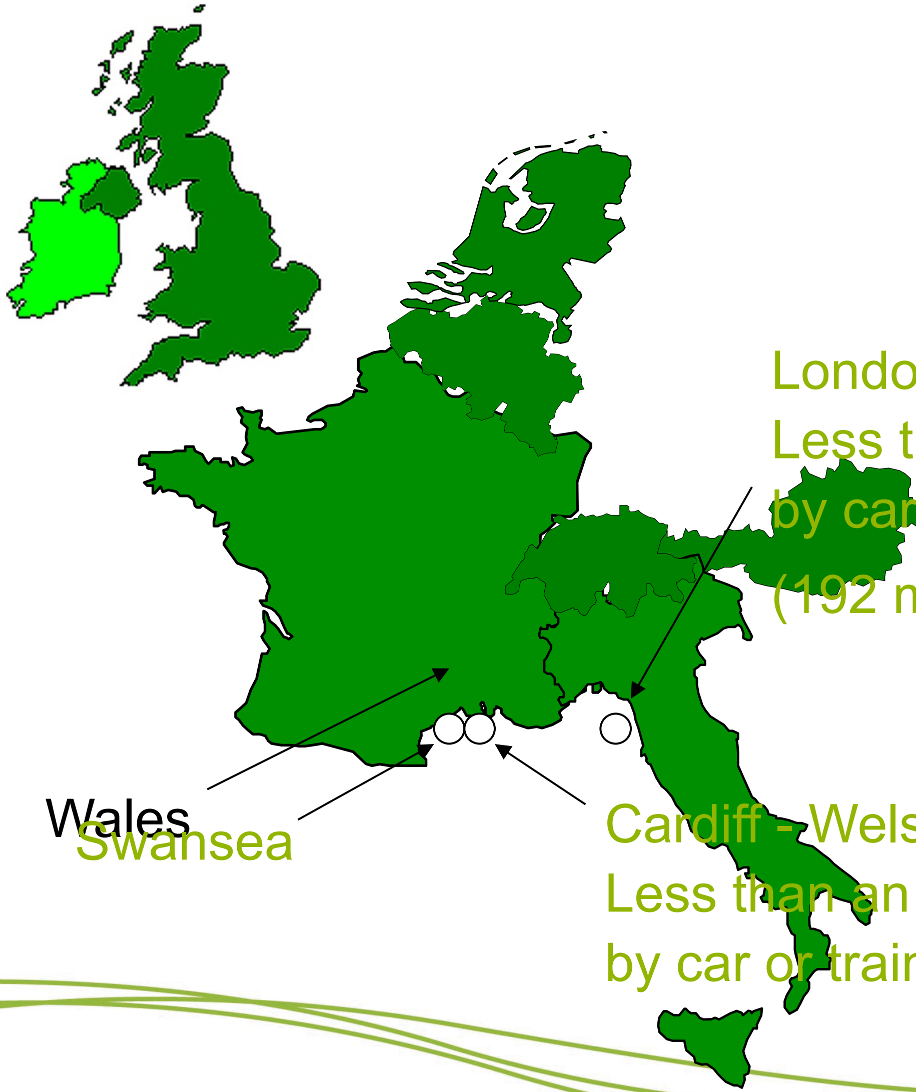
Overview

- Introduction – Swansea University
- College of Engineering – Aerospace program
- My research overview
- Nanotubes, Graphene, Fullerenes: static and dynamic analysis, buckling, composites
- Nanobio sensors: vibrating nanotube and graphene based mass sensor
- DNA mechanics
- Conclusions

Overview

- Introduction – Swansea University
- College of Engineering – Aerospace program
- My research interests
- Stochastic dynamic analysis
- Vibration energy harvesting
- Nanotubes, Graphene, Fullerenes, DNA: static and dynamic analysis, buckling, composites
- Conclusions

Where is Swansea?



London – UK Capital
Less than three hours
by car or train

(192 miles)

Wales

Swansea

Cardiff - Welsh Capital
Less than an hour away
by car or train

Swansea University

- 29th UK university to be established
- King George V laid the foundation stone of the University in July 1920
- Now over 12,500 students - 1,800 international

The College of Engineering

- Engineering established at the Universities Inception in 1920
- Formed into Multidisciplinary College in 2001
- Offering 11 undergraduate disciplines
- Wide portfolio of postgraduate options, including MSc, MRes, PhD and EngD
- Professionally accredited degrees
- Extensive Industry links, including TATA Steel, Rolls Royce, Airbus, European Space Agency, BAe systems, Siemens, IBM, Motorola, BT, Ericsson, Esso, BP Chemicals
- Friendly and supportive study environment within the College and the Campus

The College of Engineering

~ 100 academic staff

~ 45 support staff

~ 500 research staff and postgraduate students

(~150 International)

~ 1600 undergraduates

(~300 International)

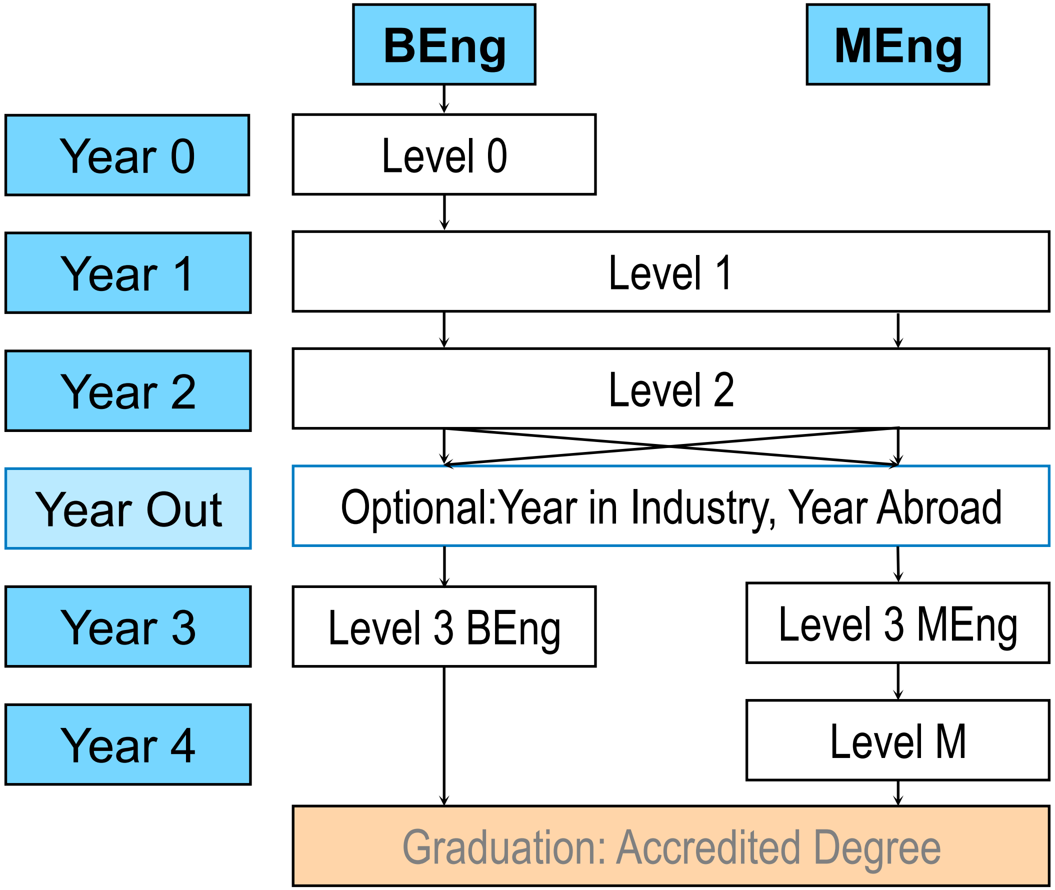
Undergraduate Degrees

Aerospace
Chemical and Biological Process
Civil
Electrical and Electronic
Materials
Mechanical
Product Design

Environmental
Medical

Sports Science & Engineering
Sports Materials

Undergraduate Degrees



BEng

MEng

Year 0

Level 0

Year 1

Level 1

Year 2

Level 2

Year Out

Optional:Year in Industry, Year Abroad

Year 3

Level 3 BEng

Level 3 MEng

Year 4

Level M

Graduation: Accredited Degree

Accreditation

Accreditation to the appropriate professional bodies:

Institute of Materials, Minerals and Mining (IOM3)

Royal Aeronautical Society (RAeS)

Institution of Chemical Engineers (IChemE)

Institution of Mechanical Engineers (IMechE)

Institute of Civil Engineers (ICE)

Institution of Electrical Engineers (IEEE)

A graduate can achieve “Chartered” (CEng) Status with additional work experience.

Postgraduate Degrees

Masters Degree Schemes:

Master of Science (MSc)

Master of Science by Research (MScR)

Master of Philosophy (MPhil)

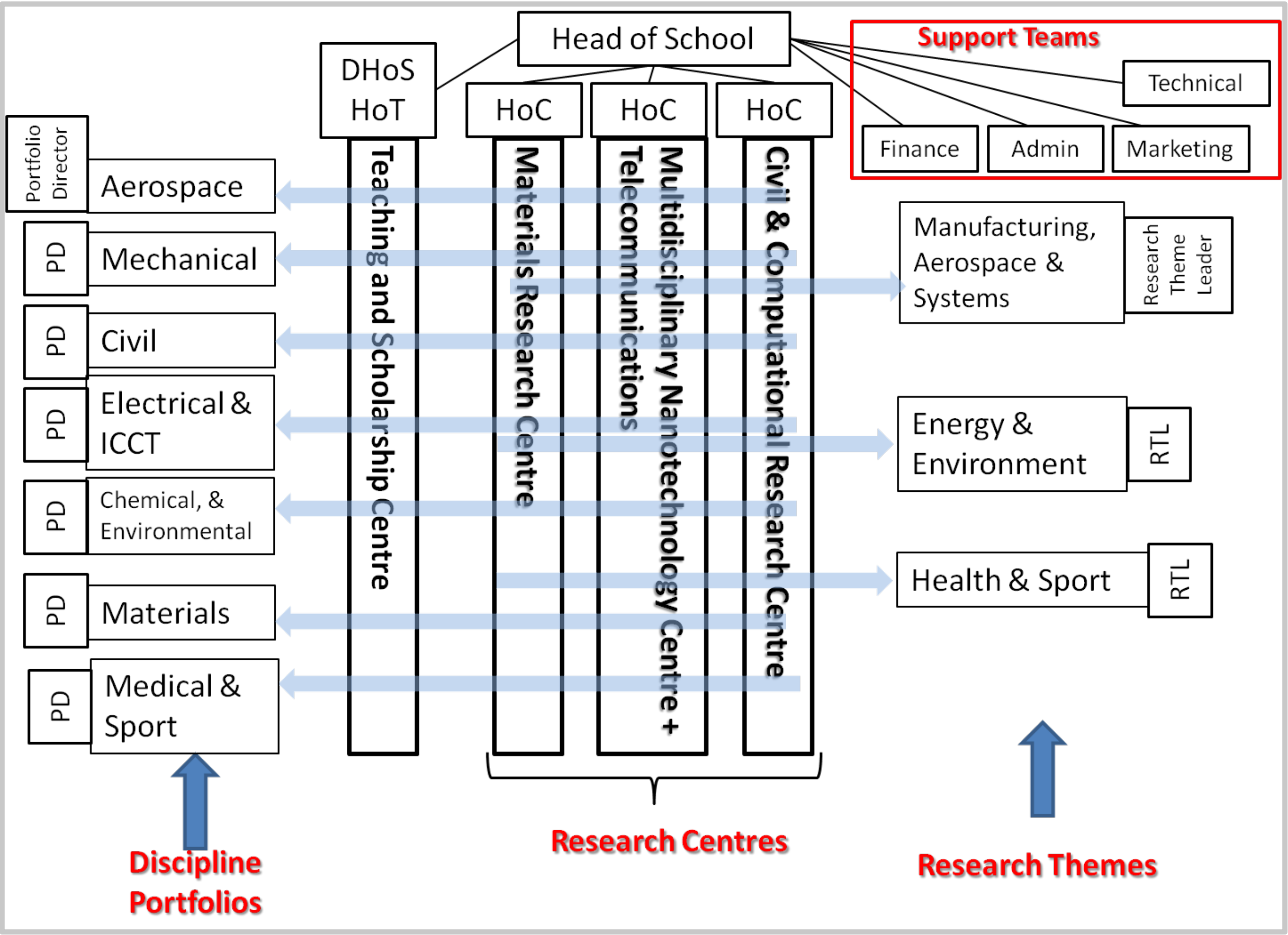
Master of Research (MRes)

Doctorate Degree Schemes:

Doctor of Philosophy (PhD)

Engineering Doctorate (EngD)

World Class Research



Head of School

DHoS
HoT

HoC

HoC

HoC

Support Teams

Technical

Finance

Admin

Marketing

Portfolio Director

Aerospace

PD

Mechanical

PD

Civil

PD

Electrical & ICCT

PD

Chemical, & Environmental

PD

Materials

PD

Medical & Sport

Teaching and Scholarship Centre

Materials Research Centre

Multidisciplinary Nanotechnology Centre + Telecommunications

Civil & Computational Research Centre

Manufacturing, Aerospace & Systems

Research Theme Leader

Energy & Environment

RTL

Health & Sport

RTL

Discipline Portfolios

Research Centres

Research Themes

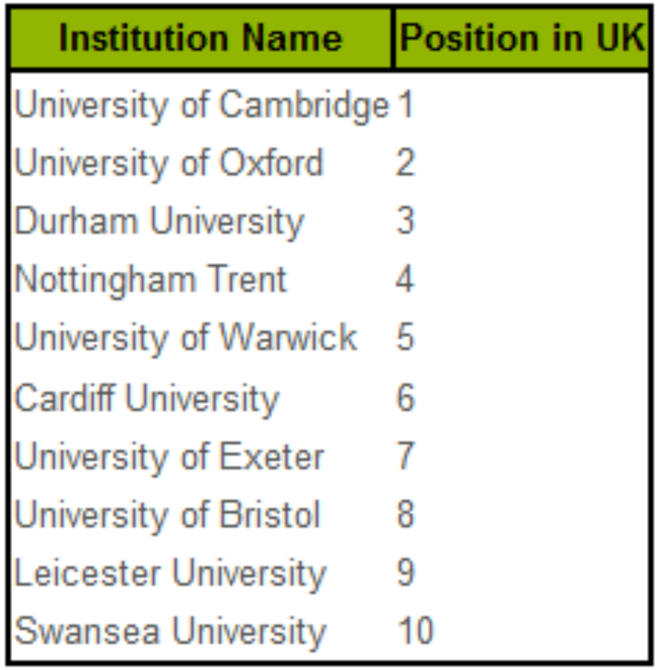
RAE Ranking

Source: Research Assessment Exercise 2008, overall summary of results using weighted averages www.rae.ac.uk)

Institution name	Staff FTE's	Overall GPA	Position in UK
University of Cambridge	210	3.321	1
University of Oxford	122.7	3.07	2
Imperial College London	293.1	3.036	3
University of Manchester	180.22	2.963	4
University of Nottingham	114.51	2.948	5
University of Surrey	110.25	2.93	6
University of Leeds	132.7	2.911	7
Swansea University	**63.5**	**2.902**	**8**
University of Bristol	88.1	2.88	9
University of Warwick	69.45	2.85	10

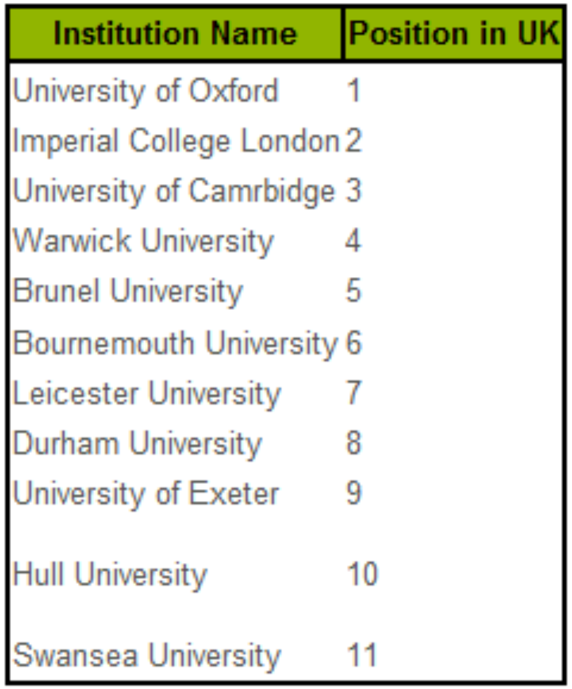
League Tables

The Guardian



Institution Name	Position in UK
University of Cambridge	1
University of Oxford	2
Durham University	3
Nottingham Trent	4
University of Warwick	5
Cardiff University	6
University of Exeter	7
University of Bristol	8
Leicester University	9
Swansea University	10

The Times

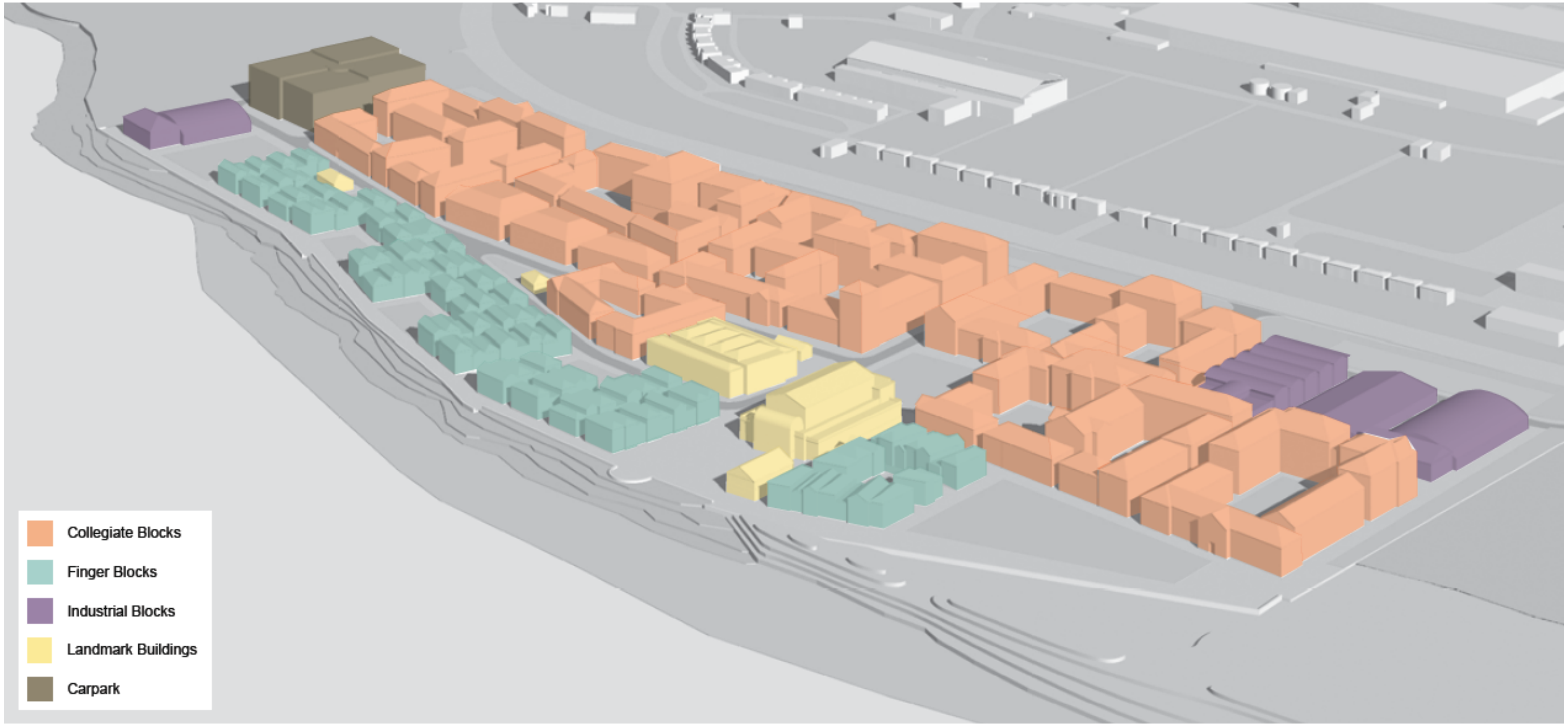


Institution Name	Position in UK
University of Oxford	1
Imperial College London	2
University of Camrbidge	3
Warwick University	4
Brunel University	5
Bournemouth University	6
Leicester University	7
Durham University	8
University of Exeter	9
Hull University	10
Swansea University	11

Science and Innovation Campus Site

Swansea University
Prifysgol Abertawe

Science and Innovation Campus



Science & Innovation Campus

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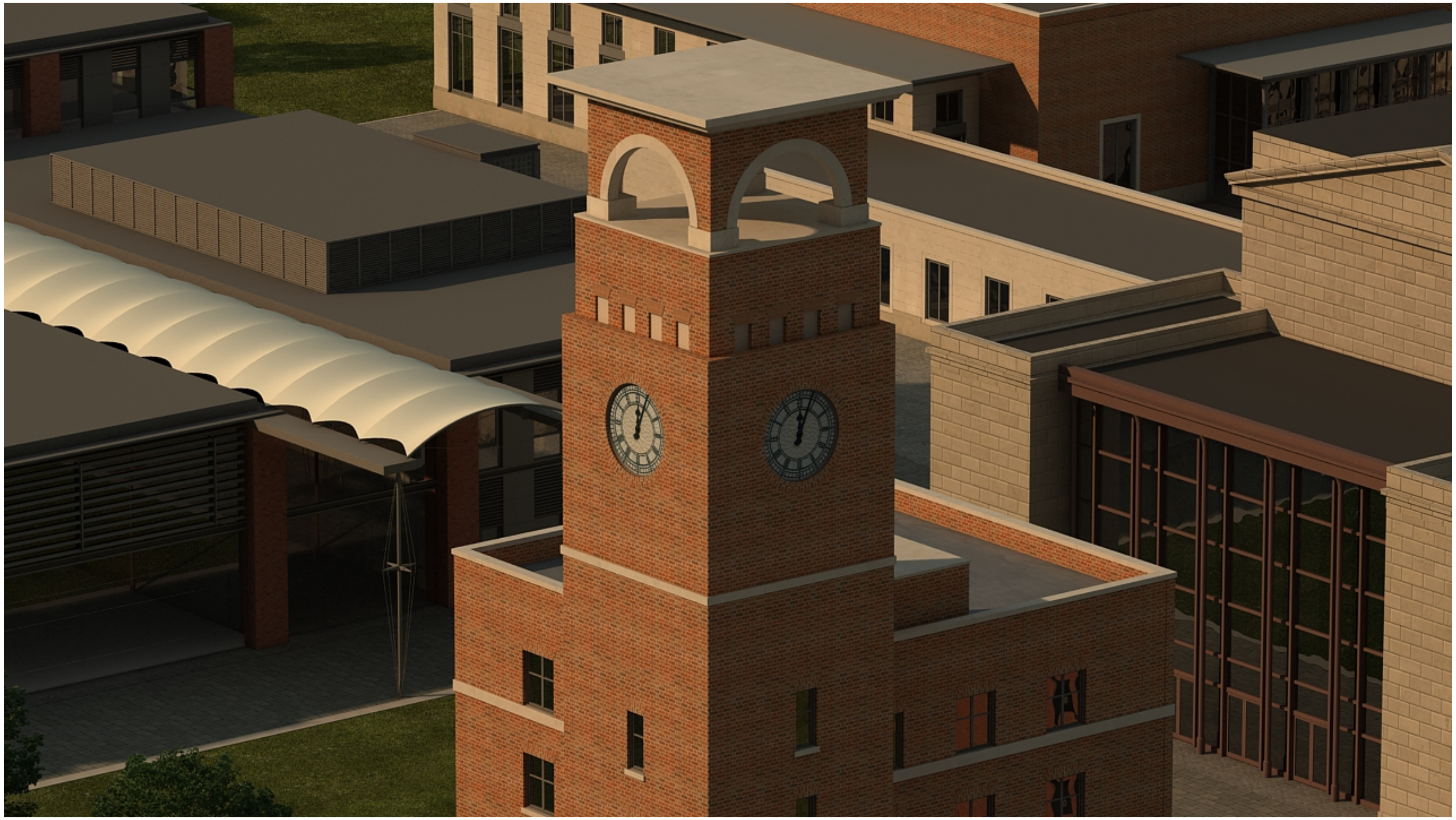


Science & Innovation Campus

bp

ST.MODWEN
ARBENIGWYR ADFYWIO MWYAF BLAENLLAW'R DU

Campws Gwyddoniaeth ac Arloesedd Arfaethedig Newydd

Swansea University

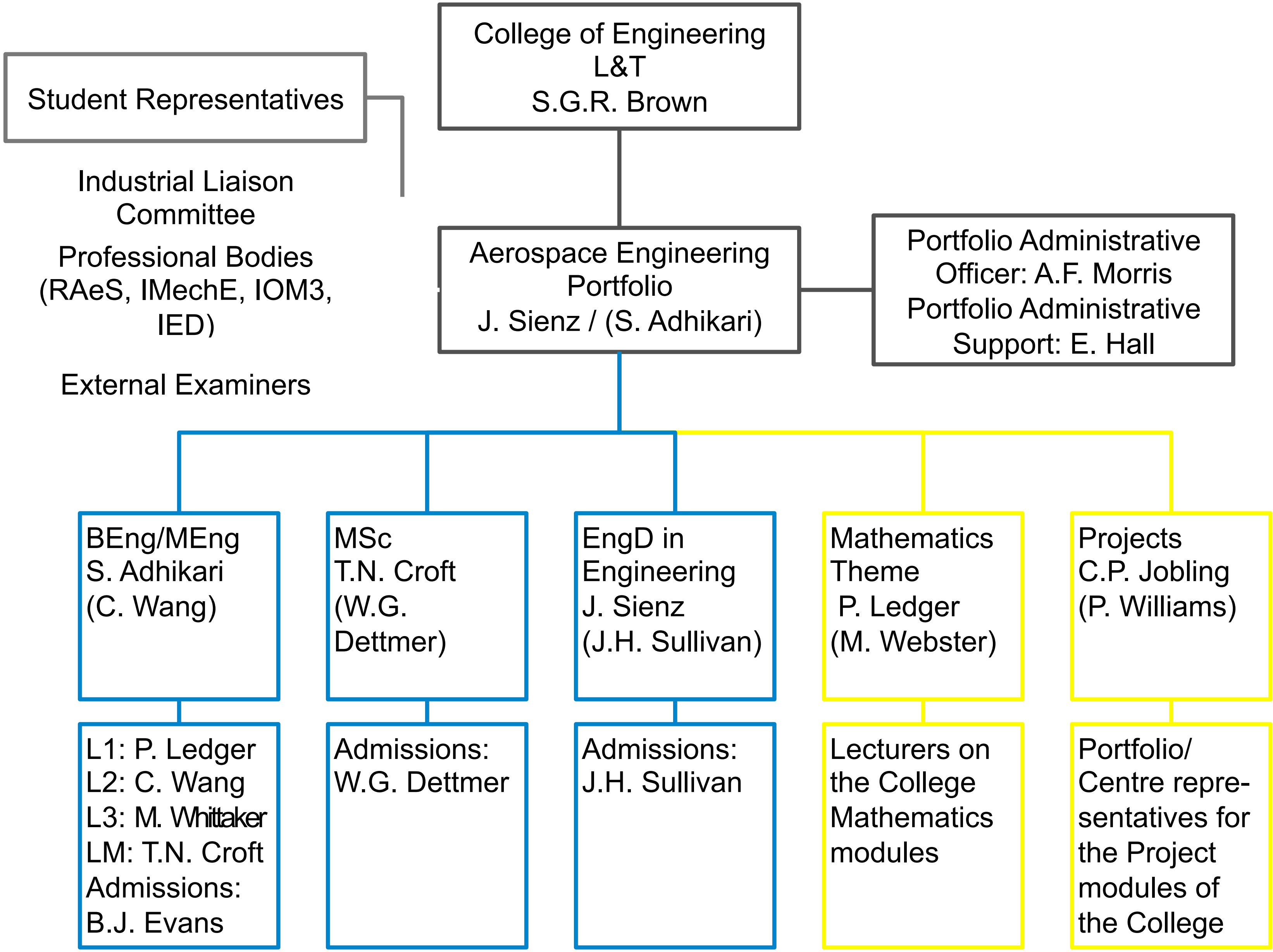
BEng/MEng Aerospace Engineering

Swansea University
Prifysgol Abertawe

College of Engineering

www.swansea.ac.uk/engineering

Aerospace Engineering Structure



College of Engineering
L&T
S.G.R. Brown

Student Representatives

Industrial Liaison Committee

Professional Bodies (RAeS, IMechE, IOM3, IED)

External Examiners

Aerospace Engineering Portfolio
J. Sienz / (S. Adhikari)

Portfolio Administrative Officer: A.F. Morris
Portfolio Administrative Support: E. Hall

BEng/MEng
S. Adhikari
(C. Wang)

L1: P. Ledger
L2: C. Wang
L3: M. Whittaker
LM: T.N. Croft
Admissions:
B.J. Evans

MSc
T.N. Croft
(W.G. Dettmer)

Admissions:
W.G. Dettmer

EngD in Engineering
J. Sienz
(J.H. Sullivan)

Admissions:
J.H. Sullivan

Mathematics Theme
P. Ledger
(M. Webster)

Lecturers on the College Mathematics modules

Projects
C.P. Jobling
(P. Williams)

Portfolio/Centre representatives for the Project modules of the College

Aerospace Summary

Accreditation: BEng/MEng/MSc/EngD with minor changes

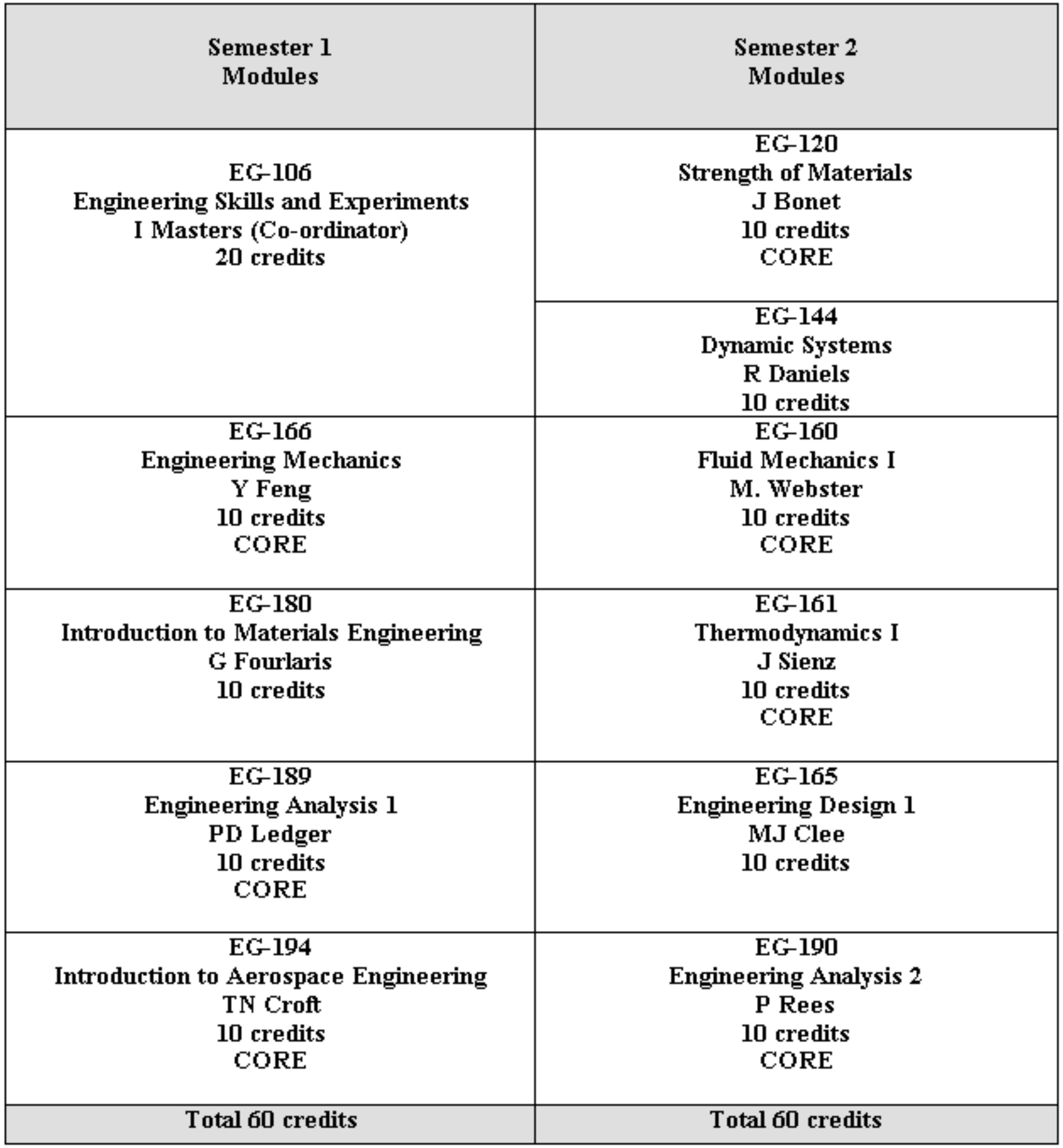
BEng/MEng:

- 60% increase in L1 students from 10/11 to 11/12
- 192 FTEs overall (4 L0, 89 L1, 65 L2, 26 L3, 8 LM)
- Second highest UCAS entry (just behind Welsh)
- Highest conversion rate in Engineering

Current Student numbers

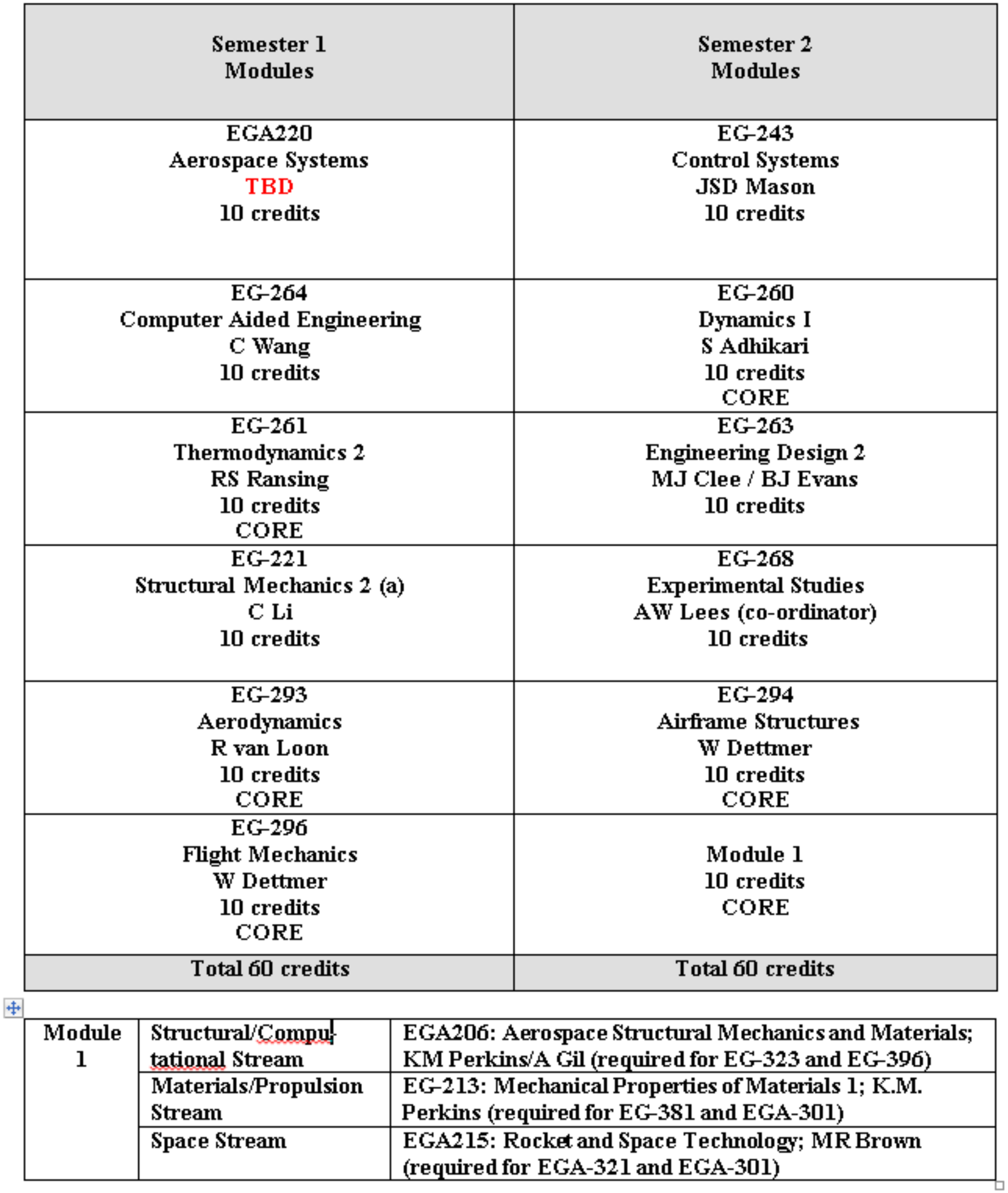
Level 1	91
Level 2	85
Level 3	71
Level M	6

Level 1



Semester 1 Modules	Semester 2 Modules
EG-106 Engineering Skills and Experiments I Masters (Co-ordinator) 20 credits	EG-120 Strength of Materials J Bonet 10 credits CORE
	EG-144 Dynamic Systems R Daniels 10 credits
EG-166 Engineering Mechanics Y Feng 10 credits CORE	EG-160 Fluid Mechanics I M. Webster 10 credits CORE
EG-180 Introduction to Materials Engineering G Fourlaris 10 credits	EG-161 Thermodynamics I J Sienz 10 credits CORE
EG-189 Engineering Analysis 1 PD Ledger 10 credits CORE	EG-165 Engineering Design 1 MJ Clee 10 credits
EG-194 Introduction to Aerospace Engineering TN Croft 10 credits CORE	EG-190 Engineering Analysis 2 P Rees 10 credits CORE
Total 60 credits	Total 60 credits

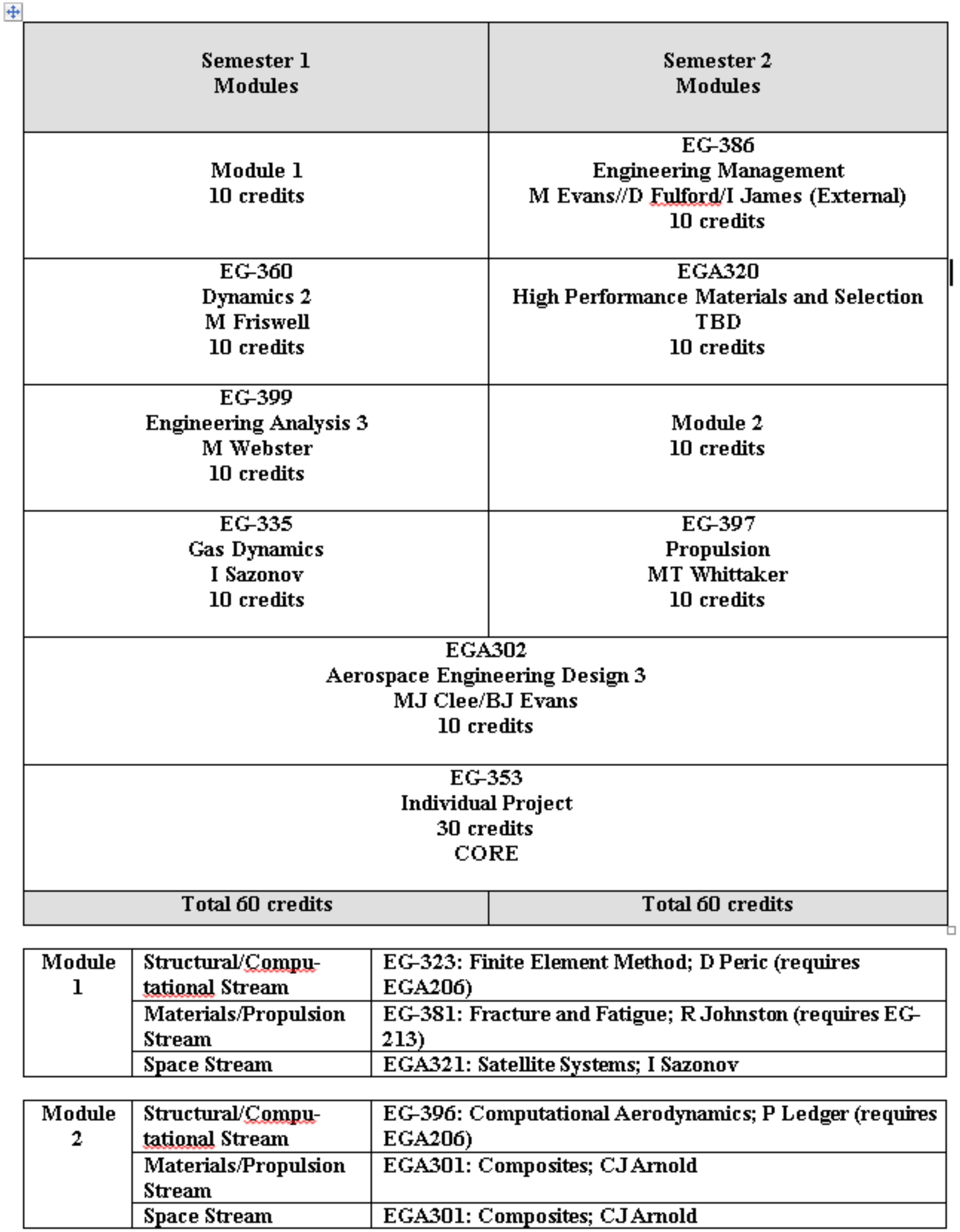
Level 2



Semester 1 Modules	Semester 2 Modules
EGA220 Aerospace Systems TBD 10 credits	EG-243 Control Systems JSD Mason 10 credits
EG-264 Computer Aided Engineering C Wang 10 credits	EG-260 Dynamics I S Adhikari 10 credits CORE
EG-261 Thermodynamics 2 RS Ransing 10 credits CORE	EG-263 Engineering Design 2 MJ Clee / BJ Evans 10 credits
EG-221 Structural Mechanics 2 (a) C Li 10 credits	EG-268 Experimental Studies AW Lees (co-ordinator) 10 credits
EG-293 Aerodynamics R van Loon 10 credits CORE	EG-294 Airframe Structures W Dettmer 10 credits CORE
EG-296 Flight Mechanics W Dettmer 10 credits CORE	Module 1 10 credits CORE
Total 60 credits	Total 60 credits

Module 1	Structural/Computational Stream	EGA206: Aerospace Structural Mechanics and Materials; KM Perkins/A Gil (required for EG-323 and EG-396)
	Materials/Propulsion Stream	EG-213: Mechanical Properties of Materials 1; K.M. Perkins (required for EG-381 and EGA-301)
	Space Stream	EGA215: Rocket and Space Technology; MR Brown (required for EGA-321 and EGA-301)

Level 3

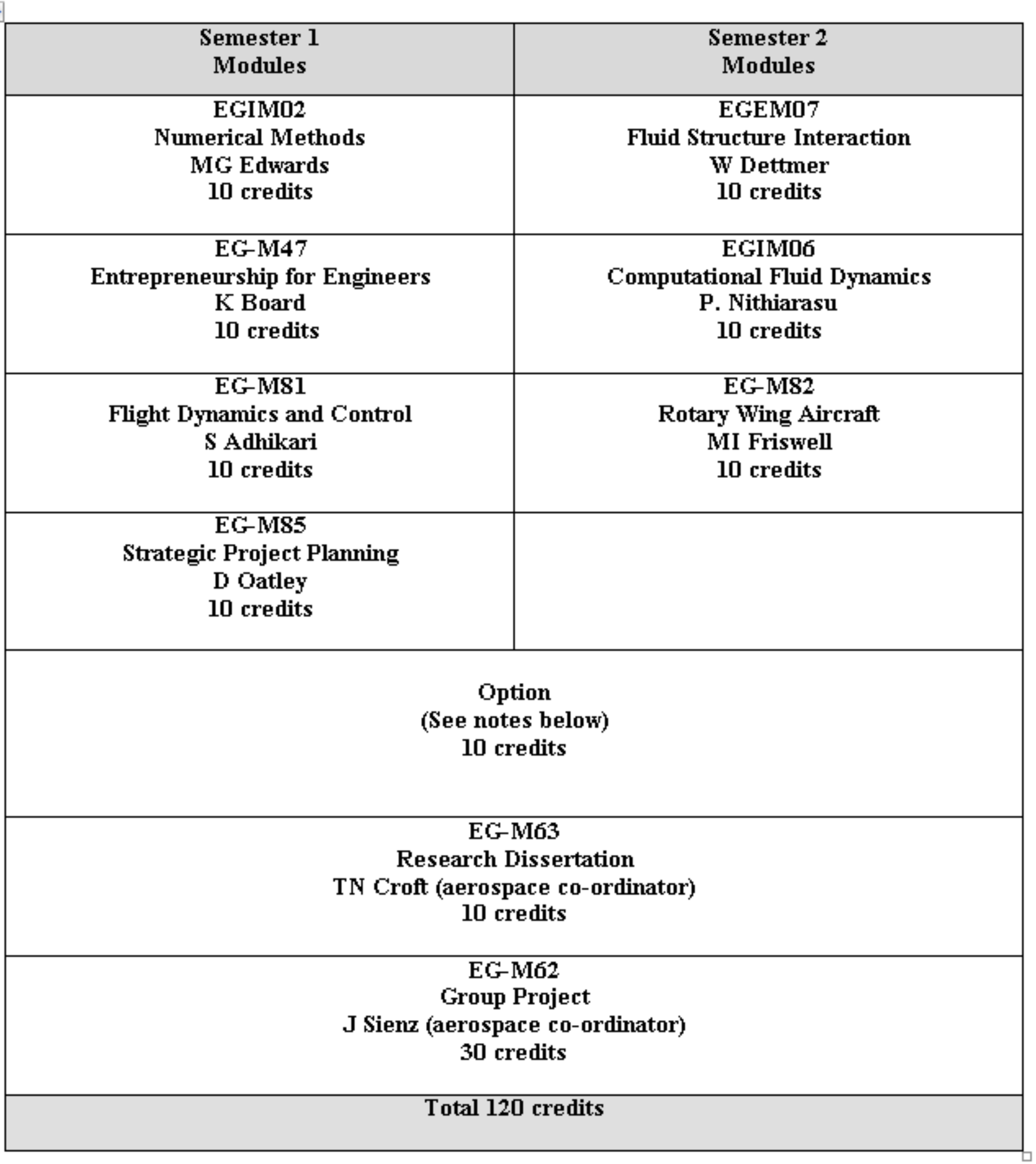


Semester 1 Modules	Semester 2 Modules
Module 1 10 credits	EG-386 Engineering Management M Evans//D Fulford/I James (External) 10 credits
EG-360 Dynamics 2 M Friswell 10 credits	EGA320 High Performance Materials and Selection TBD 10 credits
EG-399 Engineering Analysis 3 M Webster 10 credits	Module 2 10 credits
EG-335 Gas Dynamics I Sazonov 10 credits	EG-397 Propulsion MT Whittaker 10 credits
EGA302 Aerospace Engineering Design 3 MJ Clee/BJ Evans 10 credits	
EG-353 Individual Project 30 credits CORE	
Total 60 credits	Total 60 credits

Module 1	Structural/Computational Stream	EG-323: Finite Element Method; D Peric (requires EGA206)
	Materials/Propulsion Stream	EG-381: Fracture and Fatigue; R Johnston (requires EG-213)
	Space Stream	EGA321: Satellite Systems; I Sazonov

Module 2	Structural/Computational Stream	EG-396: Computational Aerodynamics; P Ledger (requires EGA206)
	Materials/Propulsion Stream	EGA301: Composites; CJ Arnold
	Space Stream	EGA301: Composites; CJ Arnold

Level M

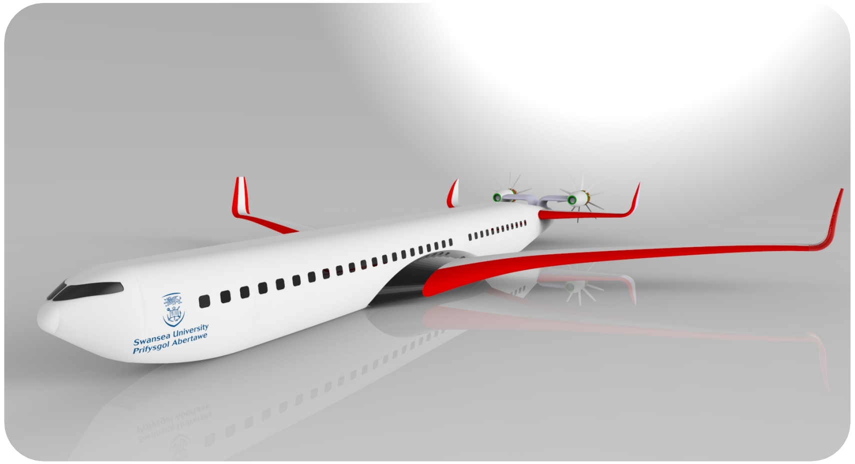


Semester 1 Modules	Semester 2 Modules
EGIM02 Numerical Methods MG Edwards 10 credits	EGEM07 Fluid Structure Interaction W Dettmer 10 credits
EG-M47 Entrepreneurship for Engineers K Board 10 credits	EGIM06 Computational Fluid Dynamics P. Nithiarasu 10 credits
EG-M81 Flight Dynamics and Control S Adhikari 10 credits	EG-M82 Rotary Wing Aircraft MI Friswell 10 credits
EG-M85 Strategic Project Planning D Oatley 10 credits	
Option (See notes below) 10 credits	
EG-M63 Research Dissertation TN Croft (aerospace co-ordinator) 10 credits	
EG-M62 Group Project J Sienz (aerospace co-ordinator) 30 credits	
Total 120 credits	

Level M Design project

Winner of Merlin Design and Aircraft Handling Competition:

- IT FLIES UK 2011
- IT FLIES US 2012
- Swansea is the first university to hold both titles at the same time

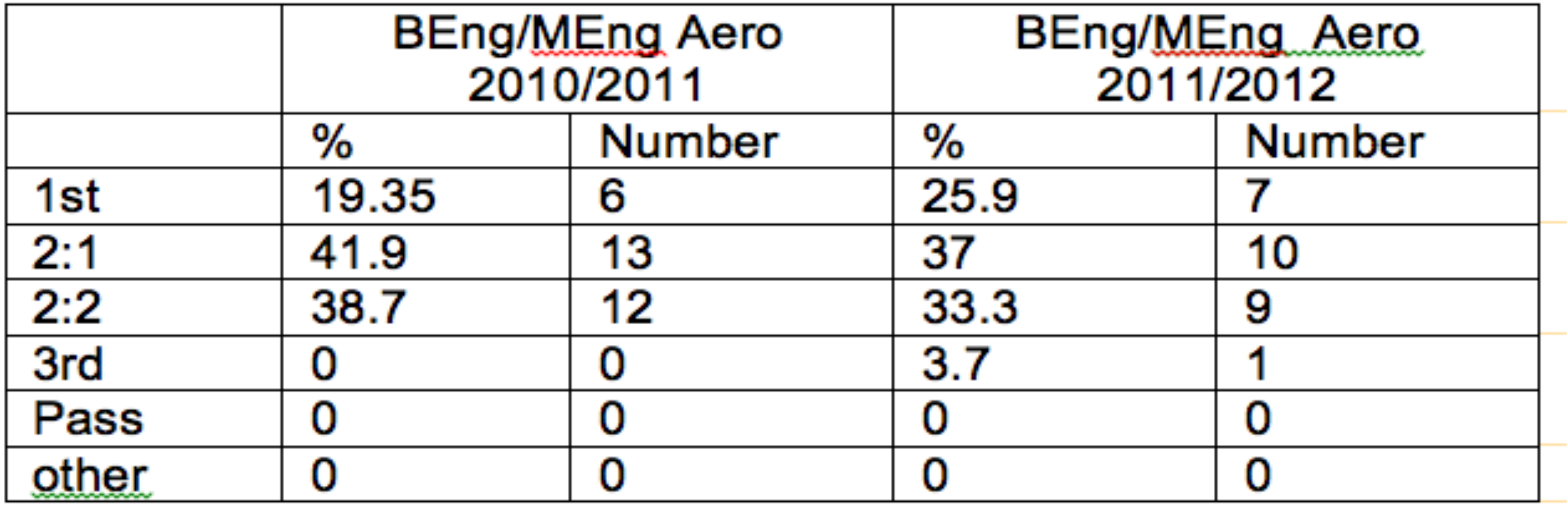


Site visits

Site visits to GE and Airbus, and also to Bloodhound Technical Centre

Flight training

Progression/Award Statistics



	BEng/MEng Aero 2010/2011		BEng/MEng Aero 2011/2012	
	%	Number	%	Number
1st	19.35	6	25.9	7
2:1	41.9	13	37	10
2:2	38.7	12	33.3	9
3rd	0	0	3.7	1
Pass	0	0	0	0
other	0	0	0	0

% Good Honours 10/11 = (6+13)/(6+13+12) x 100 = 19/31 x 100 = 61.3

% Good Honours 11/12 = (7+10)/(7+10+9+1) x 100 = 17/27 x 100 = 62.96

Executive Summary

5% improvement to 87% of students satisfied or very satisfied with the overall quality of their course.

Swansea University climbed 38 positions in UK rankings for student satisfaction to 42nd.

Swansea has climbed 12 places in the Sunday Times League Table to 45th position.

11 subject areas now in upper quartile, with 3 ranked in 1st position.

Student Recommendation

89% of final year and 91% of taught postgraduate students would recommend Swansea to a friend or relative

Research

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College of Engineering

www.swansea.ac.uk/engineering

Civil & Computational Research Centre

- Computational Mechanics
- Optimisation
- Computational Fluid dynamics
- Computational electromagnetics
- Rotordynamics
- Morphing wing aircraft
- Energy harvesting
- Computational Biomechanics
- Uncertainty quantification

My Research Areas

- Uncertainty quantification in modelling and simulation
- Dynamic analysis of complex structures
- Vibration energy harvesting
- Atomistic finite element method
- Dynamics of nanoscale structures
- Nanoscale bio sensors

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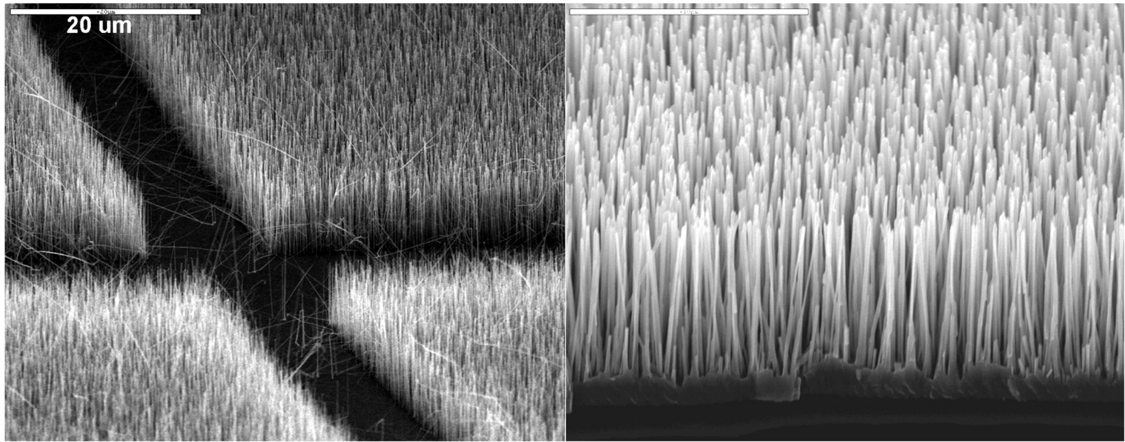
Uncertainty quantification

Uncertainty in Structural Dynamics

Stochastic dynamical systems across the length-scale



Equation of Motion of Dynamical Systems

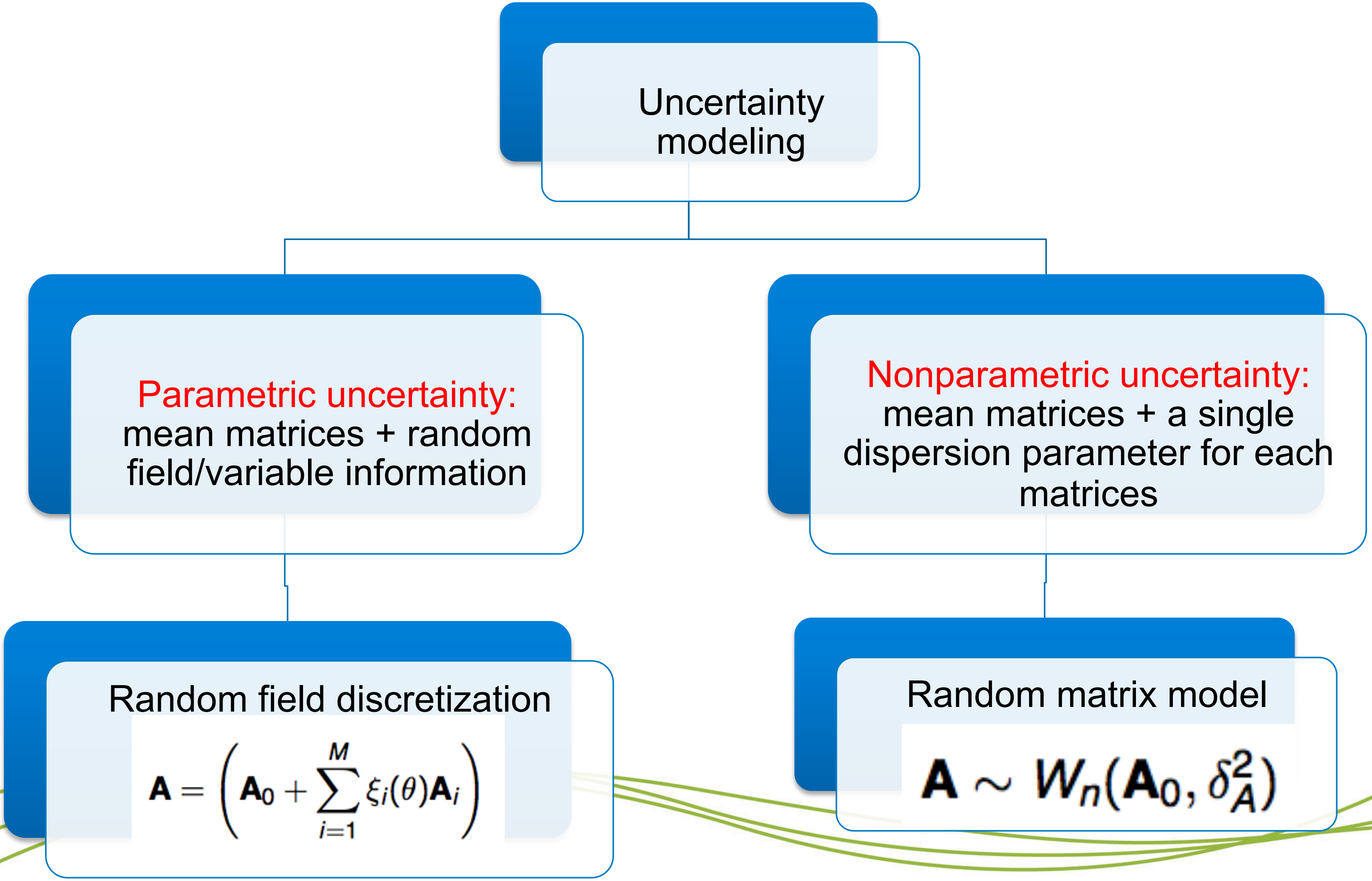
- The Equation of motion of all these systems (and many other) about an equilibrium point can be expressed by:

$$\mathbf{M}(\theta)\ddot{\mathbf{u}}(\theta, t) + \mathbf{C}(\theta)\dot{\mathbf{u}}(\theta, t) + \mathbf{K}(\theta)\mathbf{u}(\theta, t) = \mathbf{f}(t)$$

- $\mathbf{M}(\theta) \in \mathbb{R}^{n \times n}$ is the random mass matrix, $\mathbf{K}(\theta) \in \mathbb{R}^{n \times n}$ is the random stiffness matrix, $\mathbf{C}(\theta) \in \mathbb{R}^{n \times n}$ is the random damping matrix and $\mathbf{f}(t)$ is the forcing vector. We use (θ) to denote that the quantity is random.

The uncertainty propagation problem:
Given the stochastic description of the three systems matrices and the input forcing function, obtain the stochastic description of the response

Uncertainty modeling in structural dynamics



Uncertainty modeling

Parametric uncertainty: mean matrices + random field/variable information

Nonparametric uncertainty: mean matrices + a single dispersion parameter for each matrices

Random field discretization

$$\mathbf{A} = \left(\mathbf{A}_0 + \sum_{i=1}^{M} \xi_i(\theta) \mathbf{A}_i \right)$$

Random matrix model

$$\mathbf{A} \sim W_n(\mathbf{A}_0, \delta_A^2)$$

Dynamic Response

- For parametric uncertainty propagation:

$$\mathbf{u}(\omega,\theta)=\sum_{k=1}^{n_r}\frac{\phi_k^T\mathbf{f}(\omega)}{-\omega^2+2i\omega\zeta_k\omega_0^2+\omega_{0_k}^2+\sum_{i=1}^{M}\xi_i(\theta)\Lambda_{i_k}(\omega)}\phi_k$$

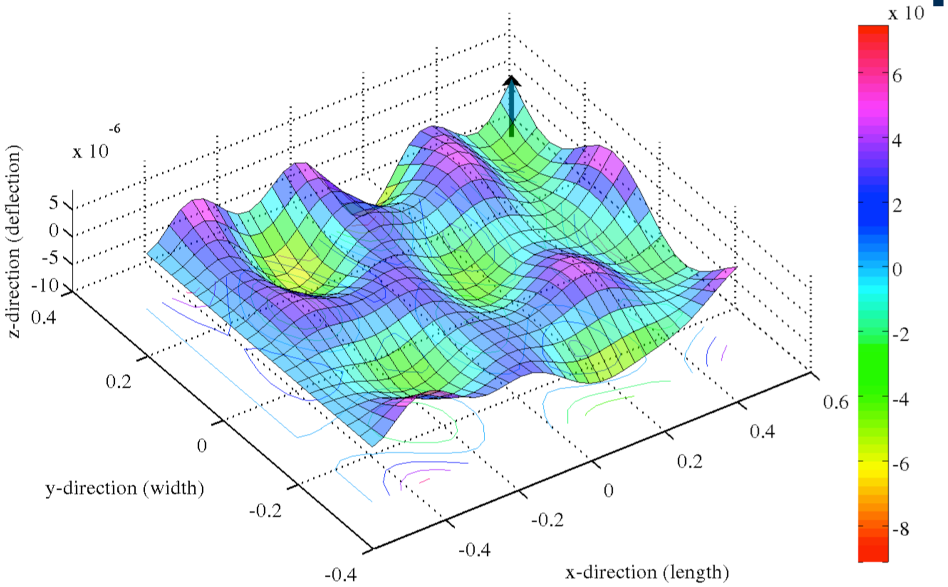
- For nonparametric uncertainty propagation

$$\mathbf{u}(\omega,\theta)=\sum_{k=1}^{n_r}\frac{\mathbf{x}_{r_k}(\theta)^T\mathbf{f}(s)}{-\omega^2+2i\omega\zeta_k\omega_{r_k}(\theta)+\omega_{r_k}^2(\theta)}\mathbf{x}_{r_k}(\theta)$$

$$\mathbf{X}_r(\theta)=\mathbf{\Phi}\mathbf{\Psi}_r,\quad \mathbf{\Psi}_r^T\mathbf{W}\mathbf{\Psi}_r=\mathbf{\Omega}_r^2$$

- Unified mathematical representation
- Can be useful for hybrid experimental-simulation approach for uncertainty quantification

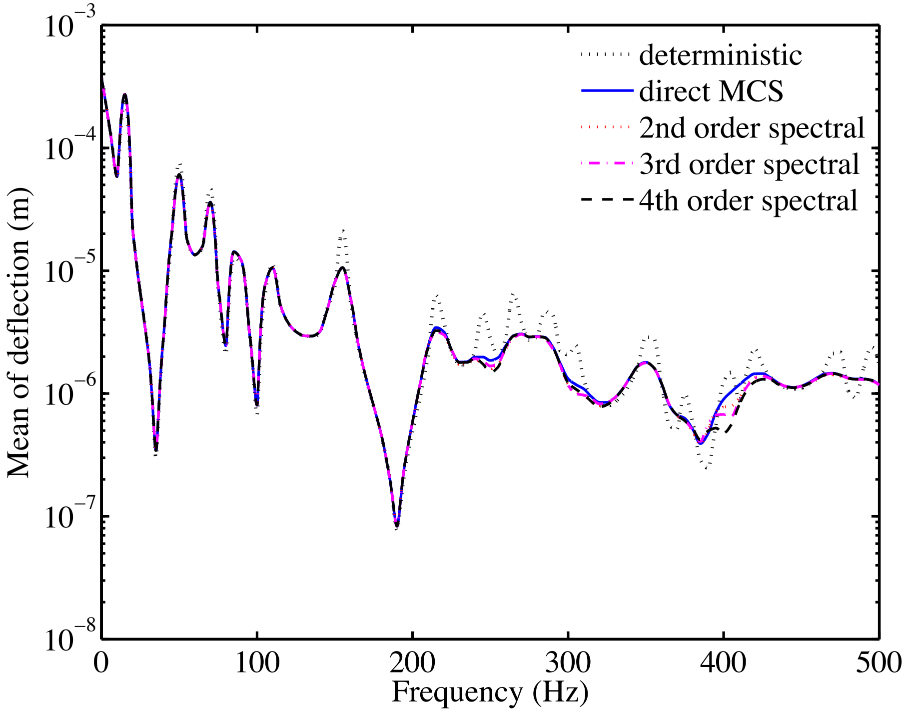
Plate with Stochastic Properties



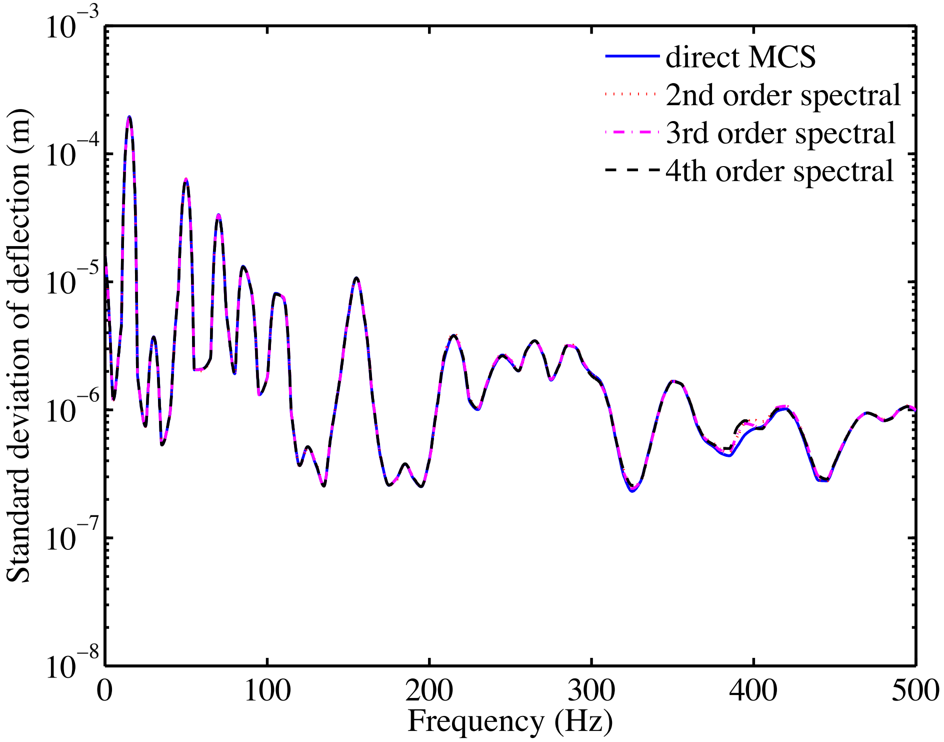
- An Euler-Bernoulli cantilever beam with stochastic bending modulus (nominal properties 1m x 0.6m, t=03mm, E=2 x 10^{11} Pa)
- We use n=1881, M=16

- We study the deflection of the beam under the action of a point load on the free end.
- The bending modulus is taken to be a homogeneous stationary Gaussian random field with exponential autocorrelation function (correlation lengths L/5)
- Constant modal damping is taken with 1% damping factor for all modes.

Response Statistics



Mean with $\sigma_a = 0.1$

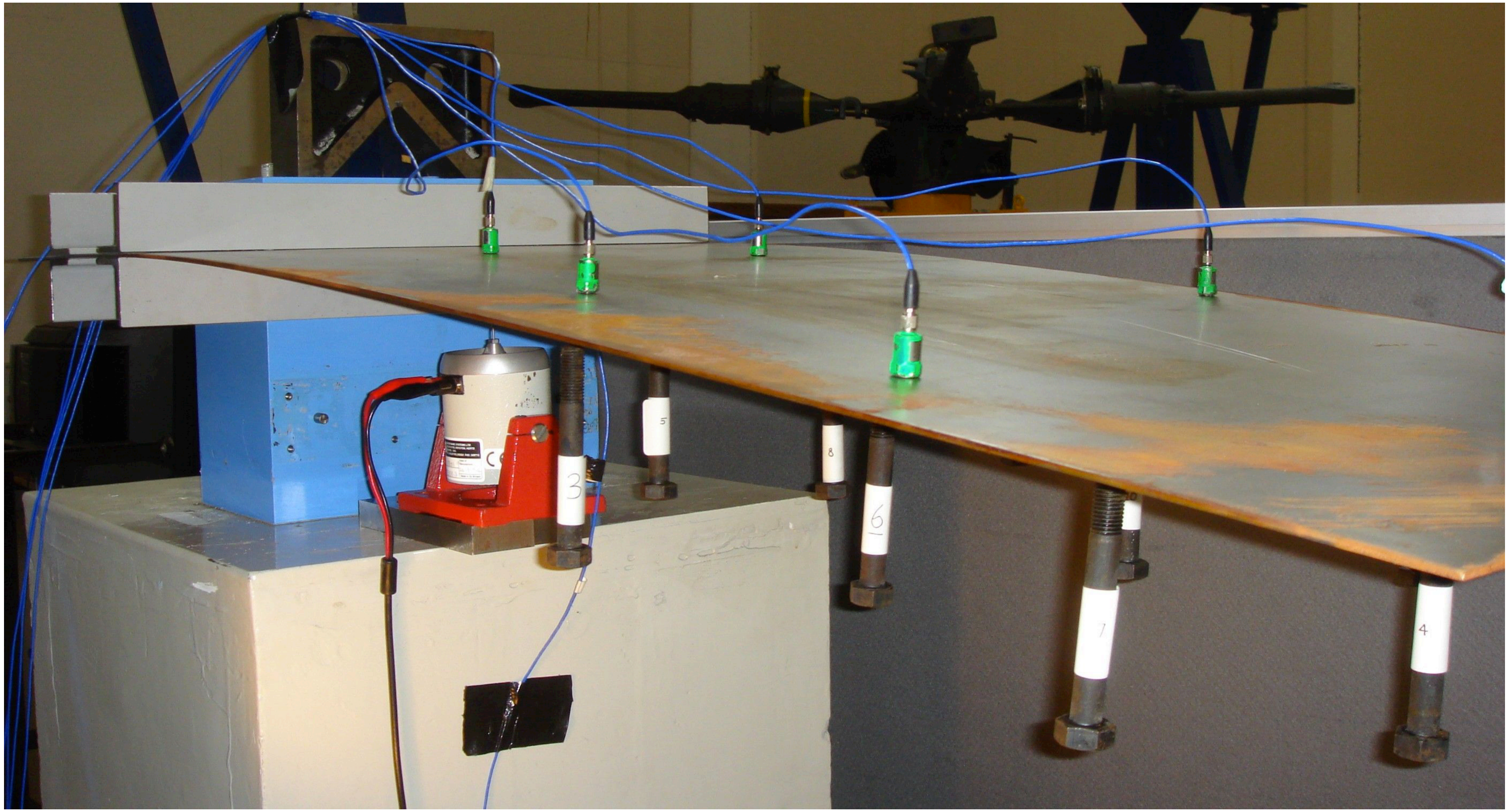


Standard deviation with $\sigma_a = 0.1$

Proposed approach: 150 x 150 equations

4th order Polynomial Chaos: 9113445 x 9113445 equations

Plate with randomly placed oscillators



10 oscillators with random stiffness values are attached at random locations in the plate by magnet

Mean of a cross-FRF

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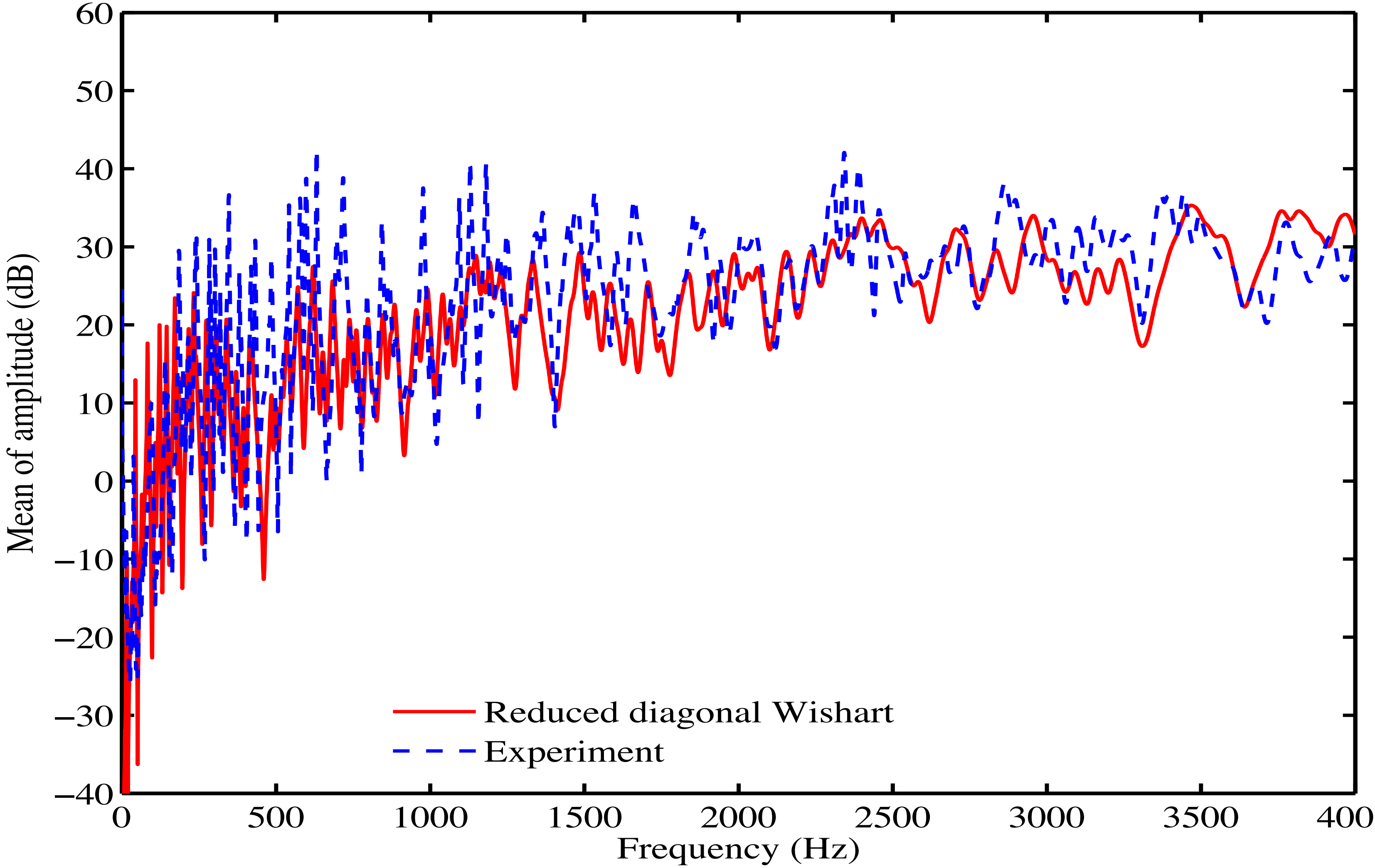

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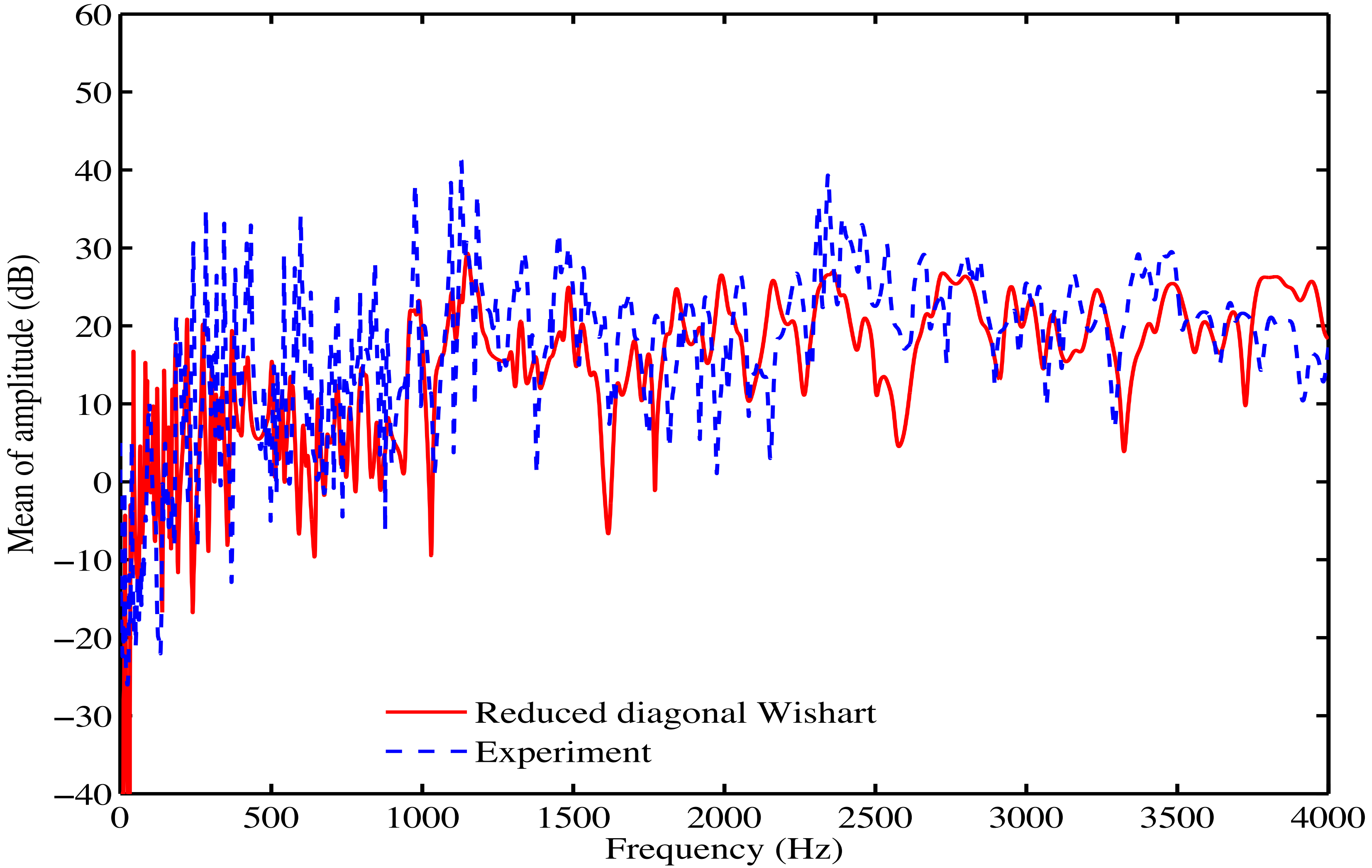
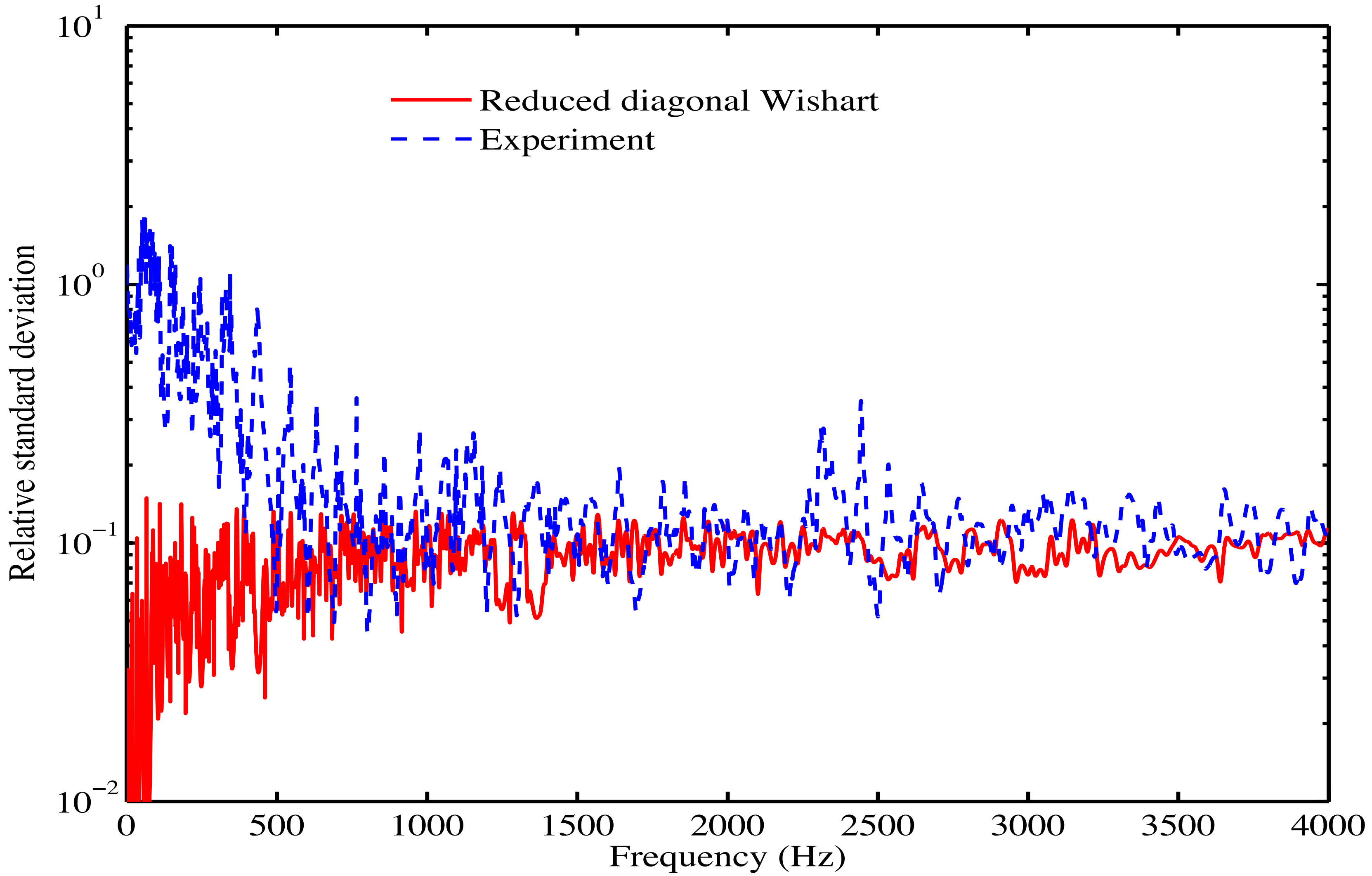
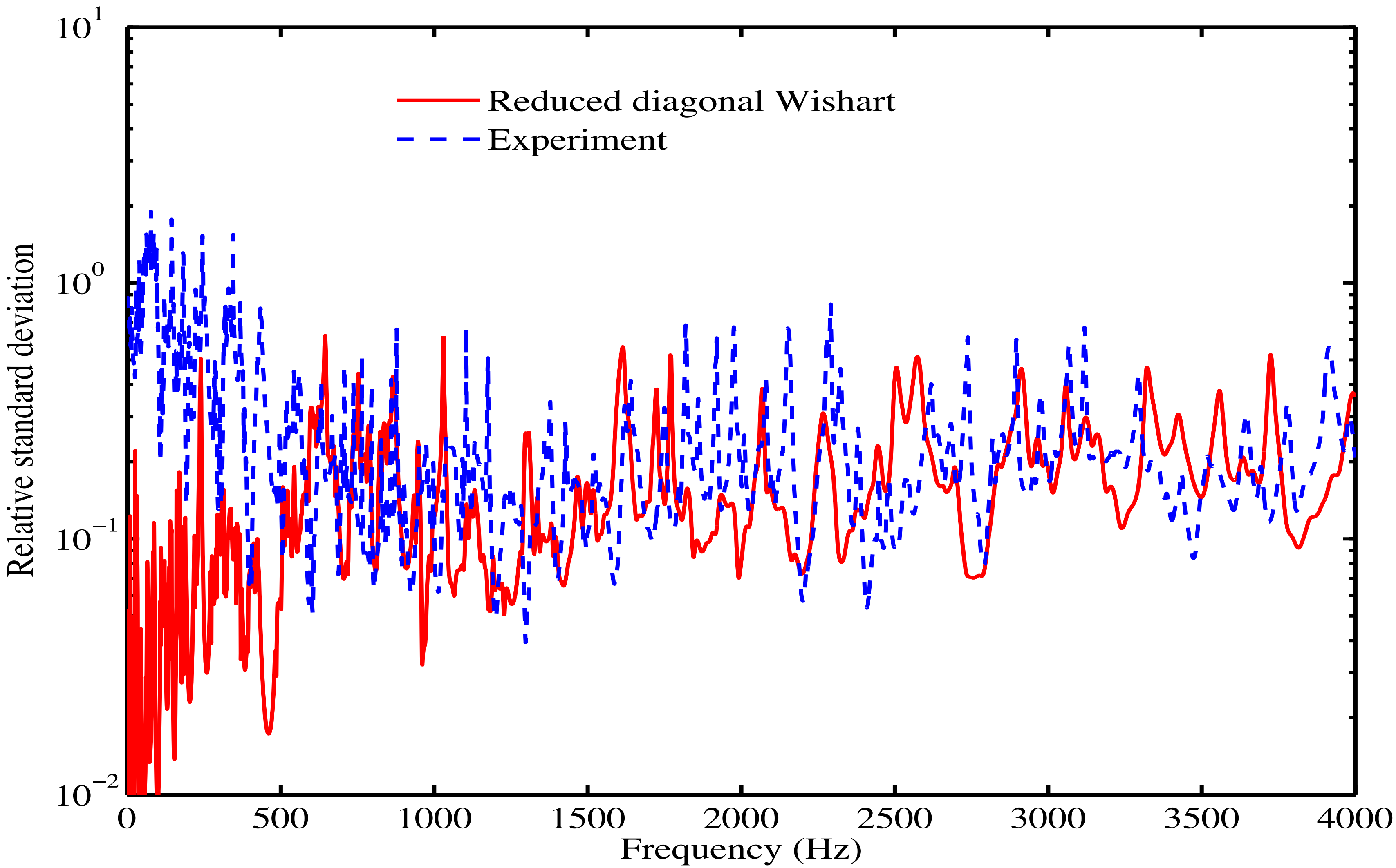
Mean of the driving-point-FRF



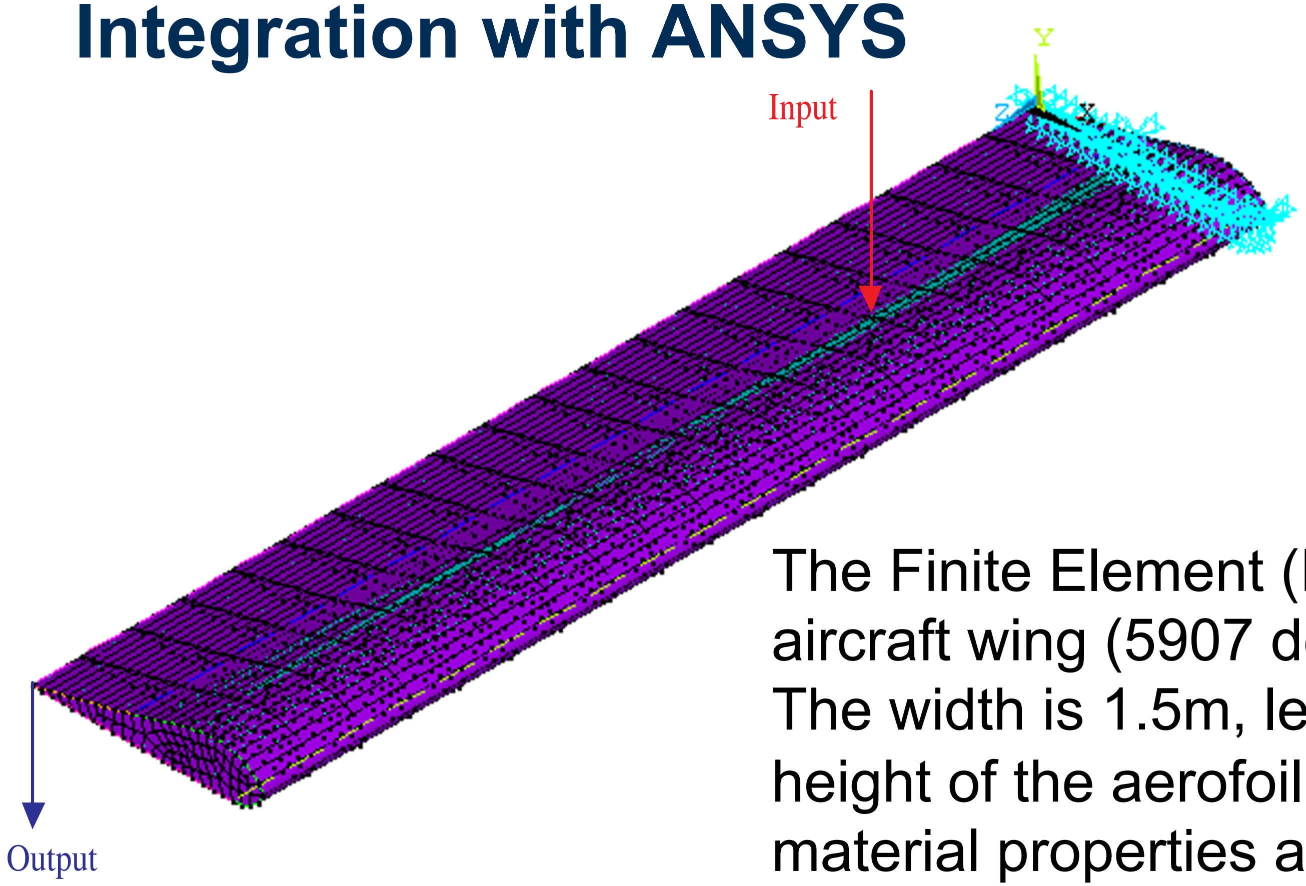
Standard deviation of a cross-FRF



Standard deviation of the driving-point-FRF

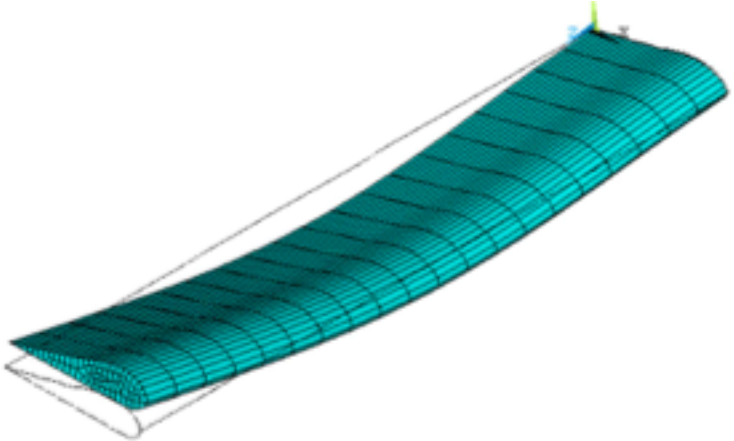


Integration with ANSYS

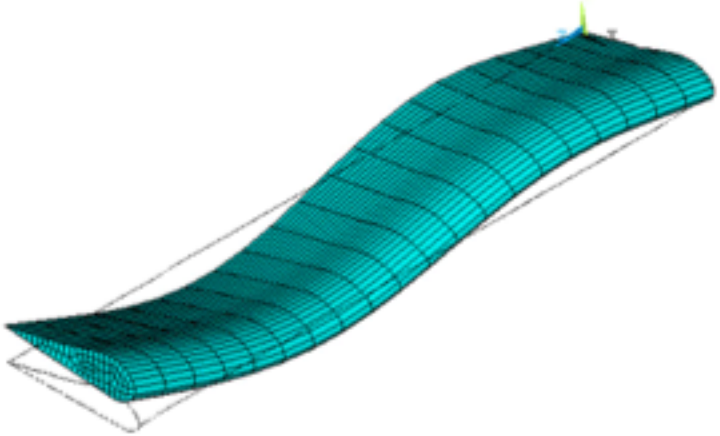


The Finite Element (FE) model of an aircraft wing (5907 degrees-of-freedom). The width is 1.5m, length is 20.0m and the height of the aerofoil section is 0.3m. The material properties are: Young's modulus 262Mpa, Poisson's ratio 0.3 and mass density 888.10kg/m^3. Input node number: 407 and the output node number 96. A 2% modal damping factor is assumed for all modes.

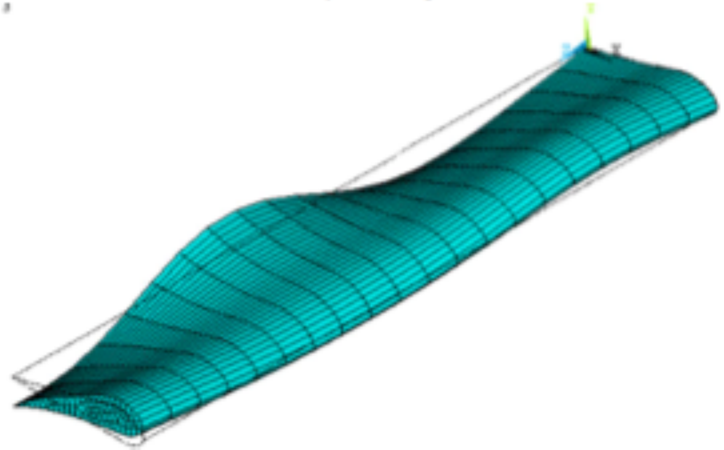
Vibration modes



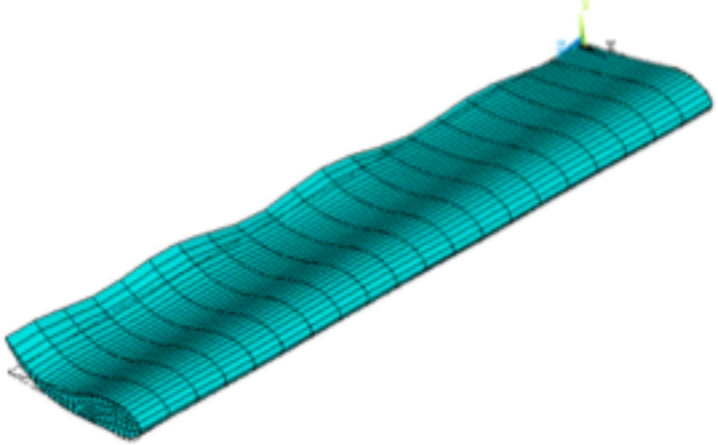
Mode 3, frequency 19.047Hz,



Mode 5, frequency 53.628Hz

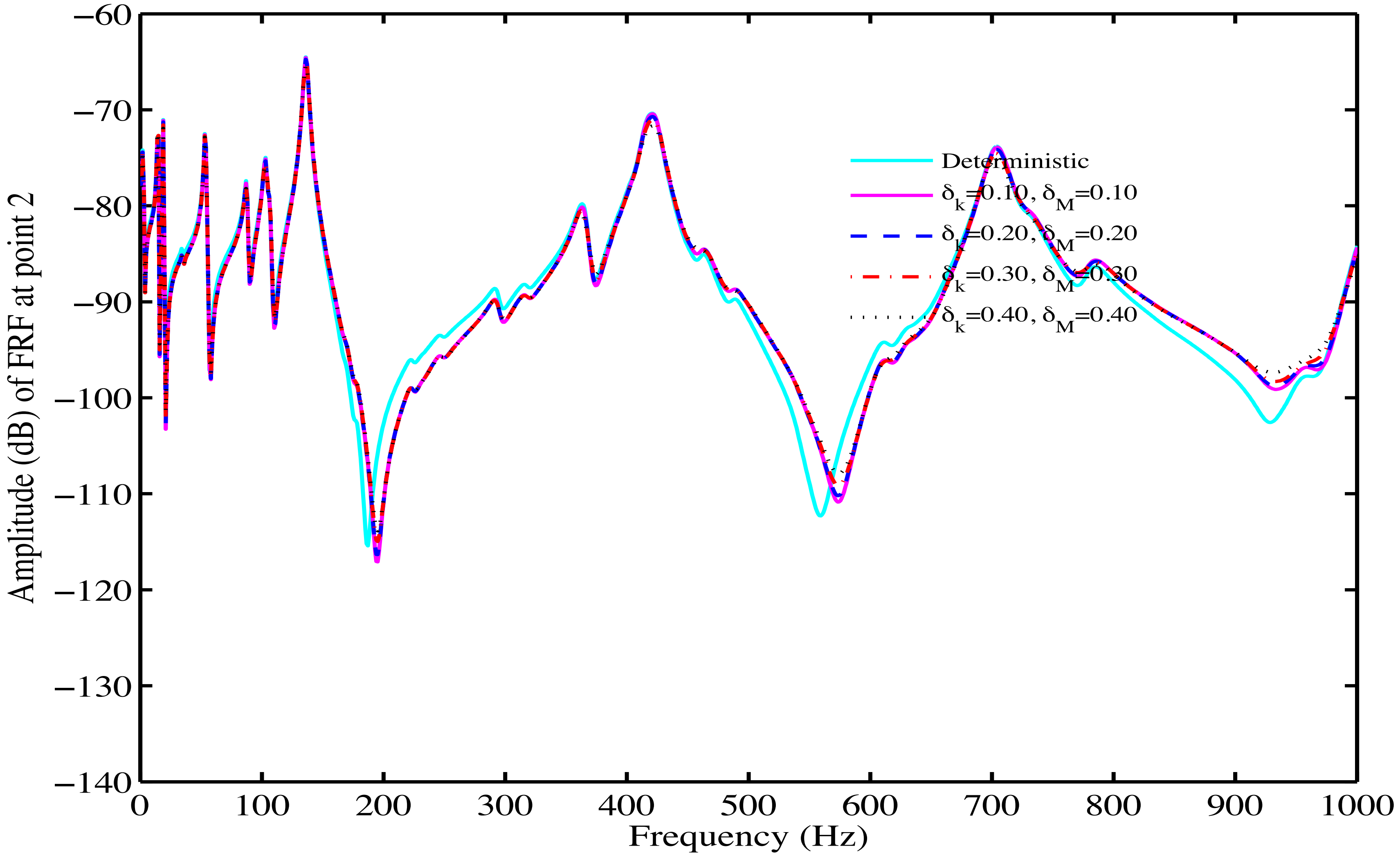


Mode 10, frequency 168.249Hz,



Mode 20, frequency 403.711Hz

Mean of a cross-FRF



Standard deviation of a cross-FRF

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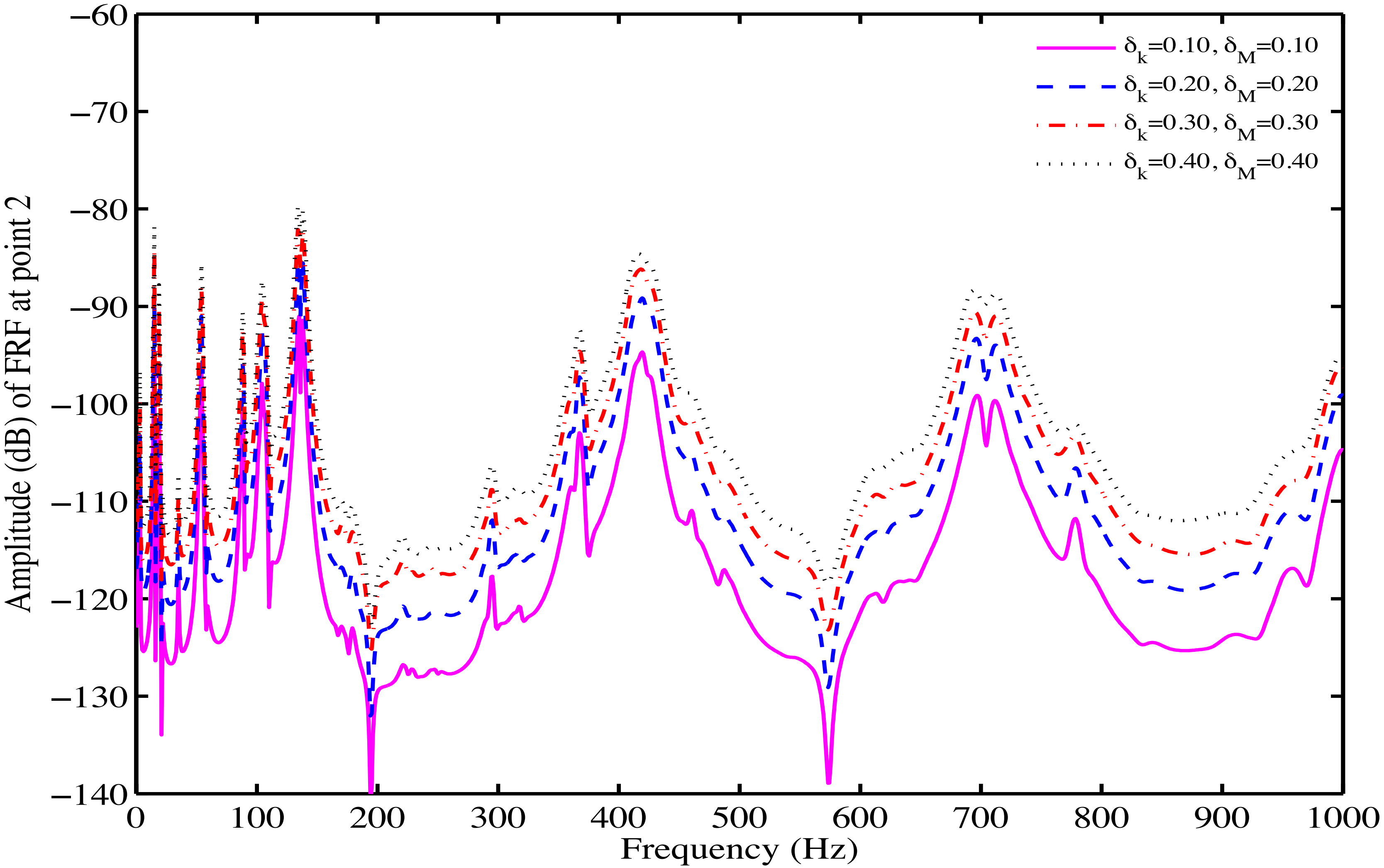

Energy harvesting under uncertainty

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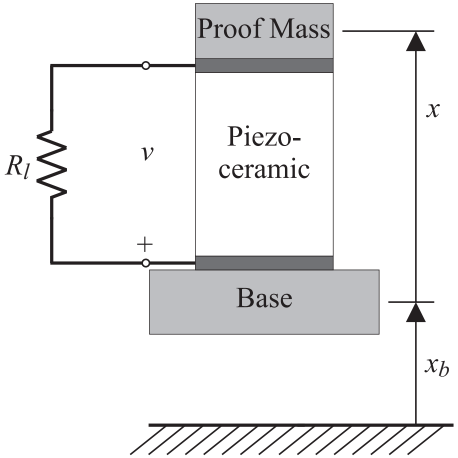
- Wireless sensor network for structural health monitoring
- Self-powered sustainable sensors – vibration energy harvesting

Energy harvesting under uncertainty

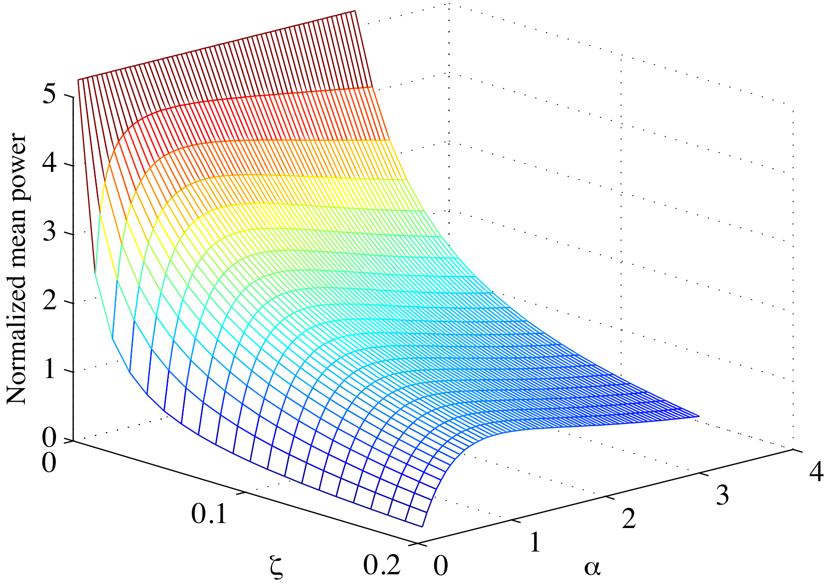


$$m\ddot{x}(t) + c\dot{x}(t) + kx(t) - \theta v(t) = -m\ddot{x}_b(t)$$

$$\theta\dot{x}(t) + C_p\dot{v}(t) + \frac{1}{R_l}v(t) = 0$$

The average harvested power due to white-noise base acceleration with a circuit without an inductor can be obtained as

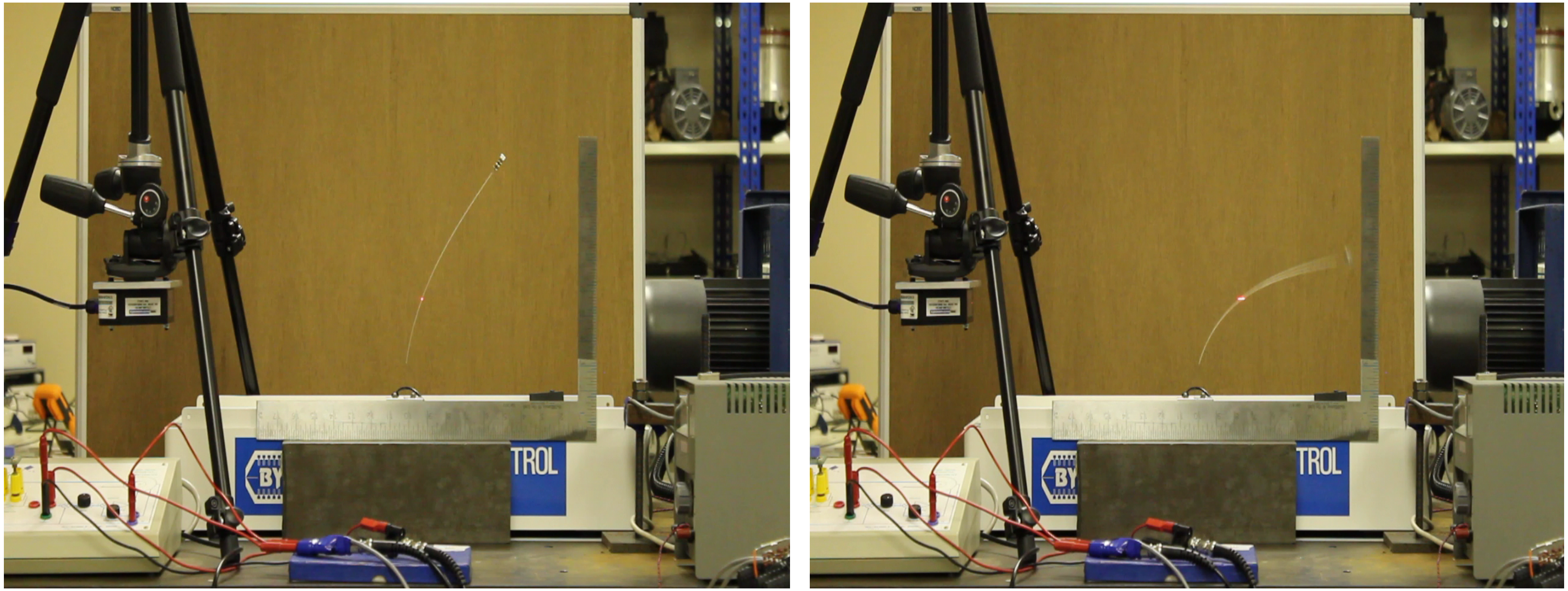
$$\mathrm{E}\left[\widetilde{P}\right] = \mathrm{E}\left[\frac{|V|^2}{(R_l\omega^4\Phi_{x_bx_b})}\right] = \frac{\pi\, m\,\alpha\,\kappa^2}{(2\,\zeta\,\alpha^2 + \alpha)\,\kappa^2 + 4\,\zeta^2\alpha + (2\,\alpha^2 + 2)\,\zeta}$$



The optimal condition is

$$R_l^2 C_p\left(kC_p + \theta^2\right) = m.$$

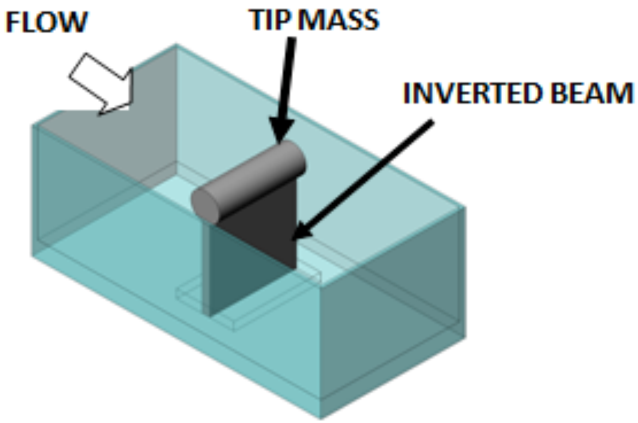
Vibration energy harvesting



Vibration energy harvesting

1. Borowiec, B., Litak, G., Friswell, M. I., Ali, S. F., Adhikari, S. and Lees, A. W. and Bilgen, O., "Energy harvesting in piezoelastic systems driven by random excitations", International Journal of Structural Stability and Dynamics.
2. Ali, S. F. and Adhikari, S., "Energy harvesting dynamic vibration absorbers", Transactions of ASME, Journal of Applied Mechanics.
3. Friswell, M. I., Ali, S. F., Adhikari, S., Lees, A.W. , Bilgen, O. and Litak, G., "Nonlinear piezoelectric vibration energy harvesting from an inverted cantilever beam with tip mass", Journal of Intelligent Material Systems and Structures, 23[3] (2012), pp. 1505-1521.
4. Litak, G., Friswell, M. I., Kitio Kwuimy, C. A., Adhikari, S. and Borowiec, B., "Energy harvesting by two magnetopiezoelastic oscillators with mistuning", Theoretical & Applied Mechanics Letters, 2[4] (2012), pp. 043009.
5. Ali, S. F., Friswell, M. I. and Adhikari, S., "Analysis of energy harvesters for highway bridges", Journal of Intelligent Material Systems and Structures, 22[16] (2011), pp. 1929-1938.
6. Jacquelin, E., Adhikari, S. and Friswell, M. I., "Piezoelectric device for impact energy harvesting", *Smart Materials and Structures*, 20[10] (2011), pp. 105008:1-12.
7. Ali, S. F., Adhikari, S., Friswell, M. I. and Narayanan, S., "The analysis of piezomagnetoelastic energy harvesters under broadband random excitations", *Journal of Applied Physics*, 109[7] (2011), pp. 074904:1-8.
8. Ali, S. F., Friswell, M. I. and Adhikari, S., "Piezoelectric energy harvesting with parametric uncertainty", *Smart Materials & Structures*, 19[10] (2010), pp. 105010:1-9.
9. Friswell, M. I. and Adhikari, S., "Sensor shape design for piezoelectric cantilever beams to harvest vibration energy", *Journal of Applied Physics*, 108[1] (2010), pp. 014901:1-6.
10. Litak, G., Friswell, M. I. and Adhikari, S., "Magnetopiezoelastic energy harvesting driven by random excitations", *Applied Physics Letters*, 96[5] (2010), pp. 214103:1-3.
11. Adhikari, S., Friswell, M. I. and Inman, D. J., "Piezoelectric energy harvesting from broadband random vibrations", *Smart Materials & Structures*, 18[11] (2009), pp. 115005:1-7.

Energy harvesting from fluid flow



TEST SECTION WITH INVERTED BEAM ENERGY HARVESTER

The objective:

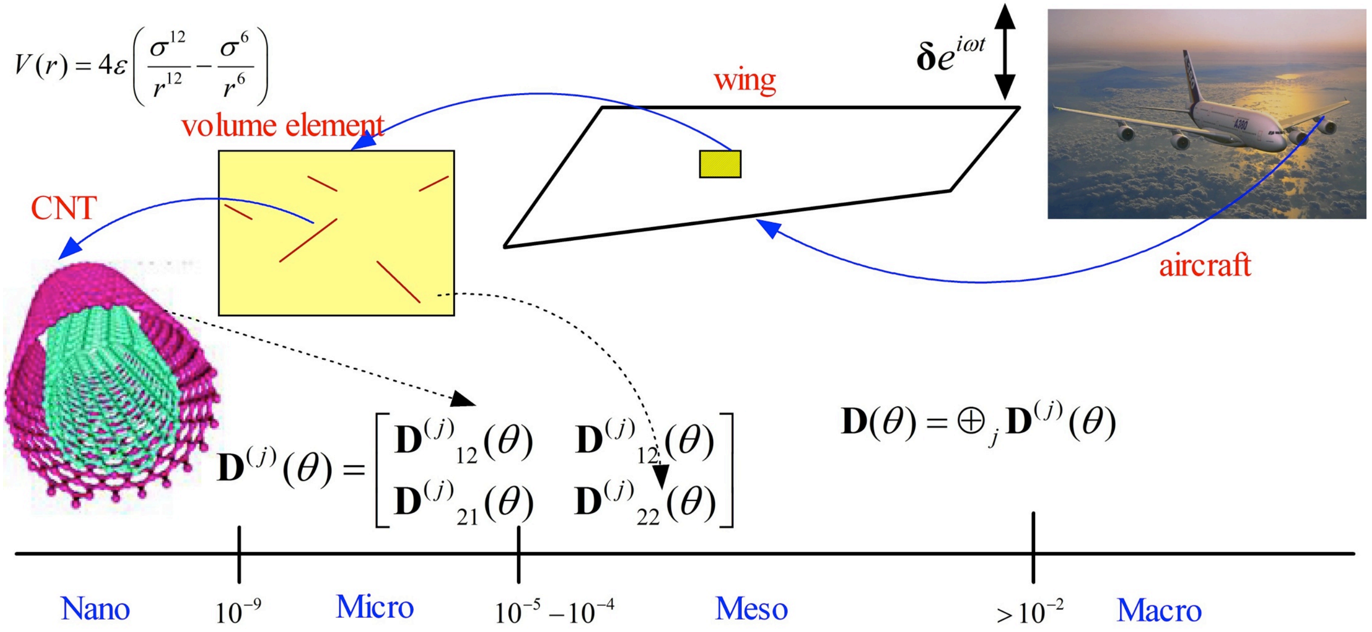
- *To harvest energy from flow induced vibration (inverted piezo beam with tip mass)*
- Useful for structural health monitoring in pipelines in nuclear power plants
- Power future generation of medical devices implanted within arteries and blood vessels.

Wind Energy Energy Quantification

- Fluid-structure interaction under stochastic loading
- Wind-velocity modeling
- Ensemble behavior of wind turbines

1. Adhikari, S. and Bhattacharya, S., "Dynamic analysis of wind turbine towers on flexible foundations", *Shock and Vibration*, 19[1] (2012), pp. 37-56.
2. Adhikari, S. and Bhattacharya, S., "Vibrations of wind-turbines considering soil-structure interaction", *Wind and Structures, An International Journal*, 14[2] (2011), pp. 85-112.
3. Bhattacharya, S. and Adhikari, S., "Experimental validation of soil-structure interaction of offshore wind turbines", *Soil Dynamics and Earthquake Engineering*, 31[5-6] (2011), pp. 805-816.
4. Adhikari, S., *On the Application of ANOVA method for Wind Energy Predictions*, Report prepared for Garrad Hassan Ltd, March 2007.
5. Adhikari, S., *Uncertainty Quantification in the Prediction of Wind Velocities*, Report prepared for Garrad Hassan Ltd, April 2006.

Stochastic multiscale method



$$V(r)=4\varepsilon\left(\frac{\sigma^{12}}{r^{12}}-\frac{\sigma^{6}}{r^{6}}\right)$$

$$\boldsymbol{\delta}e^{i\omega t}$$

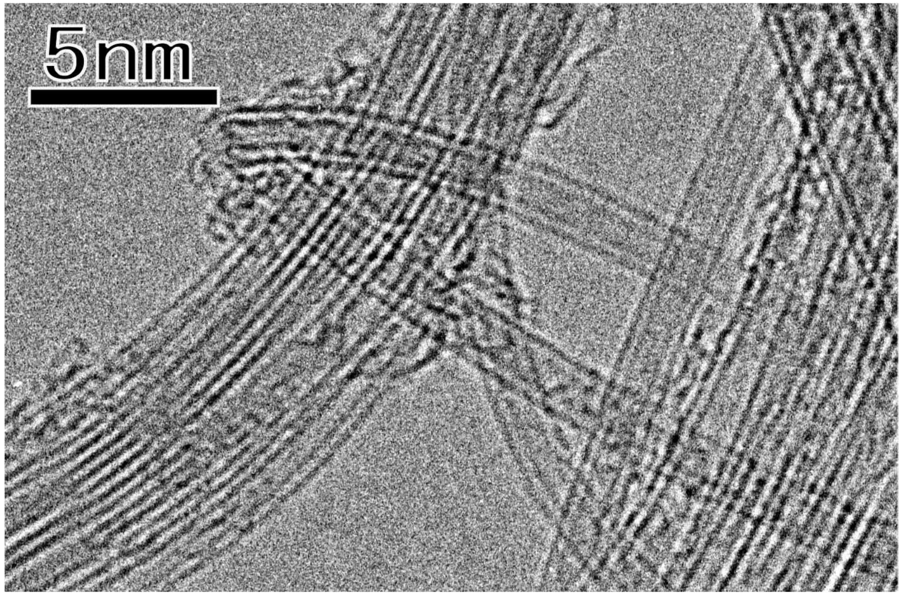
$$\mathbf{D}^{(j)}(\theta)=\begin{bmatrix}\mathbf{D}^{(j)}{}_{12}(\theta) & \mathbf{D}^{(j)}{}_{12}(\theta)\\ \mathbf{D}^{(j)}{}_{21}(\theta) & \mathbf{D}^{(j)}{}_{22}(\theta)\end{bmatrix}$$

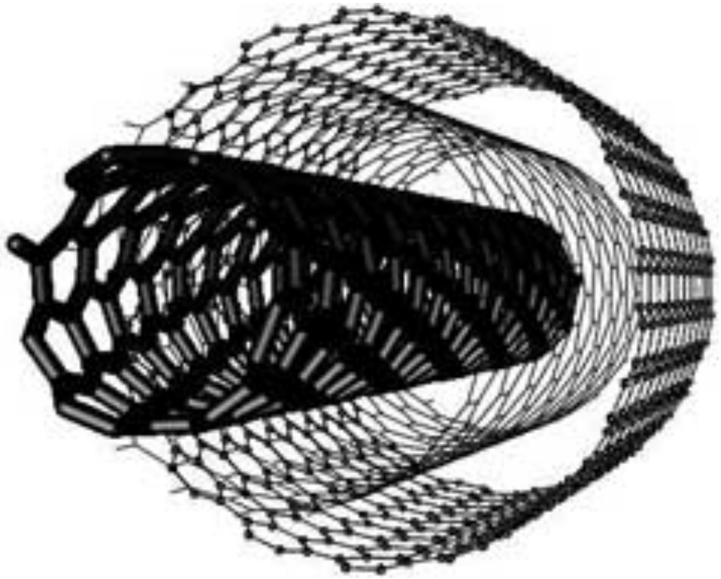
$$\mathbf{D}(\theta)=\oplus_j\mathbf{D}^{(j)}(\theta)$$

10^{-9} $10^{-5}-10^{-4}$ $>10^{-2}$

- New generation of structural materials
- Nano-composites, bio-composites
- Self-sensing, multifunctional, self-healing and sustainable materials – high strength to weight ratio
- Structural mechanics community needs to embrace new materials and develop next generation of analysis and design tools
- Requires multiscale and multiphysics approach

Nano-scale stochastic mechanics





- Uncertainty in modeling (geometry, boundary condition, system parameters)
- There are defects which may not be known a-priori
- Analysis using the principles of structural mechanics, dynamics, stochastic finite element method
- Propagation of uncertainty across the length and time-scale

Main research themes

1997

- Stochastic finite element
- Spectral methods
- High-frequency analysis

2000

- Structural dynamics
- Damping analysis
- Experimental methods
- System identification

2003

- Probabilistic reliability analysis
- Random eigenvalue problem
- Model updating
- Mode veering

2006

- Nonparametric UQ
- Random matrix theory
- Parametric sensitivity analysis
- Nonlocal finite element method
- Wind energy quantification

2008

- Atomistic finite element method
- Mechanics of CNT, Graphene, buckyball
- Dynamics of Viscoelastic systems
- Gaussian process (GP) emulators
- High dimensional model representation (HDMR)

2010-

- Nanoscale biosensors
- Vibration energy harvesting
- Computational Biomechanics
- Nanocomposites
- Dynamics of wind turbines
- Magneto elastodynamics
- Stochastic projection methods

Future

- **Computational stochastic dynamics – model calibration and validation**
- **Stochastic multiscale method for bio and nano structures**
- **Vibration/wind energy harvesting under uncertainty**

Central Underlying Themes
(1) Stochastic mechanics
(2) Structural dynamics
(3) Atomistic finite element method

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AgustaWestland

THE ROYAL SOCIETY
CELEBRATING 350 YEARS

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Prifysgol Abertawe

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Pioneering research and skills

newton
international fellowships

GL Garrad Hassan

MARIE CURIE ACTIONS

Collaborators, Students and Postdocs

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Bristol: F Scarpa, N Lieven, J DuBois, S Bhattacharya
Limerick: M McCarthy, T Murmu
Michigan: DJ Inman
Lyon: E Jacquelin
IIT Madras: S Narayanan, SF Ali
Kharkov: L Pastur
University of British Columbia: AS Phani
Johannesburg: T Marwala
Ottawa: M Khalil, A Sarkar
Swansea: MI Friswell, CW Wang, R Chowdhury, B Pascual, F DiazDelaO, A Potrykus

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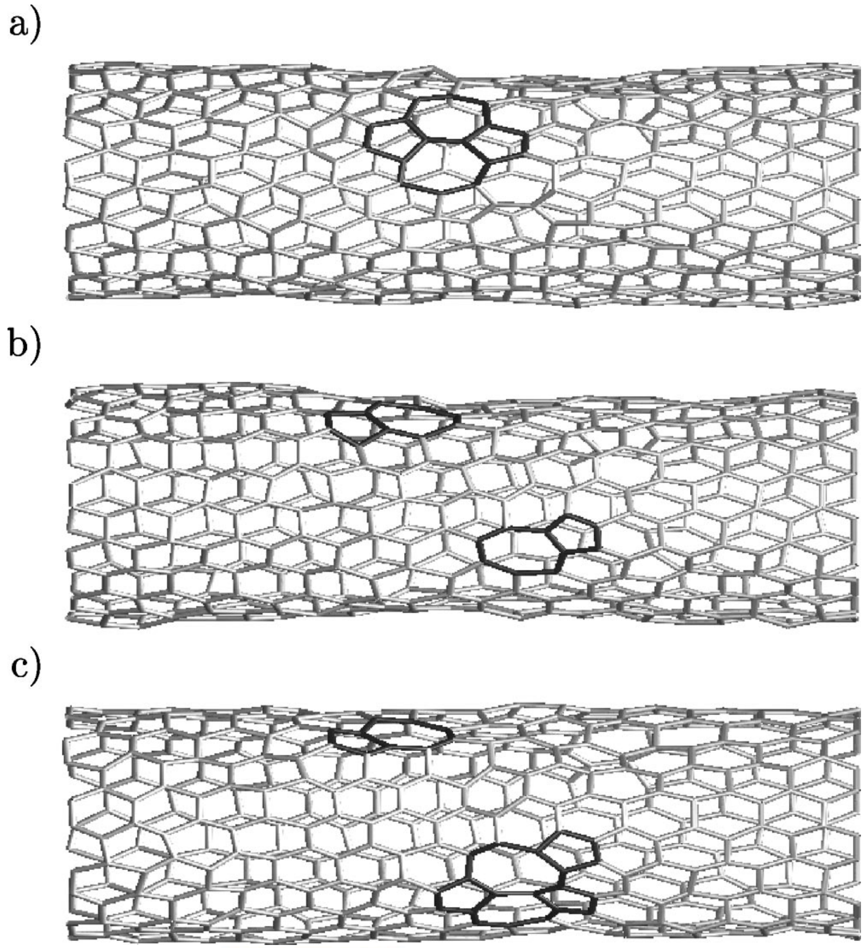
Atomistic finite element method

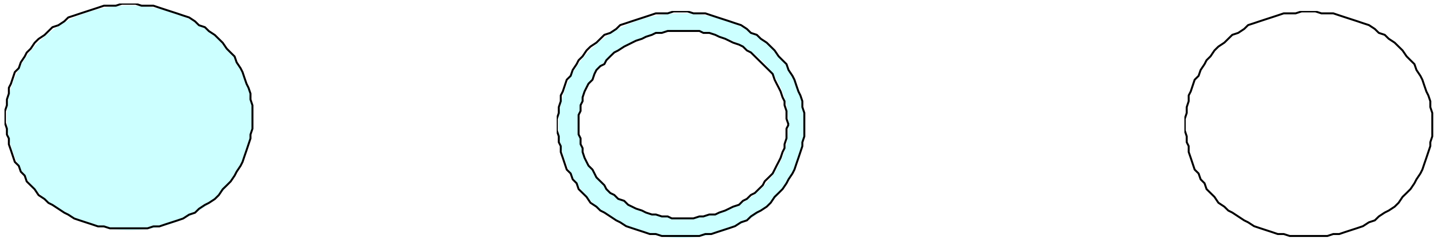
Can we use continuum mechanics at the nanoslace?



- What about the "holes"?
- Can we have an "equivalent" continuum model with "correct" properties?
- How defects can be taken into account ?

Which Young's modulus?

Effective **Longitudinal** **Surface**

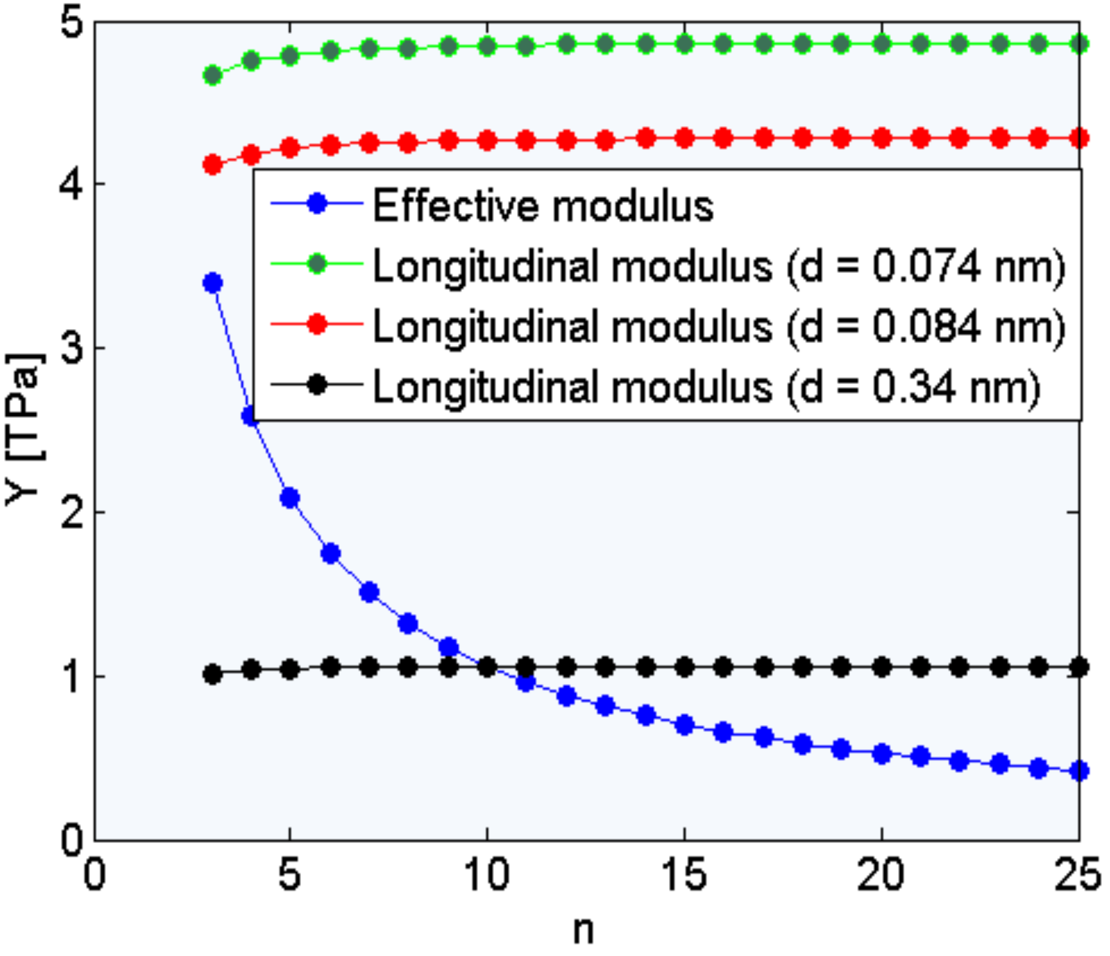


$$\bar{Y}_{11} = \frac{F}{\pi R^2 \varepsilon_{11}}$$

$$Y_{11} = \frac{F}{2\pi R d\, \varepsilon_{11}}$$

$$Y_{11}^{s} = \frac{F}{2\pi R\, \varepsilon_{11}}$$

Which Young's modulus?



Atomistic finite element method

- Atomic bonds are represented by beam elements
- Beam properties are obtained by energy balance

$$U_{total} = U_r + U_\theta + U_\tau$$

$$U_r = \frac{1}{2}k_r\left(\Delta r\right)^2 \quad U_\theta = \frac{1}{2}k_\theta\left(\Delta \theta\right)^2 \quad U_\tau = \frac{1}{2}k_\tau\left(\Delta \phi\right)^2$$

$$U_{axial} = \frac{1}{2}K_{axial}(\Delta L)^2 = \frac{EA}{2L}(\Delta L)^2$$

$$U_{torsion} = \frac{1}{2}K_{torsion}(\Delta \beta)^2 = \frac{GJ}{2L}(\Delta \beta)$$

$$U_{bending} = \frac{1}{2}K_{bending}(2\alpha)^2 = \frac{EI}{2L}\frac{4+\Phi}{1+\Phi}(2\alpha)^2$$

Scarpa, F. and Adhikari, S., "A mechanical equivalence for the Poisson's ratio and thickness of C-C bonds in single wall carbon nanotubes", Journal of Physics D: Applied Physics, 41 (2008) 085306

Atomistic finite element method

- All parameters of the beam can be obtained in closed-form:

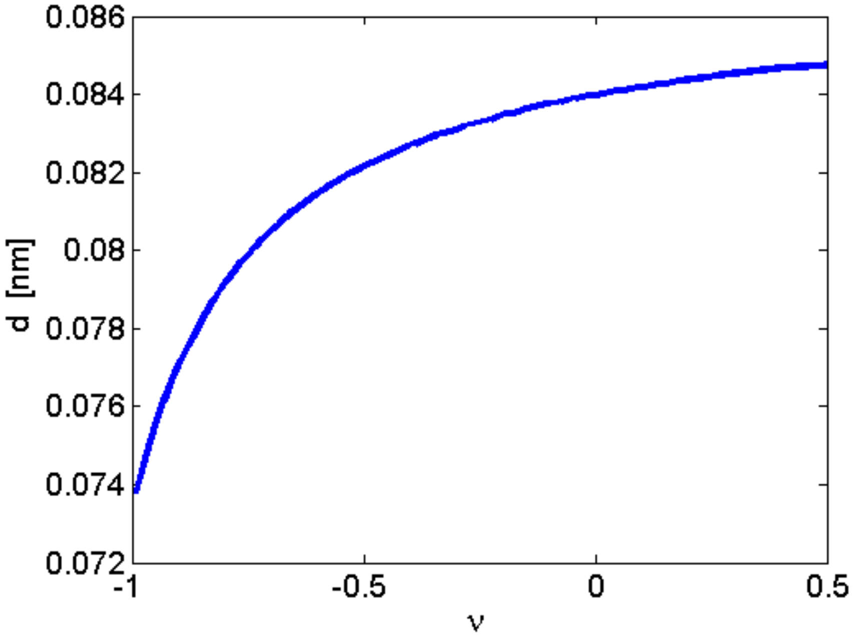
$$E = \frac{4k_r L}{\pi d^2}, \quad G = \frac{32 k_\tau L}{\pi d^4}$$

$$\Phi = \frac{3k_r d^4 \left(6+12\nu+6\nu^2\right)}{32 k_\tau L^2 \left(7+12\nu+4\nu^2\right)}$$

$$k_\theta = \frac{k_r d^2}{16}\frac{4\mathrm{A}+\mathrm{B}}{\mathrm{A}+\mathrm{B}} \qquad d < 2\sqrt{6}\sqrt{\frac{k_\tau}{k_r}}$$

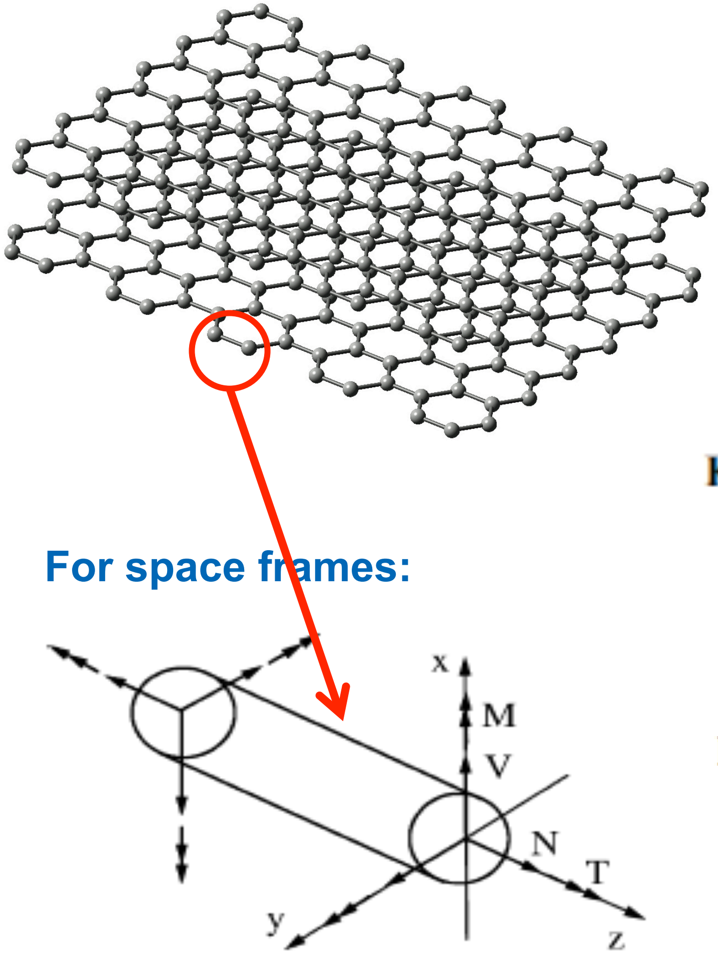
$$\mathrm{A} = 112L^2 k_\tau + 192 L^2 k_\tau \nu + 64 L^2 k_\tau \nu^2$$

$$\mathrm{B} = 9k_r d^4 + 18 k_r d^4 \nu + 9 k_r d^4 \nu^2$$



Scarpa, F. and Adhikari, S., "A mechanical equivalence for the Poisson's ratio and thickness of C-C bonds in single wall carbon nanotubes", Journal of Physics D: Applied Physics, 41 (2008) 085306

Atomistic Structural Mechanics



$$[\mathbf{K}]\{\mathbf{u}\}=\{\mathbf{f}\}$$

[K] → stiffness matrix
{u} → nodal displacement vector
{f} → nodal force vector

$$\mathbf{u}=[u_{xi},u_{yi},u_{zi},\theta_{xi},\theta_{yi},\theta_{zi},u_{xj},u_{yj},u_{zj},\theta_{xj},\theta_{yj},\theta_{zj}]^{\mathrm{T}}$$

$$\mathbf{f}=[f_{xi},f_{yi},f_{zi},m_{xi},m_{yi},m_{zi},f_{xj},f_{yj},f_{zj},m_{xj},m_{yj},m_{zj}]^{\mathrm{T}}$$

$$\mathbf{K}=\begin{bmatrix}\mathbf{K}_{ii} & \mathbf{K}_{ij}\\ \mathbf{K}_{ij}^{\mathrm{T}} & \mathbf{K}_{jj}\end{bmatrix};$$

For space frames:

$$\mathbf{K}_{ii}=\begin{bmatrix}EA/L & 0 & 0 & 0 & 0 & 0\\ 0 & 12EI_x/L^3 & 0 & 0 & 0 & 6EI_x/L^2\\ 0 & 0 & 12EI_y/L^3 & 0 & -6EI_y/L^2 & 0\\ 0 & 0 & 0 & GJ/L & 0 & 0\\ 0 & 0 & -6EI_y/L^2 & 0 & 4EI_y/L & 0\\ 0 & 6EI_x/L^2 & 0 & 0 & 0 & 4EI_x/L\end{bmatrix}$$

Atomistic FE – bending deformation of SWCNTs

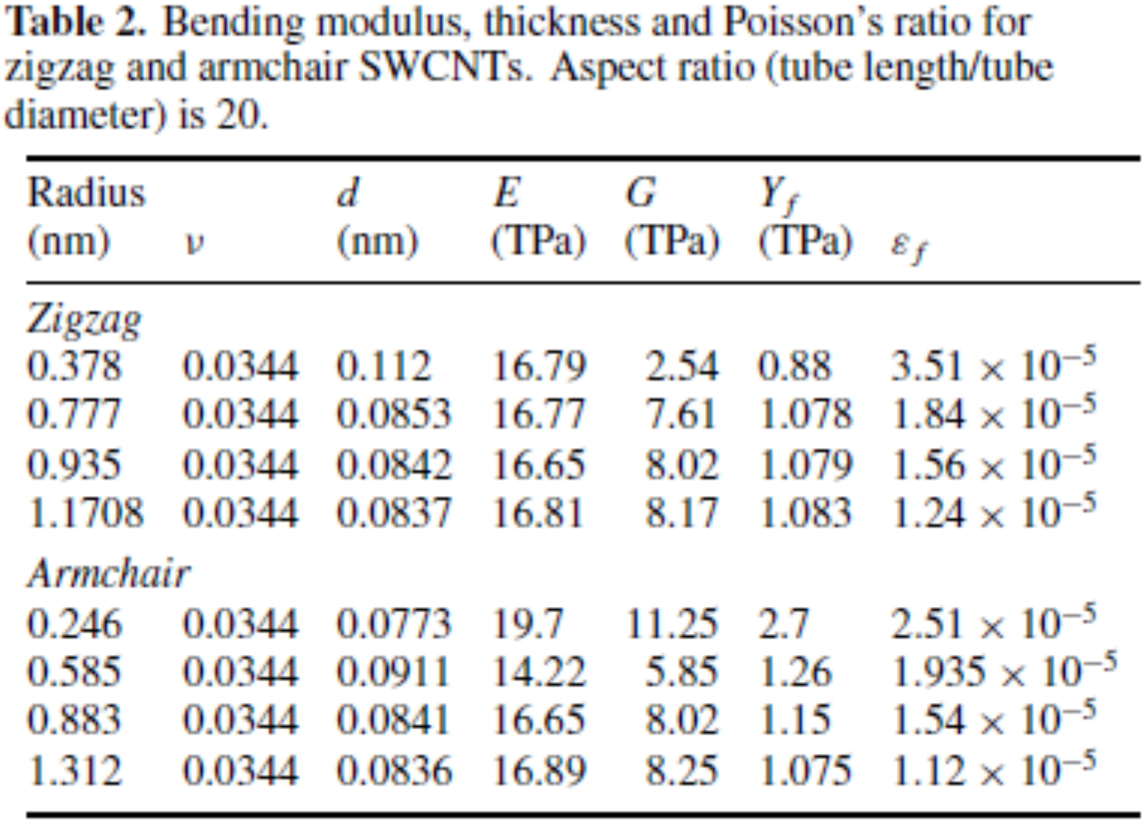
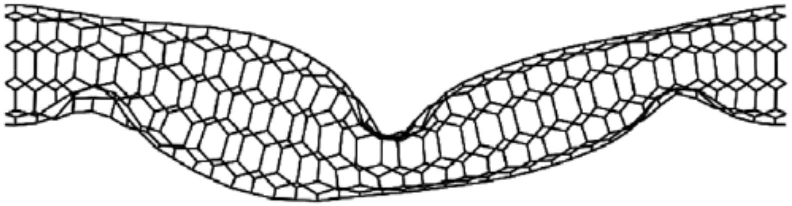


Table 2. Bending modulus, thickness and Poisson's ratio for zigzag and armchair SWCNTs. Aspect ratio (tube length/tube diameter) is 20.

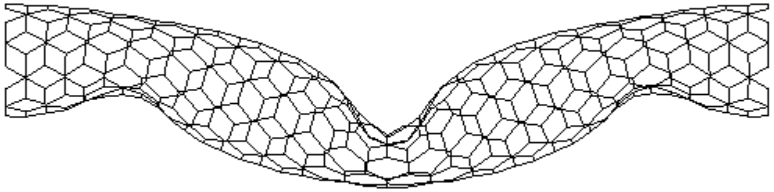
Radius (nm)	ν	d (nm)	E (TPa)	G (TPa)	Y_f (TPa)	ε_f
Zigzag						
0.378	0.0344	0.112	16.79	2.54	0.88	3.51×10^{-5}
0.777	0.0344	0.0853	16.77	7.61	1.078	1.84×10^{-5}
0.935	0.0344	0.0842	16.65	8.02	1.079	1.56×10^{-5}
1.1708	0.0344	0.0837	16.81	8.17	1.083	1.24×10^{-5}
Armchair						
0.246	0.0344	0.0773	19.7	11.25	2.7	2.51×10^{-5}
0.585	0.0344	0.0911	14.22	5.85	1.26	1.935×10^{-5}
0.883	0.0344	0.0841	16.65	8.02	1.15	1.54×10^{-5}
1.312	0.0344	0.0836	16.89	8.25	1.075	1.12×10^{-5}

(F Scarpa and S Adhikari, 2008. *J. Phys. D: App. Phys.*, 41, 085306)

Buckling of Carbon nanotubes

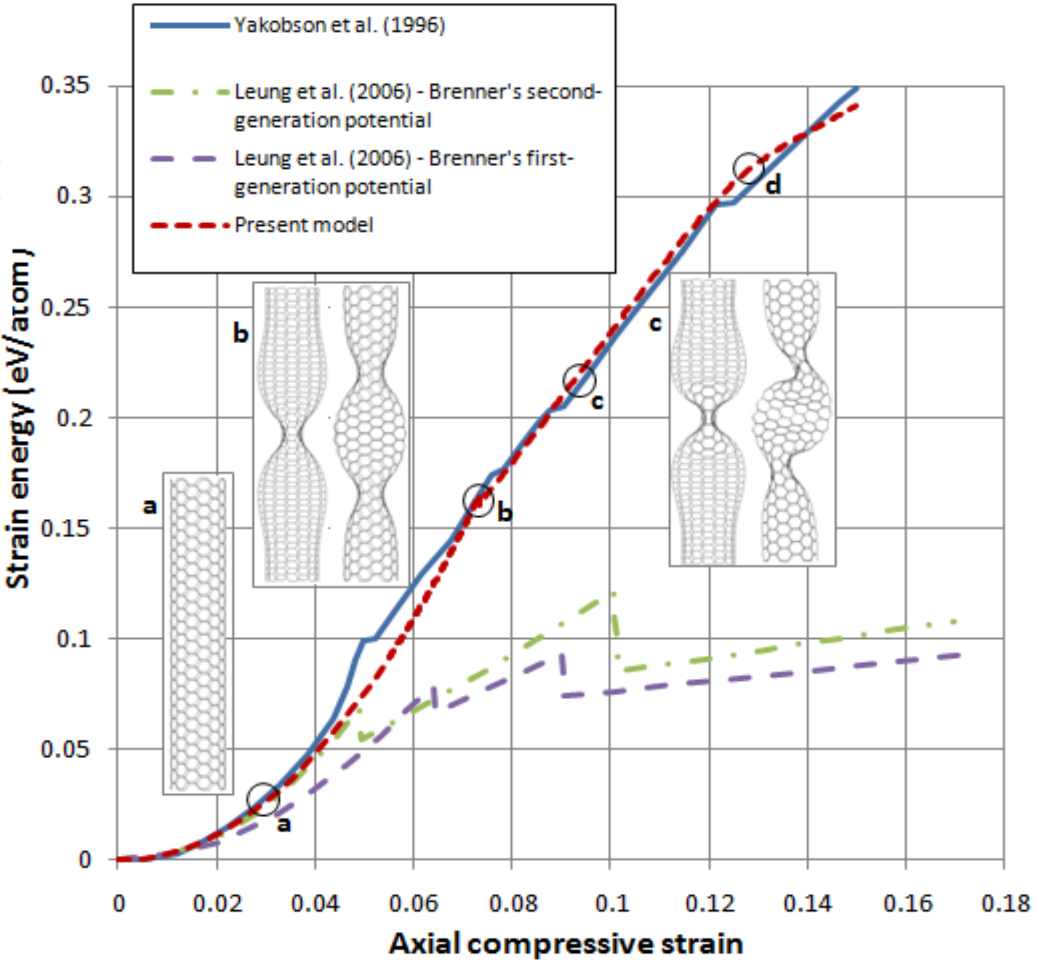


(a) Molecular dynamics



(b) Hyperplastic atomistic FE (Ogden strain energy density function)

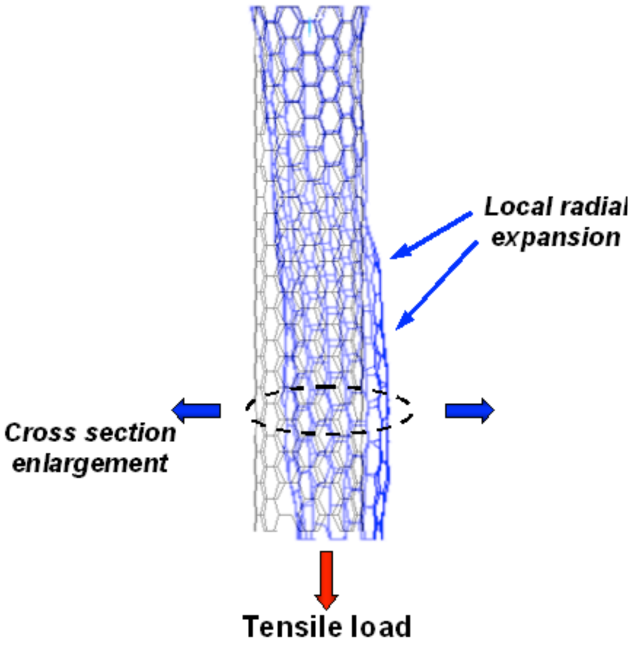
Comparison of buckling mechanisms in a (5,5) SWCNT with 5.0 nm length.

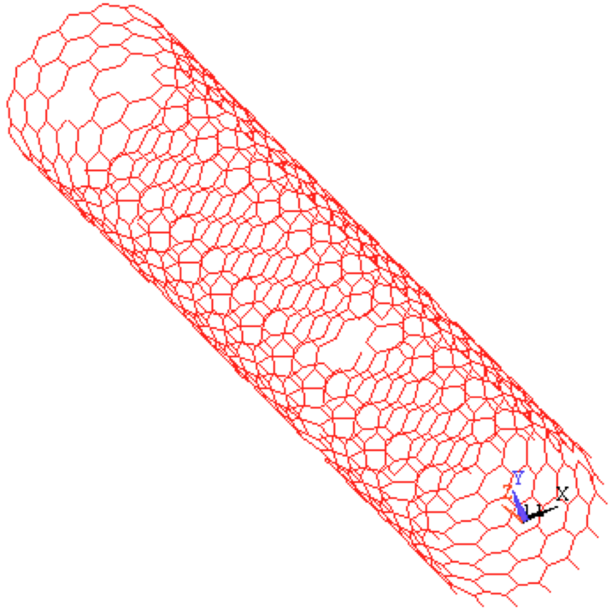


Flores, E. I. S., Adhikari, S., Friswell, M. I. and Scarpa, F., "Hyperelastic axial buckling of single wall carbon nanotubes", Physica E: Low-dimensional Systems and Nanostructures, 44[2] (2011), pp. 525-529.

Carbon nanotubes with defects

- We are interested in the changes in the mechanical properties





Scarpa, F., Adhikari, S. and Wang, C. Y., "Mechanical properties of non reconstructed defective single wall carbon nanotubes", *Journal of Physics D: Applied Physics*, 42 (2009) 142002

Carbon nanotubes with defects

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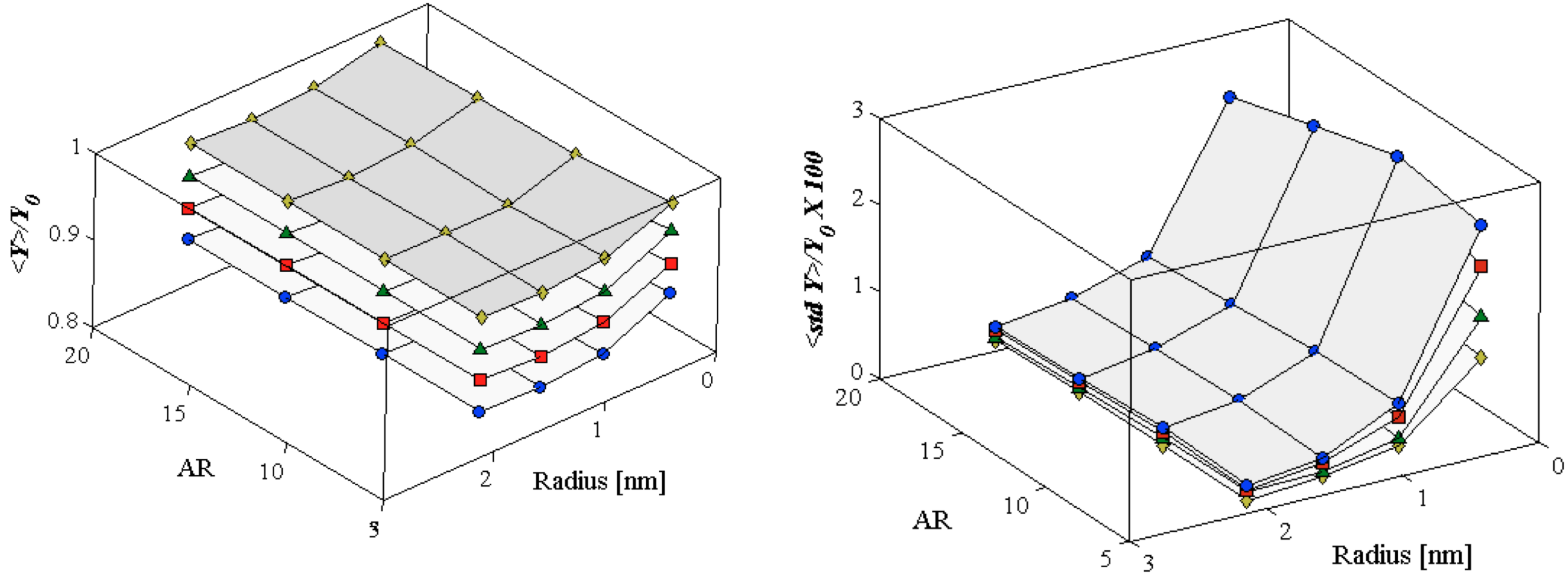

(a) Ratio between mean of axial Young's modulus and pristine stiffness and (b) between standard deviation of the Young's modulus against pristine Young's modulus for armchair (n,n). Pristine Young's modulus Y_0: 2.9, 1.36, 0.91, 0.67 TPa for a thickness d = 0.084 nm. ● = 2 % NRV; ■ = 1.5 % NRV; ▲= 1 % NRV; ♦= 0.5 % NRV

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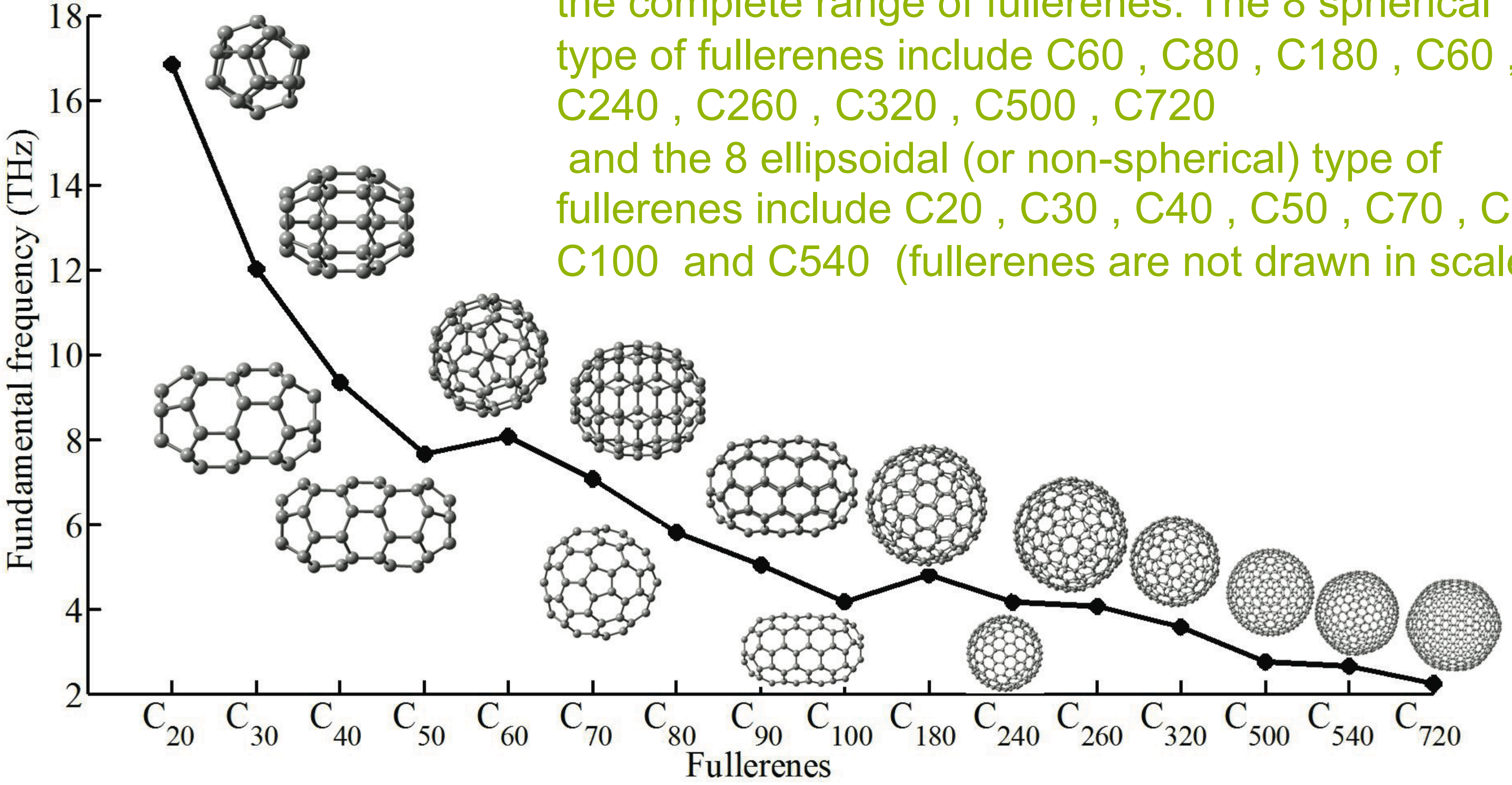
Fullerene

Vibration spectra of fullerene family

The variation of the first natural frequency across the the complete range of fullerenes. The 8 spherical type of fullerenes include C60 , C80 , C180 , C60 , C240 , C260 , C320 , C500 , C720

and the 8 ellipsoidal (or non-spherical) type of fullerenes include C20 , C30 , C40 , C50 , C70 , C90 , C100 and C540 (fullerenes are not drawn in scale).

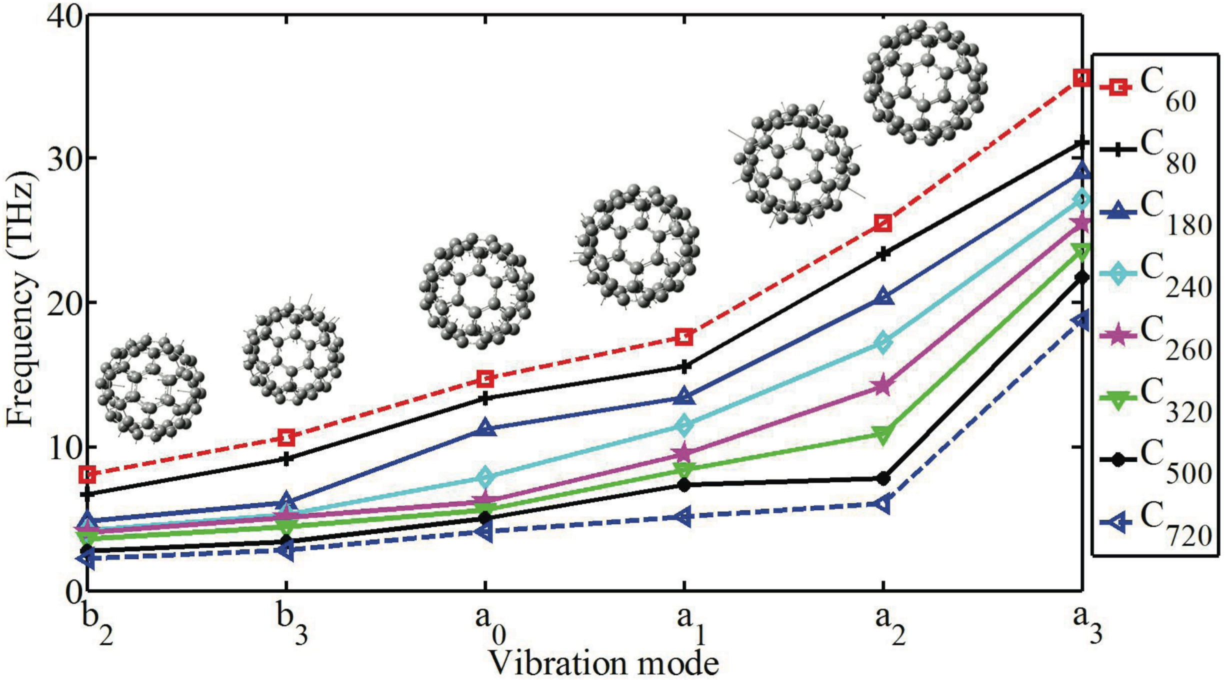


Adhikari, S. and Chowdhury, R., "Vibration spectra of fullerene family", Physics Letters A, 375[22] (2011), pp. 1276-1280.

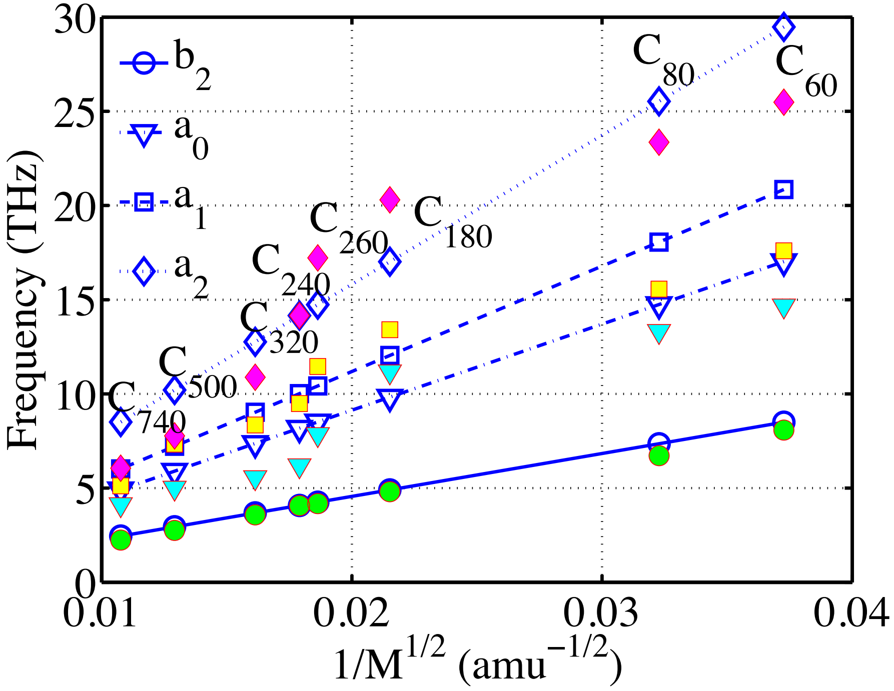
Thin shell theory

The natural frequencies of spherical fullerenes can be given by

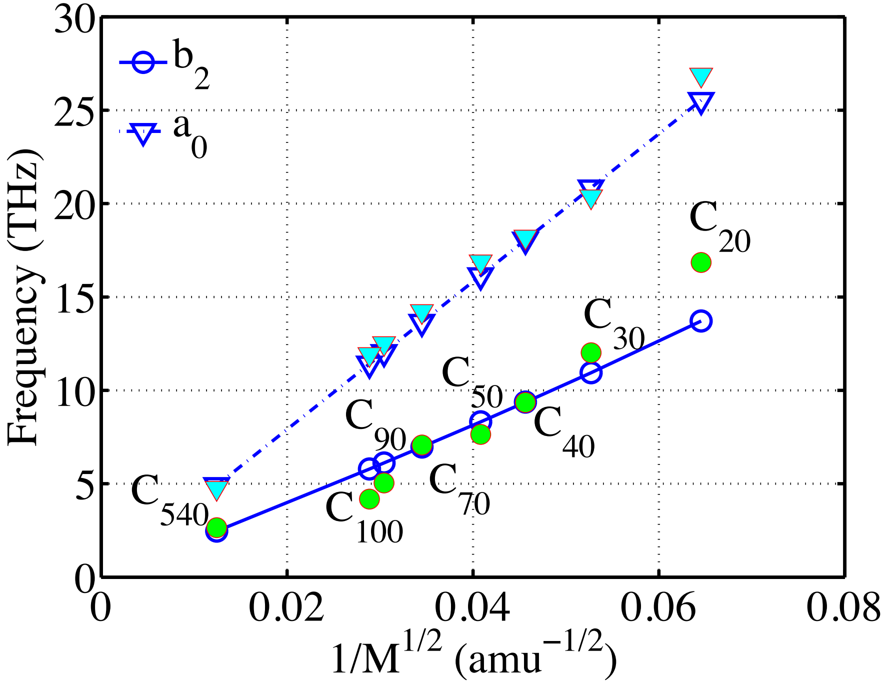
$$\omega_{n1,2}^2 = \frac{E}{R^2\rho}\Omega_{n1,2}^2 \qquad \Omega_{n1,2}^2 = \frac{1}{2(1-\mu^2)}\{n(n+1)+1+3\mu\pm \sqrt{[n(n+1)+1+3\mu]^2 - 4(1-\mu^2)[n(n+1)-2]}\}$$



Atomistic Simulation vs Shell theory



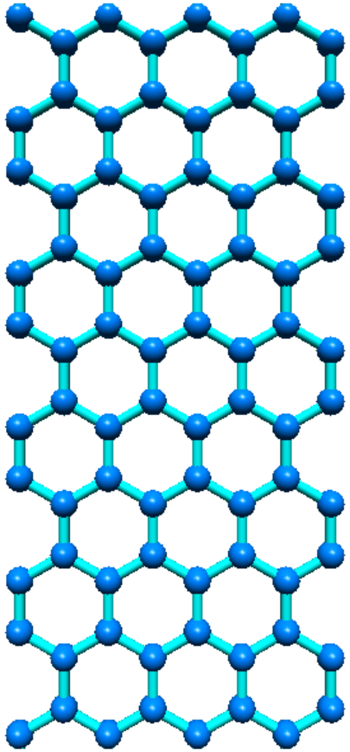
Spherical type fullerenes



Ellipsoidal type fullerenes

Graphene

Atomistic FE – in-plane SLGS



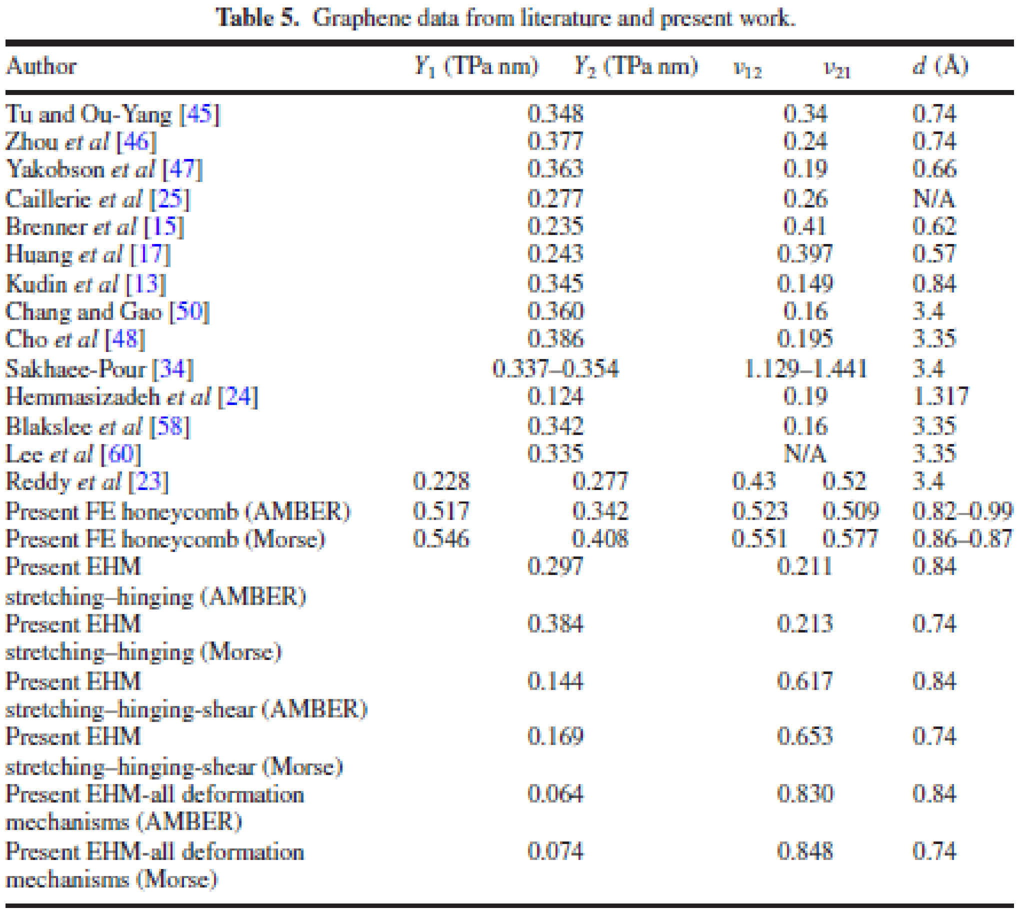
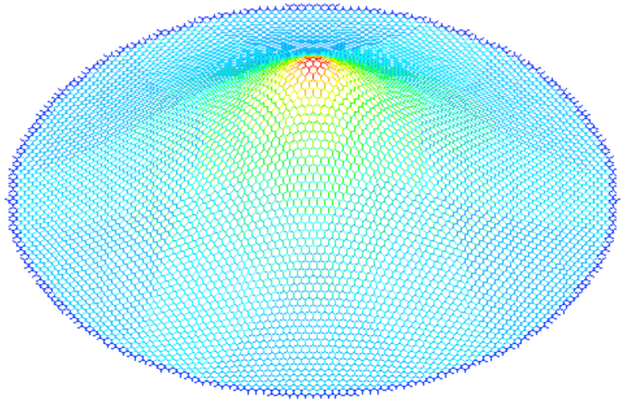


Table 5. Graphene data from literature and present work.

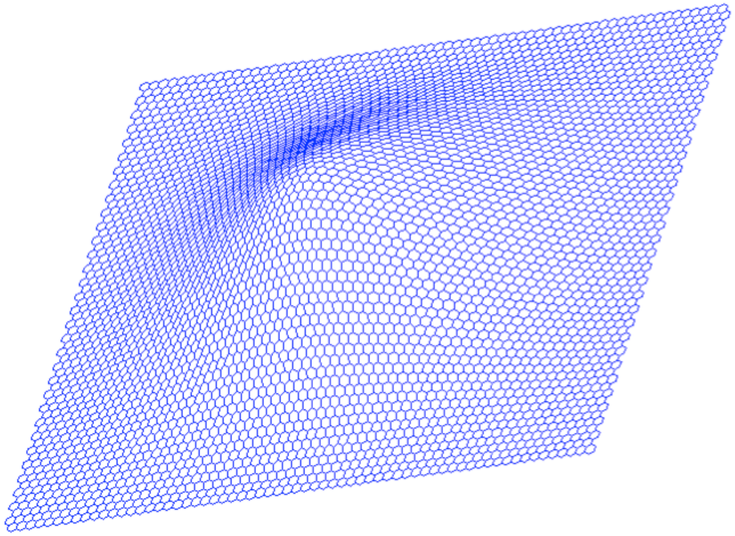
Author	Y_1 (TPa nm)	Y_2 (TPa nm)	ν_{12}	ν_{21}	d (Å)
Tu and Ou-Yang [45]	0.348		0.34		0.74
Zhou *et al* [46]	0.377		0.24		0.74
Yakobson *et al* [47]	0.363		0.19		0.66
Caillerie *et al* [25]	0.277		0.26		N/A
Brenner *et al* [15]	0.235		0.41		0.62
Huang *et al* [17]	0.243		0.397		0.57
Kudin *et al* [13]	0.345		0.149		0.84
Chang and Gao [50]	0.360		0.16		3.4
Cho *et al* [48]	0.386		0.195		3.35
Sakhaee-Pour [34]	0.337–0.354		1.129–1.441		3.4
Hemmasizadeh *et al* [24]	0.124		0.19		1.317
Blakslee *et al* [58]	0.342		0.16		3.35
Lee *et al* [60]	0.335		N/A		3.35
Reddy *et al* [23]	0.228	0.277	0.43	0.52	3.4
Present FE honeycomb (AMBER)	0.517	0.342	0.523	0.509	0.82–0.99
Present FE honeycomb (Morse)	0.546	0.408	0.551	0.577	0.86–0.87
Present EHM stretching–hinging (AMBER)	0.297		0.211		0.84
Present EHM stretching–hinging (Morse)	0.384		0.213		0.74
Present EHM stretching–hinging-shear (AMBER)	0.144		0.617		0.84
Present EHM stretching–hinging-shear (Morse)	0.169		0.653		0.74
Present EHM-all deformation mechanisms (AMBER)	0.064		0.830		0.84
Present EHM-all deformation mechanisms (Morse)	0.074		0.848		0.74

(F Scarpa, S Adhikari, A S Phani, 2009. *Nanotechnology* 20, 065709)

Atomistic FE vs Continuum – SLGS



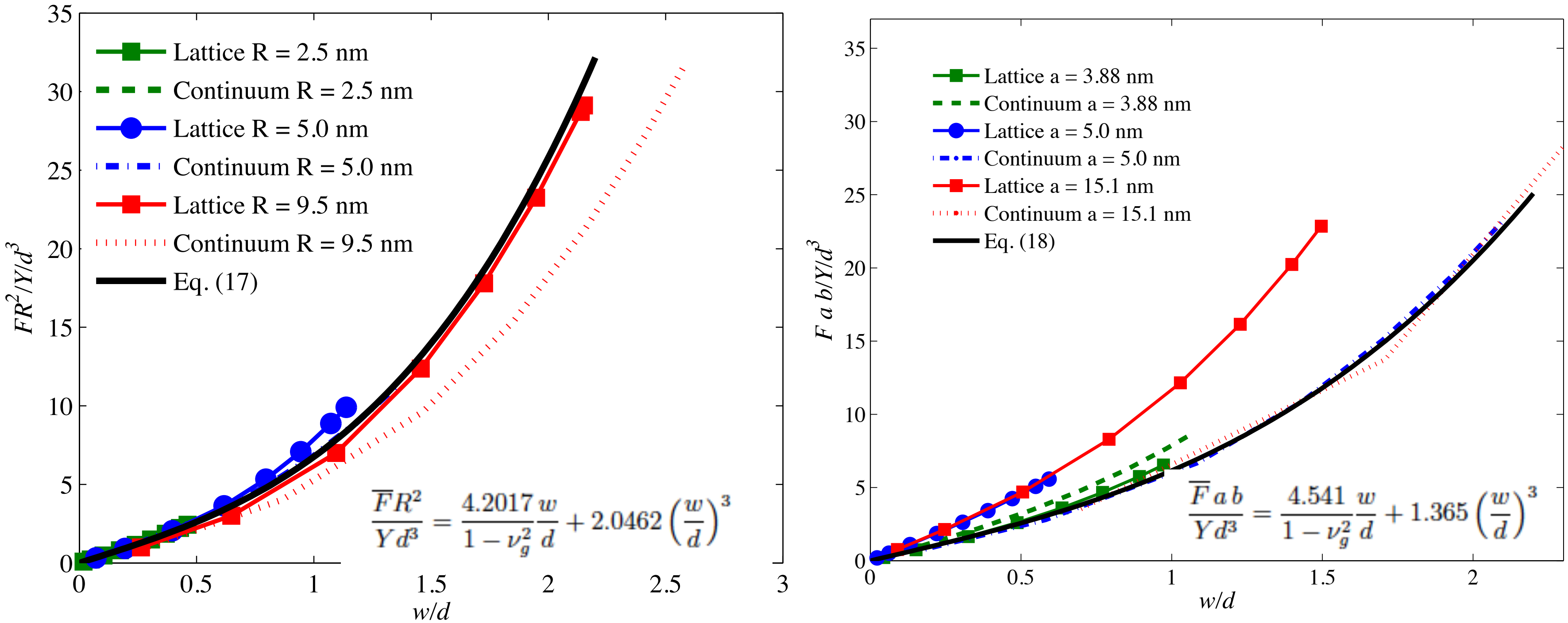
Circular SLGS (R = 9: 5 nm) under central loading. Distribution of equivalent membrane stresses.



Deformation of rectangular SLGS (15.1 x 13.03 nm^2) under central loading.

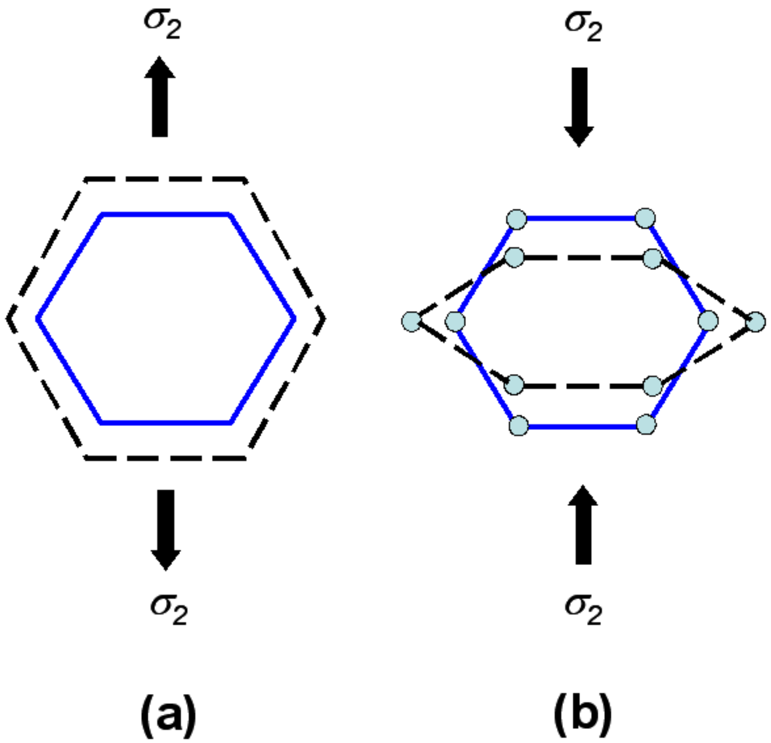
Scarpa, F., Adhikari, S., Gil, A. J. and Remillat, C., "The bending of single layer graphene sheets: Lattice versus continuum approach", Nanotechnology, 21[12] (2010), pp. 125702:1-9.

Axtomistic FE vs Continuum – SLGS



Comparison of the nondimensional force vs. nondimensional out-of-plane displacement for circular and rectangular lattice and continuum SLGS.

Analytical approach for SLGS – honeycomb structure



C-C bonds deform under stretching and hinging

$$K_h = \frac{8k_\tau}{d^2}$$ Hinging constant related to thickness d

Applying averaging of stretching and hinging deformation over unit cell:

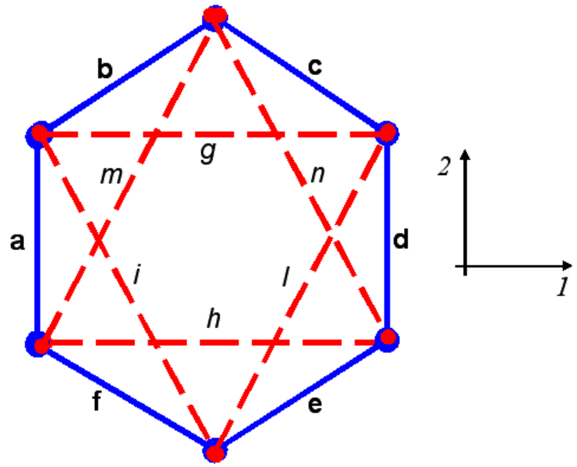
$$E_1 = \frac{4\sqrt{3}k_r K_h}{3d\left(k_r + 3K_h\right)} \qquad E_2 = \frac{4\sqrt{3}k_r K_h}{3d\left(k_r + 3K_h\right)}$$

$$\nu_{21} = \nu_{12} = \frac{1 - K_h/k_r}{1 + 3K_h/k_r} \qquad G_{12} = \frac{\sqrt{3}K_h k_r}{3d\left(k_r + K_h\right)}$$

- Isotropic for “infinite” graphene sheet
- Orthotropic for finite size graphene and considering edge effects

F Scarpa, S Adhikari, A S Phani, 2009. *Nanotechnology* **20,** 065709

Analytical approach for SLGS – honeycomb structure



Unit cell made by rods withstanding axial and bending deformation

$$Y_{\mathbf{a-f}} = \frac{4Lk_r}{\pi d_s^2}$$ Equivalent Young's modulus for axial members

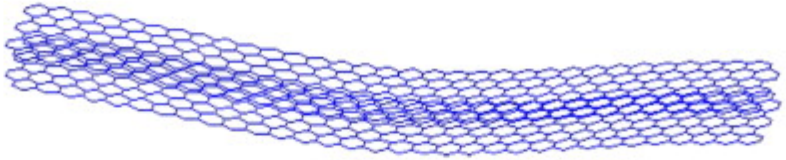
$$Y_{g-n} = \frac{16k_\theta}{\pi L d_b^2}$$ Equivalent Young's modulus for axial members

A **Rigidity** matrix is obtained using a lattice continuum modelling of space frames → equivalence with plane stress formulation for a plane sheet:

$$E = \frac{1}{d_{\max}} \frac{4\sqrt{3}}{9L^2}\left(k_r L^2 + 12k_\theta\right) \qquad \nu = \frac{1}{3}$$

F Scarpa, S Adhikari, A S Phani, 2009. *Nanotechnology* **20,** 065709
(L Kollár and I Hegedús. Analysis and design of space frames by the Continuum Method. Developments in Civil Engineering, 10. Elsevier, Amsterdam, 1985)

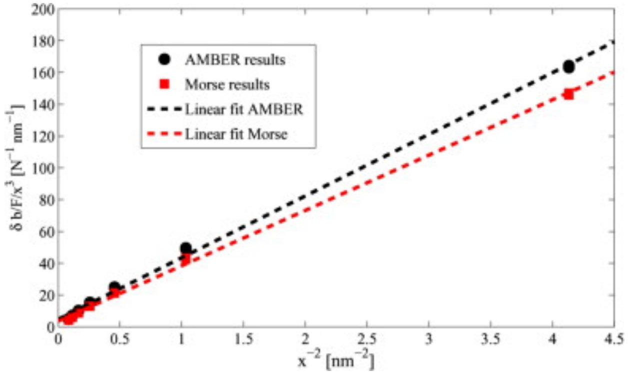
Atomistic FE – Bilayer Graphene

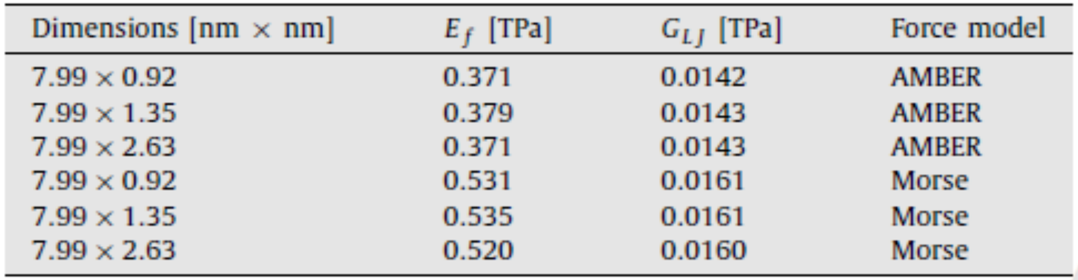


- Equivalent to structural “sandwich” beams
- C-C bonds in graphene layers represented with classical equivalent beam models
- “Core” represented by Lennard-Jones potential interactions:

$$F_{ij} = -12\epsilon\left[\left(\frac{r_{min}}{y}\right)^{13} - \left(\frac{r_{min}}{y}\right)^{7}\right]$$

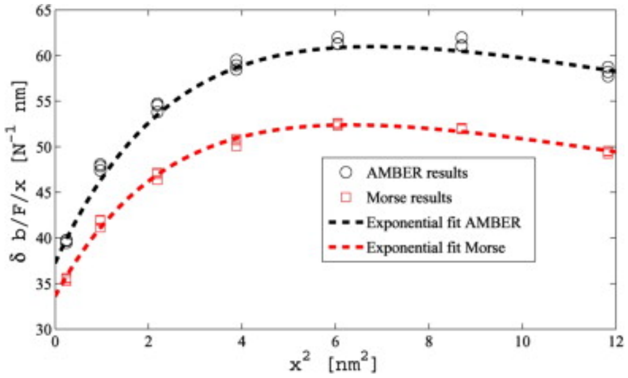
r_{min} = 0.383 nm
ε = 2.39 meV





Dimensions [nm × nm]	E_f [TPa]	G_{LJ} [TPa]	Force model
7.99 × 0.92	0.371	0.0142	AMBER
7.99 × 1.35	0.379	0.0143	AMBER
7.99 × 2.63	0.371	0.0143	AMBER
7.99 × 0.92	0.531	0.0161	Morse
7.99 × 1.35	0.535	0.0161	Morse
7.99 × 2.63	0.520	0.0160	Morse

E_f =0.5 TPa (I.W. Frank, D.M. Tanenbaum, A.M. van der Zande, P.L. McEuen, J. Vac. Sci. Technol. B 25 (2007) 2558)



Scarpa, F., Adhikari, S. and Chowdhury, R., "The transverse elasticity of bilayer graphene", Physics Letters A, 374[19-20] (2010), pp. 2053-2057.

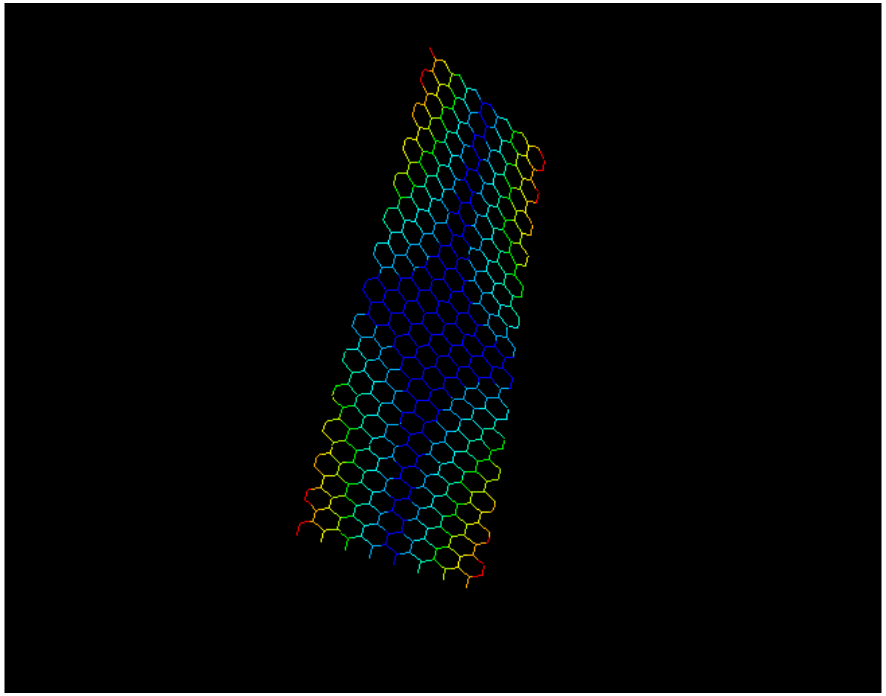
Mechanical vibration of SLGS

Lumped mass matrix:

$$[\mathrm{M}]_{\mathbf{e}} = diag\left[\ \frac{m_c}{3} \quad \frac{m_c}{3} \quad \frac{m_c}{3} \quad 0 \quad 0 \quad 0\ \right]$$

Minimisation of the Hamiltonian for the ith mode:

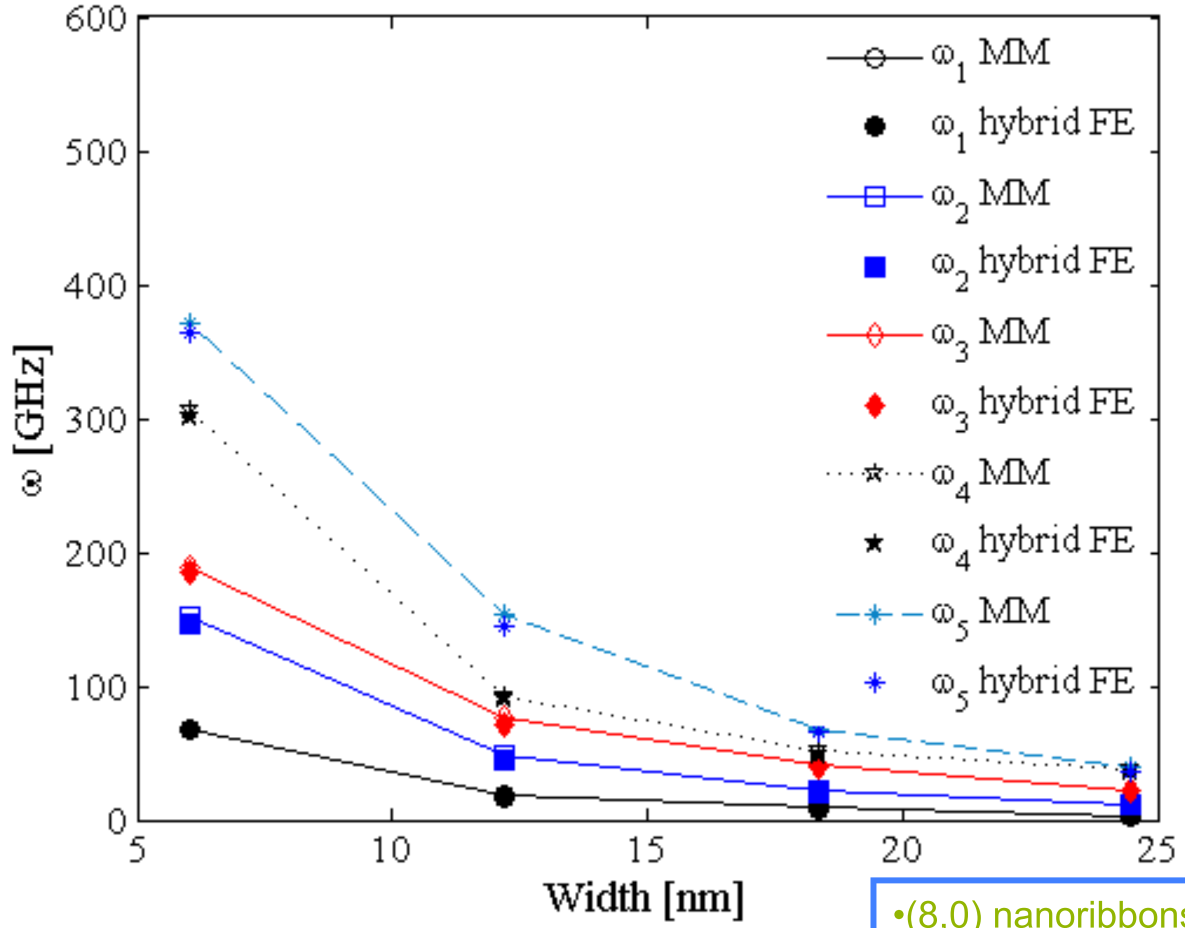
$$H_i = \frac{1}{2}\{\Phi\}_i^T [\mathrm{M}]\{\Phi\}_i \times \omega_i^2 + \frac{1}{2}\{\Phi\}_i^T [\mathbf{K}]\{\Phi\}_i = \omega_i^2$$



Comparison against Molecular Mechanics model based on the eigenvalue analysis of the system Hessian matrix

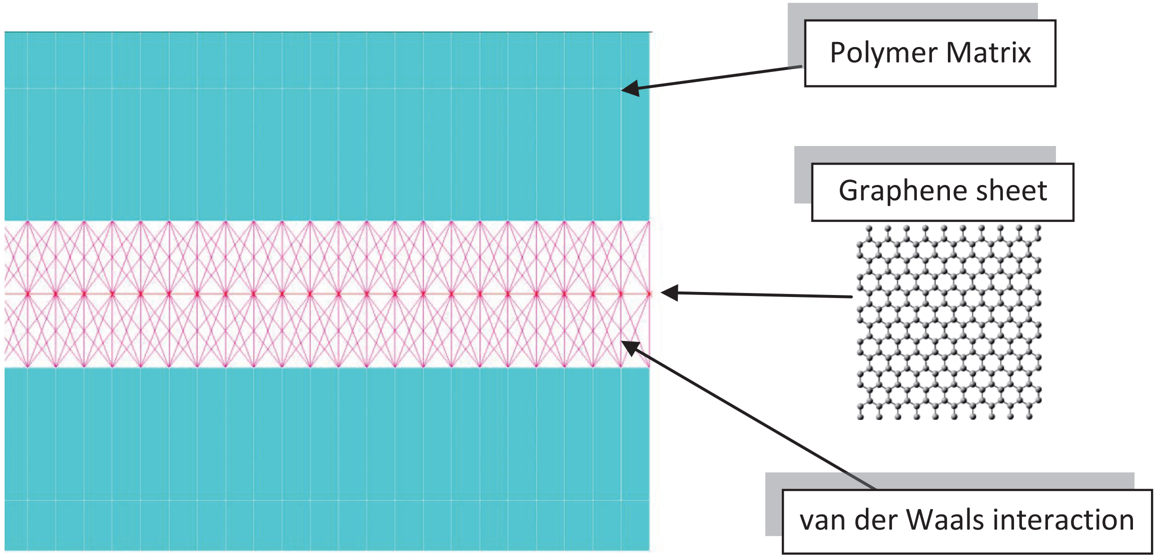
Scarpa, F., Chowdhury, R., Kam, K., Adhikari, S. and Ruzzene, M., "Wave propagation in graphene nanoribbons", Nanoscale Research Letters, 6 (2011), pp. 430:1-10.
Chowdhury, R., Adhikari, S., Scarpa, F. and Friswell, M. I., "Transverse vibration of single layer graphene sheets", Journal of Physics D: Applied Physics, 44[20] (2011), pp. 205401:1-11.

Mechanical vibration of SLGS



- (8,0) nanoribbons with different lengths
- Errors between 2 and 3 %
- Average thickness d = 0.077 nm

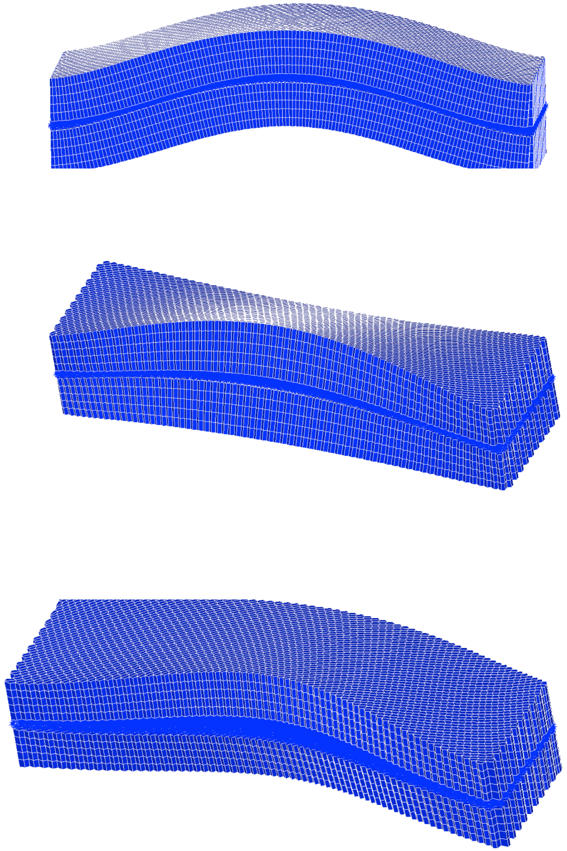
Graphene composites

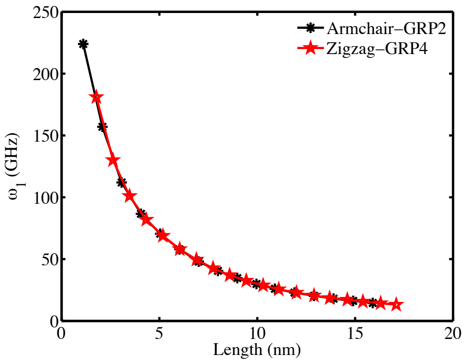


Polymer Matrix

Graphene sheet

van der Waals interaction



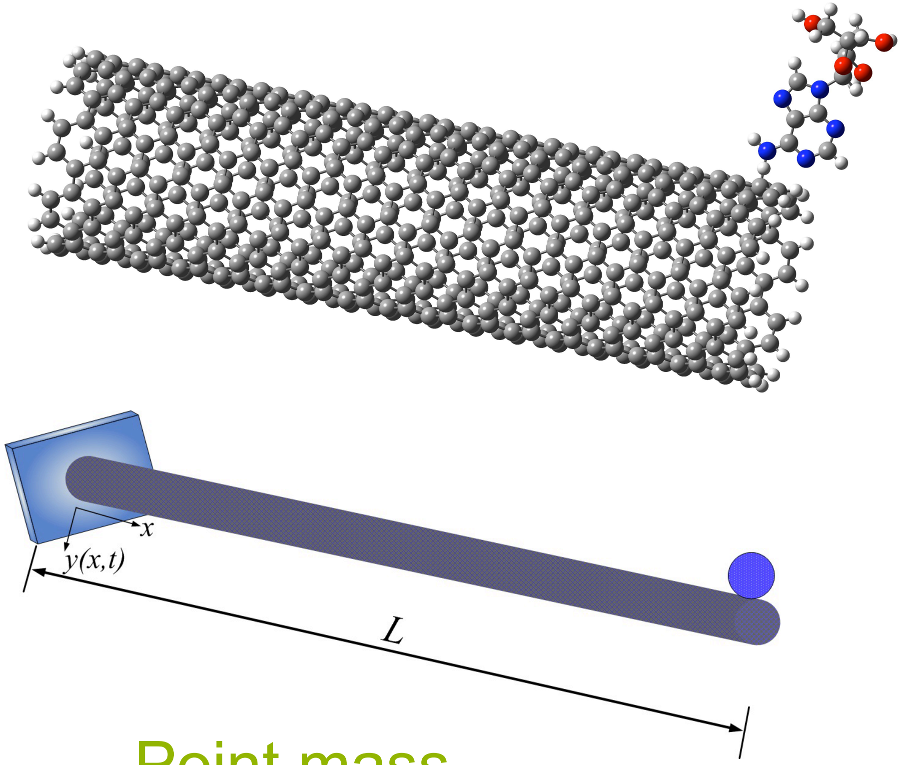


Chandra, Y., Chowdhury, R., Scarpa, F., Adhikari, S. and Seinz, J., "Multiscale modeling on dynamic behaviour of graphene based composites", Materials Science and Engineering B, in press.

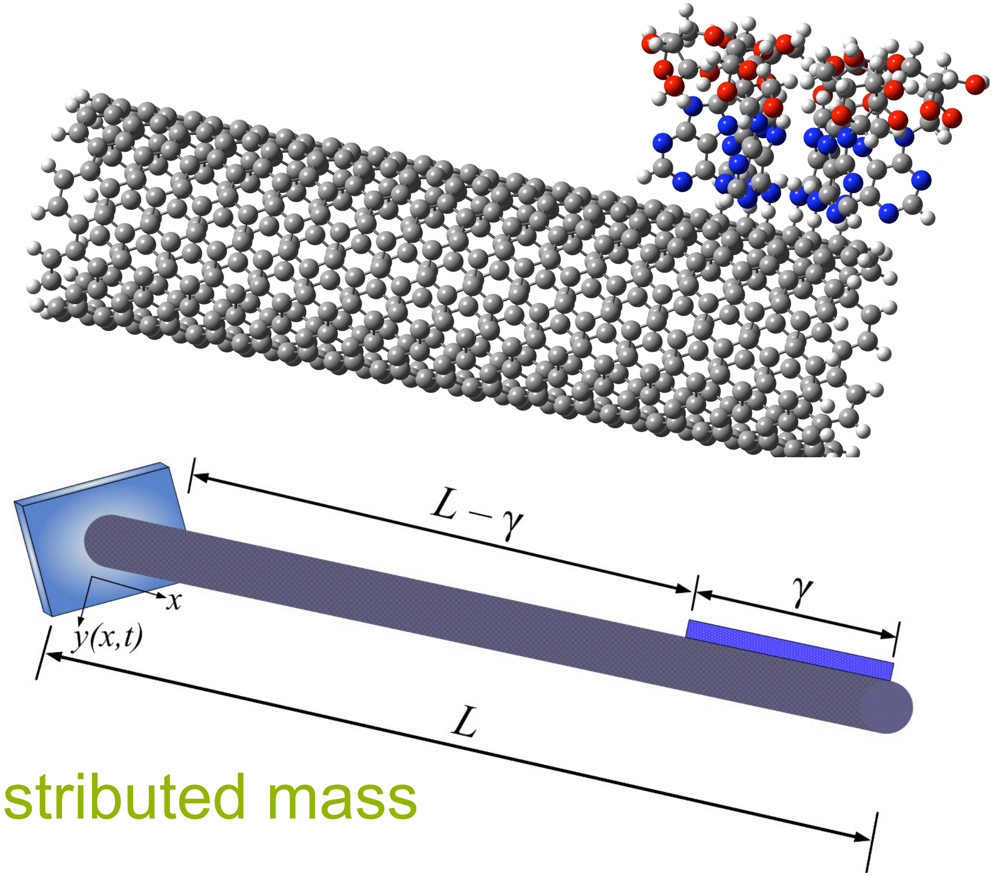
Swansea University
Prifysgol Abertawe

Nanobio Sensors

Vibration based mass sensor: CNT



Point mass



Distributed mass

Chowdhury, R., Adhikari, S. and Mitchell, J., "Vibrating carbon nanotube based bio-sensors", Physica E: Low-dimensional Systems and Nanostructures, 42[2] (2009), pp. 104-109.

Adhikari, S. and Chowdhury, R., "The calibration of carbon nanotube based bio-nano sensors", *Journal of Applied Physics*, 107[12] (2010), pp. 124322:1-8

Vibration based mass sensor: CNT

The equation of motion of free-vibration: $EI\frac{\partial^4 y(x,t)}{\partial x^4} + \rho A\frac{\partial^2 y(x,t)}{\partial t^2} = 0$

The resonance frequencies: $f_j = \frac{\lambda_j^2}{2\pi}\sqrt{\frac{EI}{\rho A L^4}}$ $\cos\lambda\cosh\lambda + 1 = 0$

The Mode shapes:
$$Y_j(\xi) = (\cosh\lambda_j\xi - \cos\lambda_j\xi) - \left(\frac{\sinh\lambda_j - \sin\lambda_j}{\cosh\lambda_j + \cos\lambda_j}\right)(\sinh\lambda_j\xi - \sin\lambda_j\xi)$$
where
$$\xi = \frac{x}{L}$$

We use energy principles to obtain the frequency shift due to the added mass.

Vibration based mass sensor: CNT

Natural frequency with the added mass:

$$f_n = \frac{1}{2\pi}\sqrt{\frac{k_{eq}}{m_{eq}}} = \frac{\beta}{2\pi}\frac{c_k}{\sqrt{1+c_m\Delta M}}$$

where

$$\beta = \sqrt{\frac{EI}{\rho A L^4}}$$

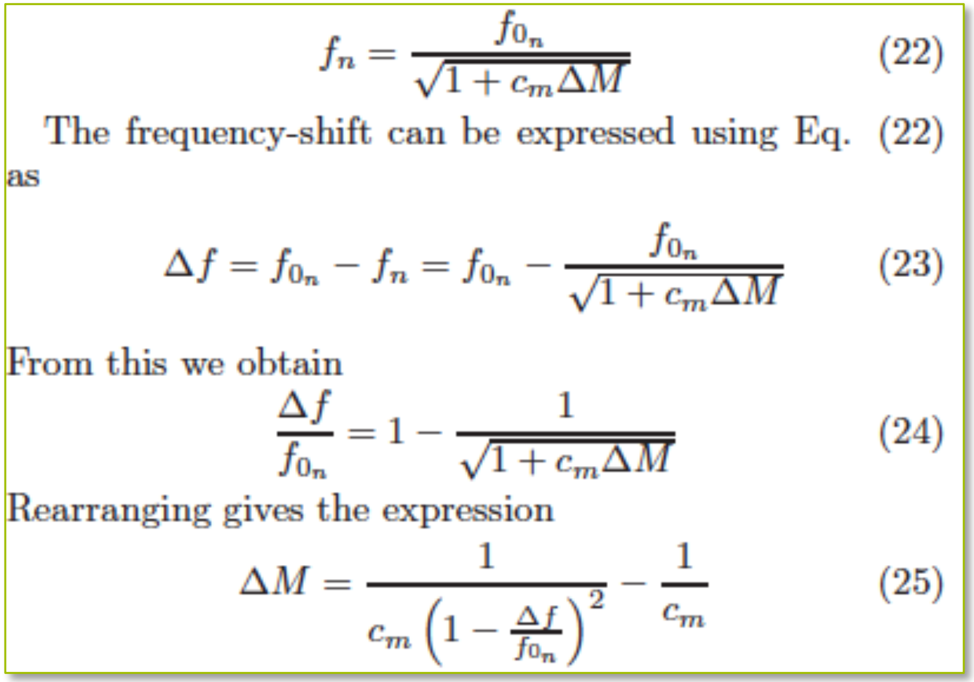
the stiffness calibration constant

$$c_k = \sqrt{\frac{I_3}{I_1}}$$

and the mass calibration constant

$$c_m = \frac{I_2}{I_1}$$

Identification of the added mass



$$f_n = \frac{f_{0_n}}{\sqrt{1+c_m\Delta M}} \tag{22}$$

The frequency-shift can be expressed using Eq. (22) as

$$\Delta f = f_{0_n} - f_n = f_{0_n} - \frac{f_{0_n}}{\sqrt{1+c_m\Delta M}} \tag{23}$$

From this we obtain

$$\frac{\Delta f}{f_{0_n}} = 1 - \frac{1}{\sqrt{1+c_m\Delta M}} \tag{24}$$

Rearranging gives the expression

$$\Delta M = \frac{1}{c_m\left(1-\frac{\Delta f}{f_{0_n}}\right)^2} - \frac{1}{c_m} \tag{25}$$

Vibration based mass sensor: CNT

Mass of a nano object can be detected from the frequency shift Δf

$$M = \frac{\rho A L}{c_m} \frac{(c_k^2 \beta^2)}{(c_k \beta - 2\pi \Delta f)^2} - \frac{\rho A L}{c_m}$$

$$I_1 = \int_0^1 Y_j^2(\xi) \mathrm{d}\xi = 1.0$$

$$I_2 = \frac{1}{\gamma} \int_{\xi=1-\gamma}^{1} Y_j^2(\xi) \mathrm{d}\xi; \quad 0 \leq \gamma \leq 1$$

$$I_3 = \int_0^1 Y_j''^2(\xi) \mathrm{d}\xi = 12.3624$$

$$c_k = \sqrt{\frac{I_3}{I_1}} = 3.5160 \quad \text{and} \quad c_m = \frac{I_2}{I_1}$$

Adhikari, S. and Chowdhury, R., "The calibration of carbon nanotube ba bio-nano sensors", *Journal of Applied Physics*, **107**[12] (2010), pp. 124322:1-8

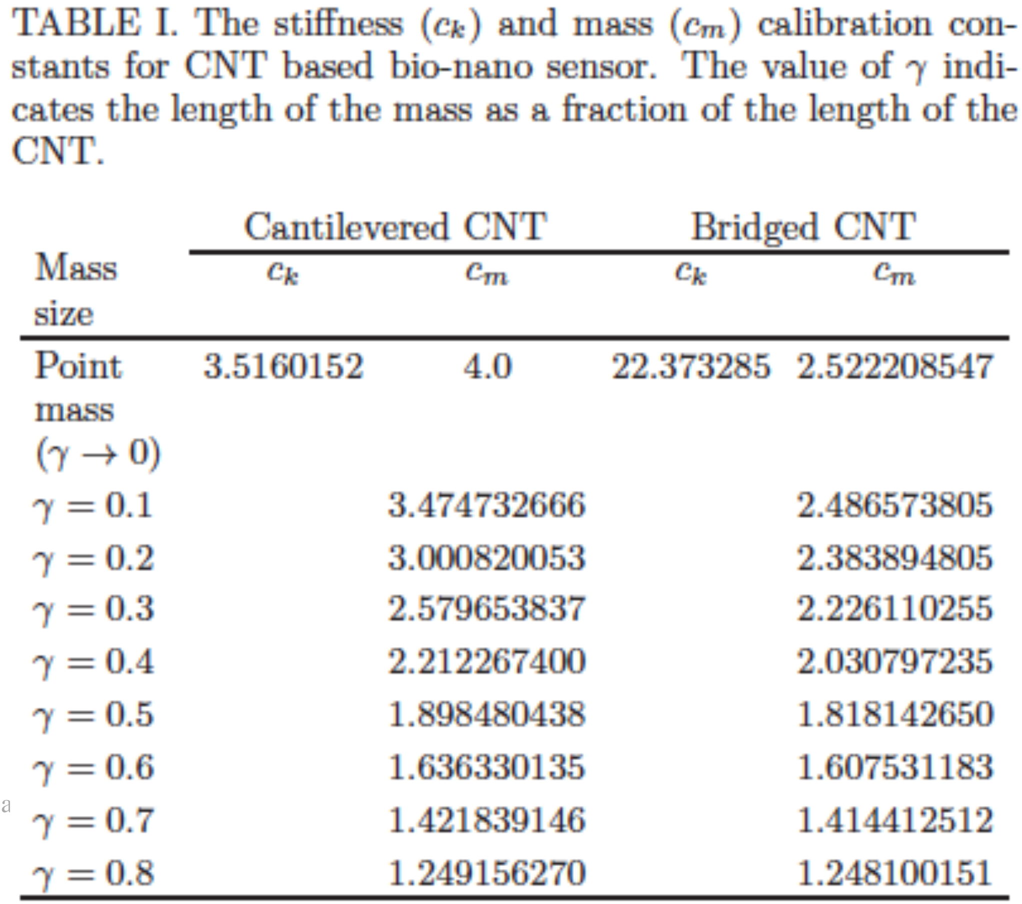


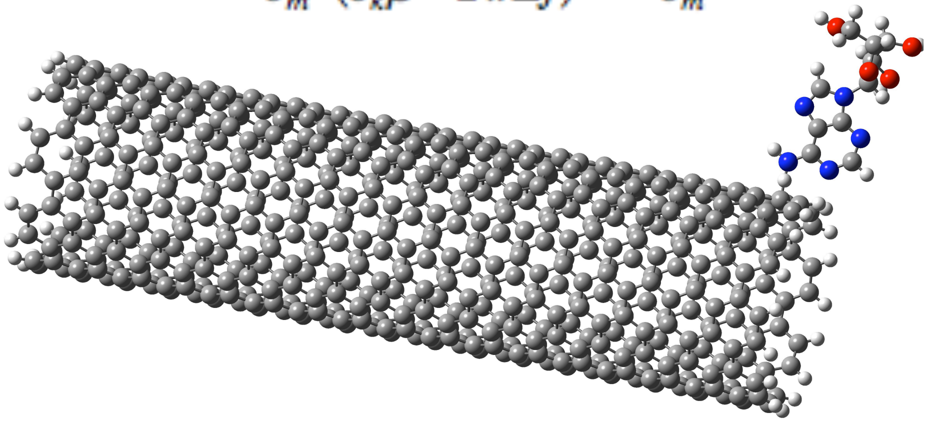
TABLE I. The stiffness (c_k) and mass (c_m) calibration constants for CNT based bio-nano sensor. The value of γ indicates the length of the mass as a fraction of the length of the CNT.

Mass size	Cantilevered CNT c_k	Cantilevered CNT c_m	Bridged CNT c_k	Bridged CNT c_m
Point mass ($\gamma \to 0$)	3.5160152	4.0	22.373285	2.522208547
$\gamma = 0.1$		3.474732666		2.486573805
$\gamma = 0.2$		3.000820053		2.383894805
$\gamma = 0.3$		2.579653837		2.226110255
$\gamma = 0.4$		2.212267400		2.030797235
$\gamma = 0.5$		1.898480438		1.818142650
$\gamma = 0.6$		1.636330135		1.607531183
$\gamma = 0.7$		1.421839146		1.414412512
$\gamma = 0.8$		1.249156270		1.248100151

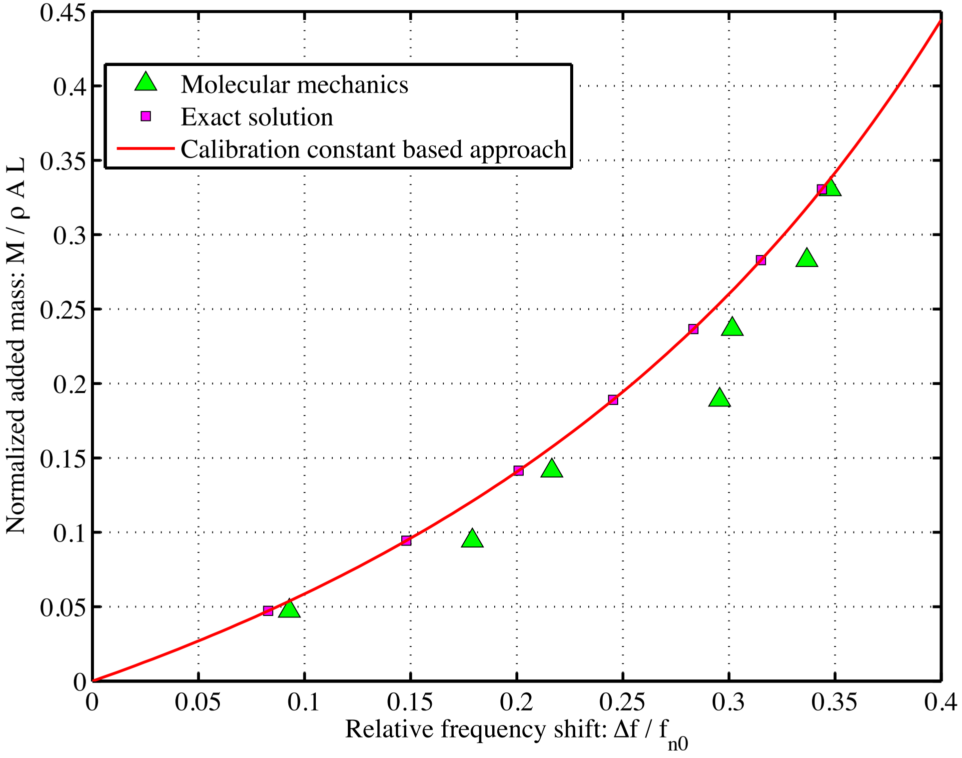
Vibration based mass sensor: CNT

Mass of a nano object can be detected from the frequency shift Δf

$$M = \frac{\rho A L}{c_m} \frac{(c_k^2 \beta^2)}{(c_k \beta - 2\pi \Delta f)^2} - \frac{\rho A L}{c_m}$$



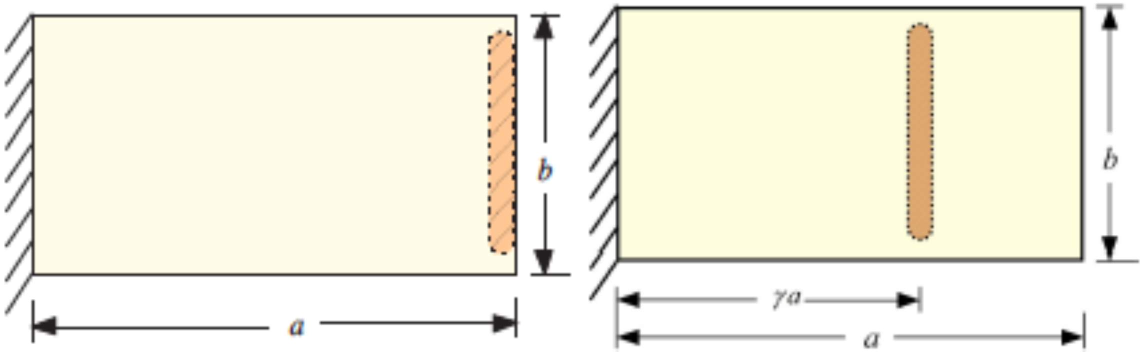
CNT with deoxythymidine



Adhikari, S. and Chowdhury, R., "The calibration of carbon nanotube based bio-nano sensors", *Journal of Applied Physics*, **107**[12] (2010), pp. 124322:1-8

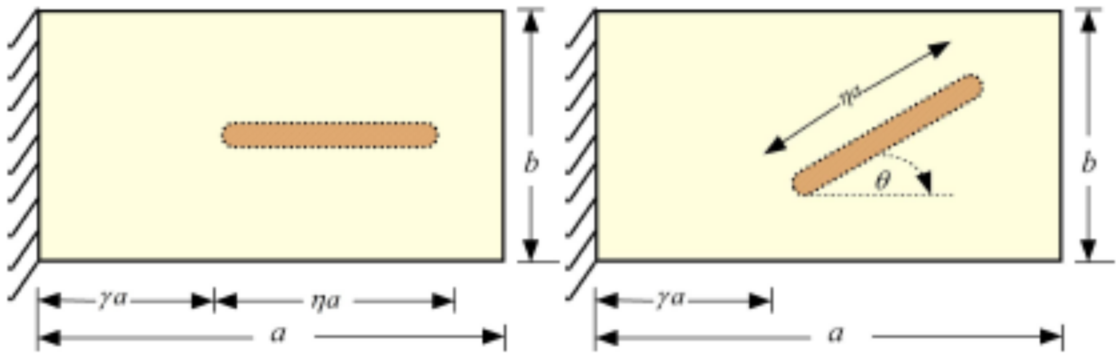
Vibration based mass sensor: Graphene

Vibrating graphene sheets can be used as sensors with different mass arrangements



(a) Masses at the cantilever tip in a line

(b) Masses in a line along the width



(c) Masses in a line along the length

(d) Masses in a line with an arbitrary angle

Vibration based mass sensor: Graphene

Relative added mass:

$$\mu = \frac{1}{c_n\left(1-\frac{\Delta f}{f_0}\right)^2} - \frac{1}{c_n}$$

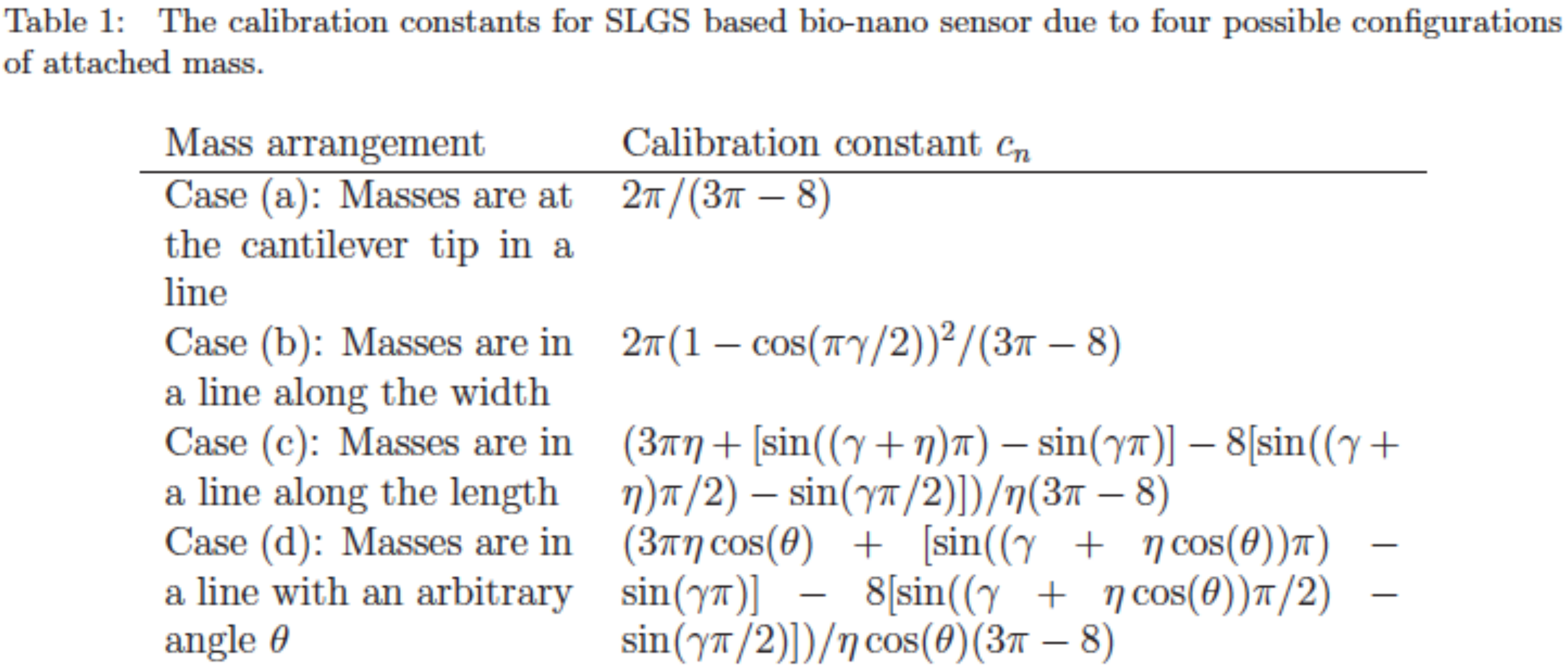
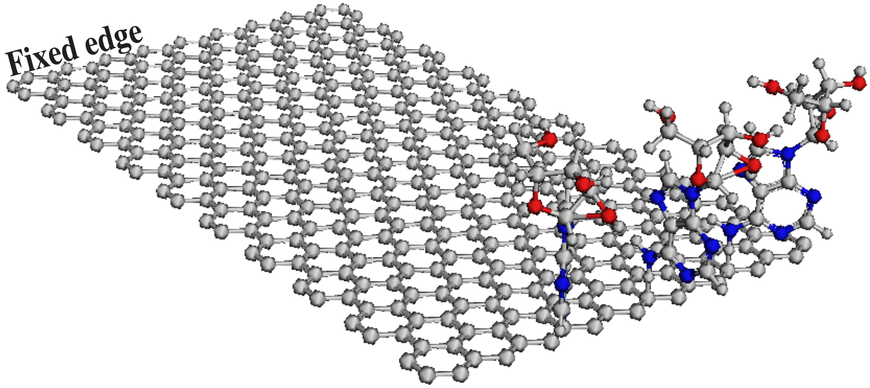


Table 1: The calibration constants for SLGS based bio-nano sensor due to four possible configurations of attached mass.

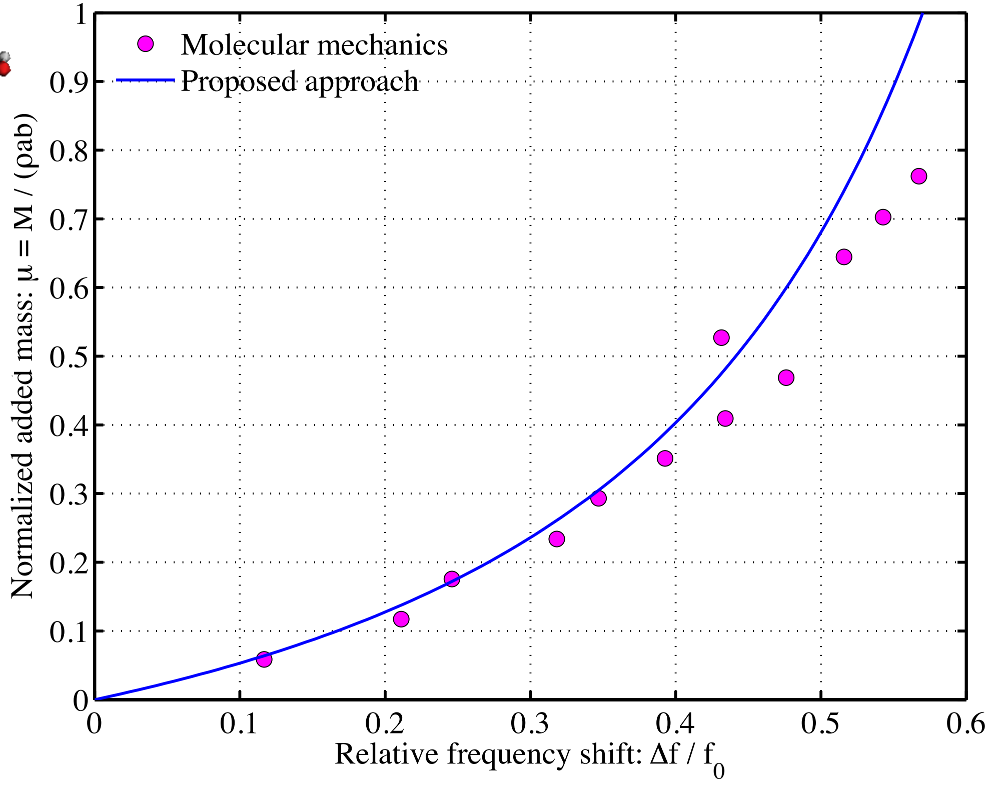
Mass arrangement	Calibration constant c_n
Case (a): Masses are at the cantilever tip in a line	$2\pi/(3\pi-8)$
Case (b): Masses are in a line along the width	$2\pi(1-\cos(\pi\gamma/2))^2/(3\pi-8)$
Case (c): Masses are in a line along the length	$(3\pi\eta+[\sin((\gamma+\eta)\pi)-\sin(\gamma\pi)]-8[\sin((\gamma+\eta)\pi/2)-\sin(\gamma\pi/2)])/\eta(3\pi-8)$
Case (d): Masses are in a line with an arbitrary angle θ	$(3\pi\eta\cos(\theta)+[\sin((\gamma+\eta\cos(\theta))\pi)-\sin(\gamma\pi)]-8[\sin((\gamma+\eta\cos(\theta))\pi/2)-\sin(\gamma\pi/2)])/\eta\cos(\theta)(3\pi-8)$

Vibration based mass sensor: Graphene

Vibrating graphene sheets can be used as sensors with different mass arrangements

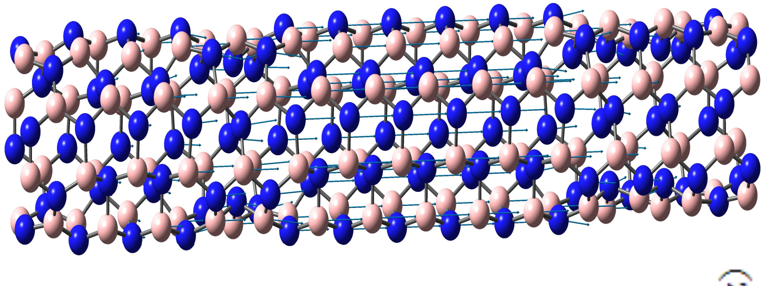


SLGS with adenosine

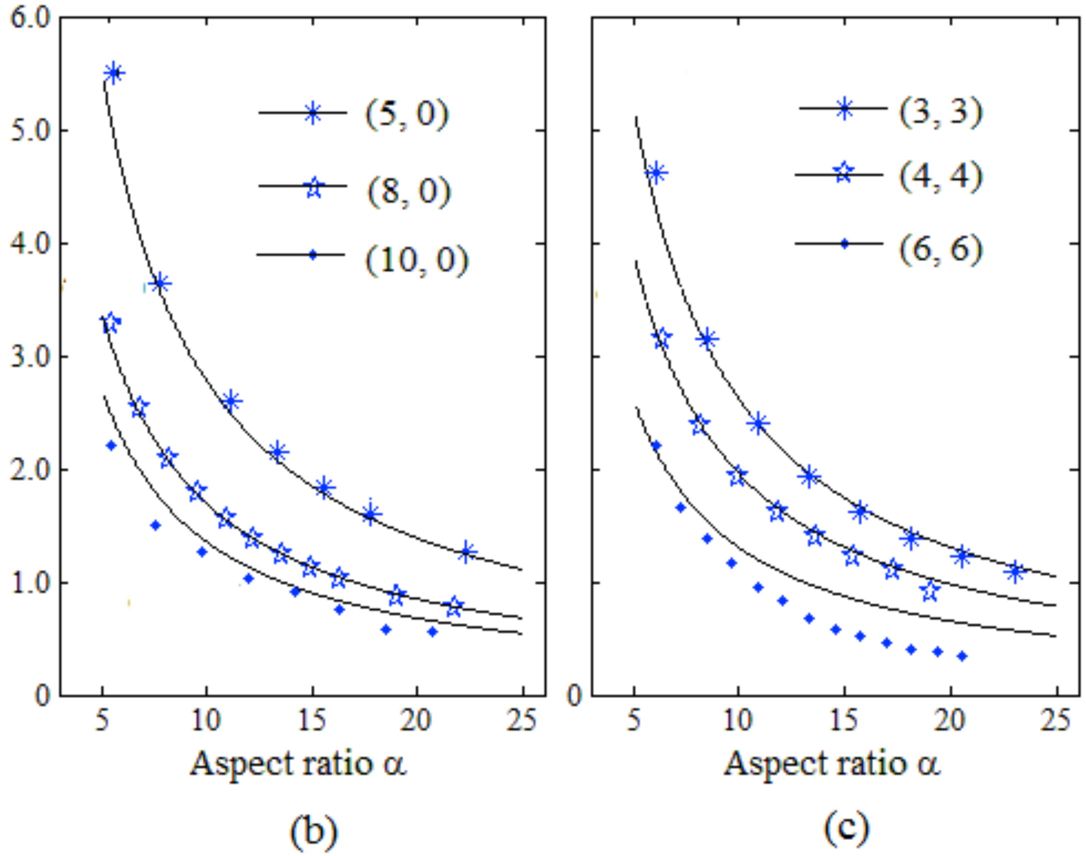


Boron Nitride Nanotube and Nanosheets

Axial vibration of BNNT



(a)



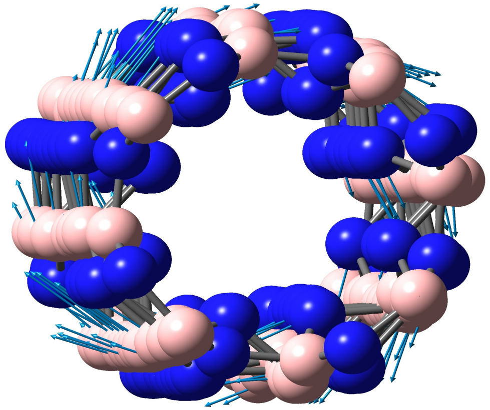
(b)

(c)

(a) Axial vibration and its associated frequency of (b) zigzag and (c) armchair BNNTs given by the MM simulations (discrete dots) and a column model with Young’s modulus 1*TPa* (solid lines).

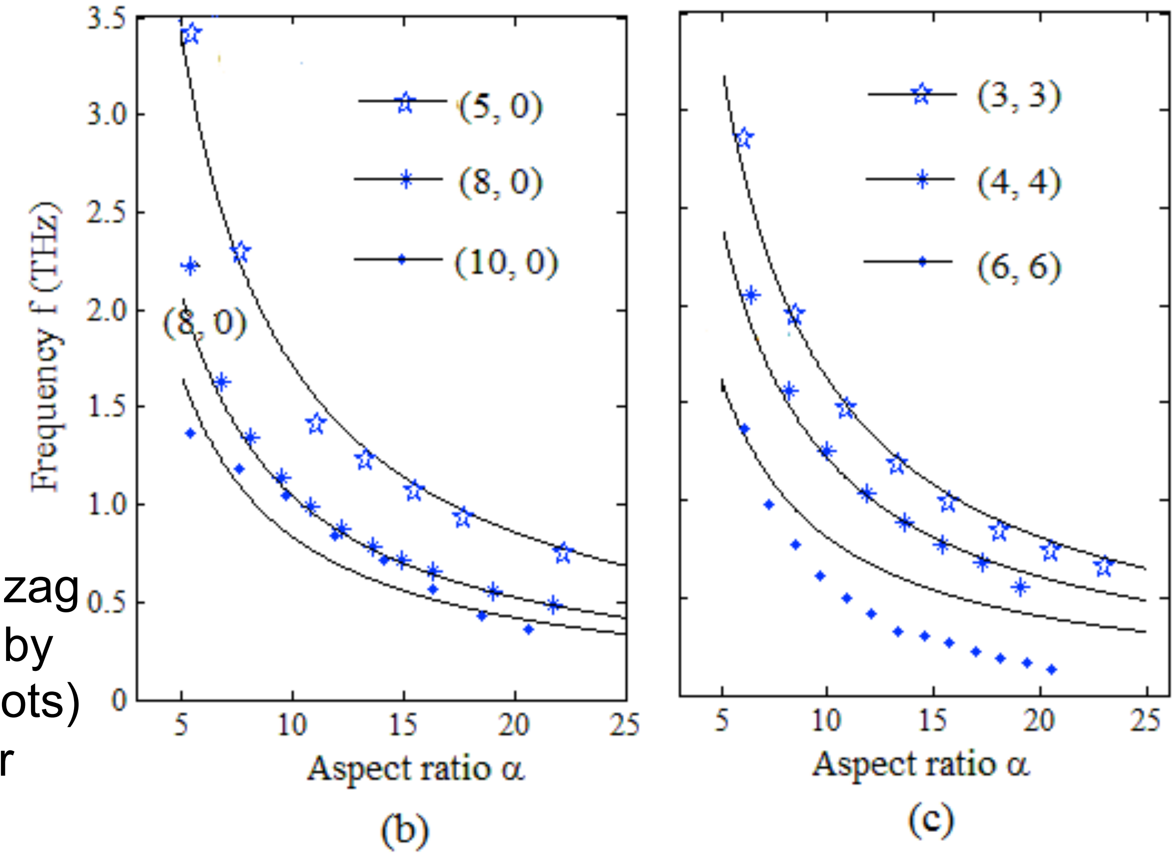
Chowdhury, R., Wang, C. W., Adhikari, S. and Scarpa, F., "Vibration and symmetry-breaking of boron nitride nanotubes", Nanotechnology, 21[36] (2010), pp. 365702:1-9.

Torsional vibration of BNNT



(a)

(a) Torsional vibration and its associated frequency of (b) zigzag and (c) armchair BNNTs given by the MM simulations (discrete dots) and a column model with shear modulus 0.41TPa (solid lines).

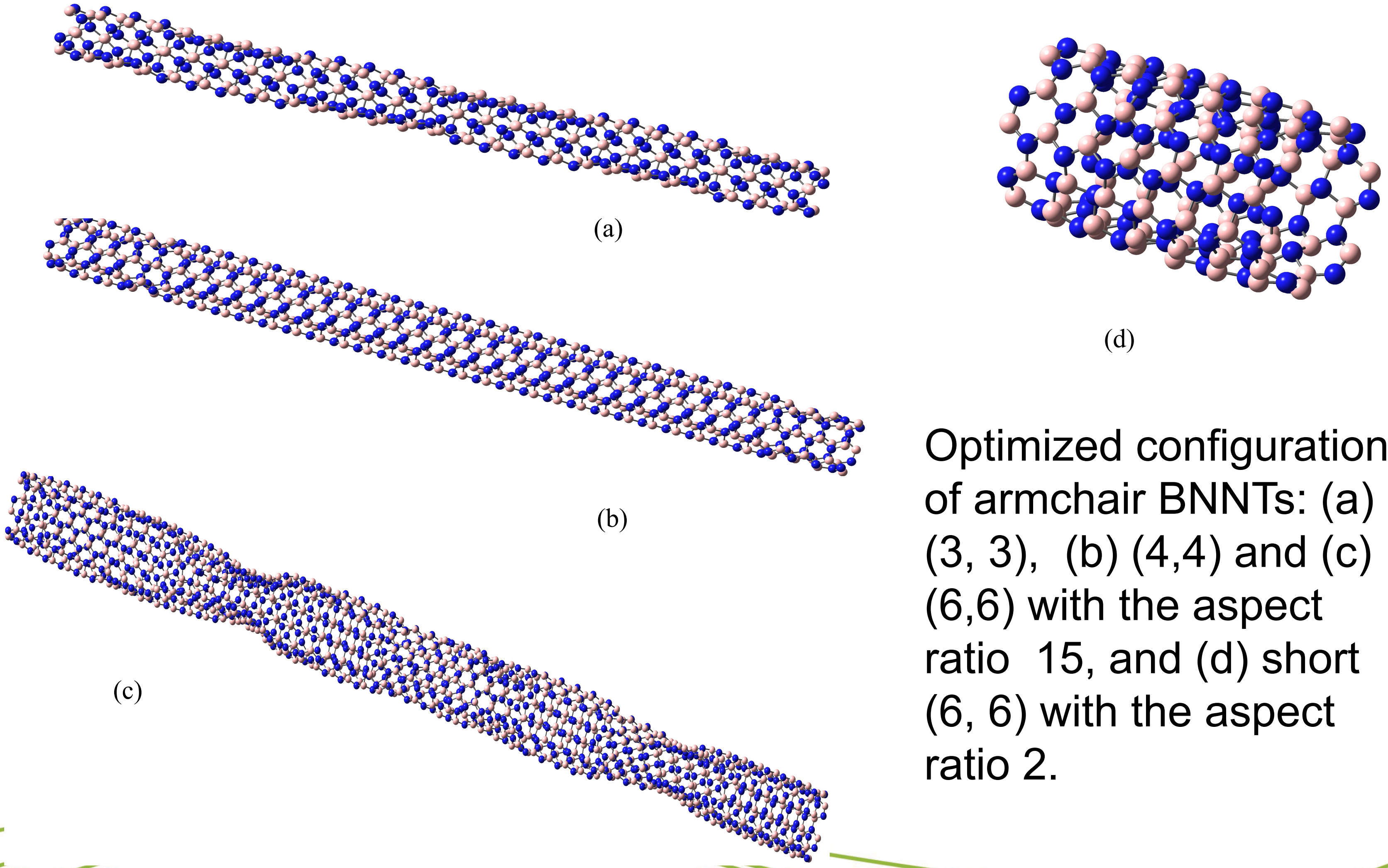


(b)

(c)

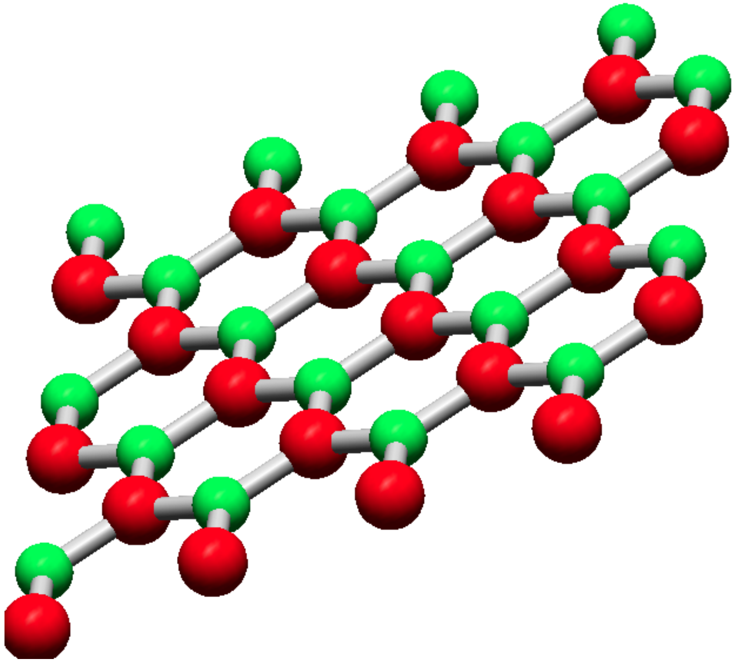
Chowdhury, R., Wang, C. W., Adhikari, S. and Scarpa, F., "Vibration and symmetry-breaking of boron nitride nanotubes", Nanotechnology, 21[36] (2010), pp. 365702:1-9.

Optimised shape of BNNT



Optimized configuration of armchair BNNTs: (a) (3, 3), (b) (4,4) and (c) (6,6) with the aspect ratio 15, and (d) short (6, 6) with the aspect ratio 2.

Mechanical property of BN Sheets



$$\bar{Y} = \frac{8\sqrt{3}\,C_\rho}{18 + r_{BN}^2\left(\frac{C_\rho}{C_\theta}\right)}$$

$$\bar{\nu} = \frac{r_{BN}^2\left(\frac{C_\rho}{C_\theta}\right) - 6}{18 + r_{BN}^2\left(\frac{C_\rho}{C_\theta}\right)}$$

$$\bar{G} = \frac{2\sqrt{3}\,C_\rho}{3 + 18\,r_{BN}^2\left(\frac{C_\rho}{C_\theta}\right)}$$

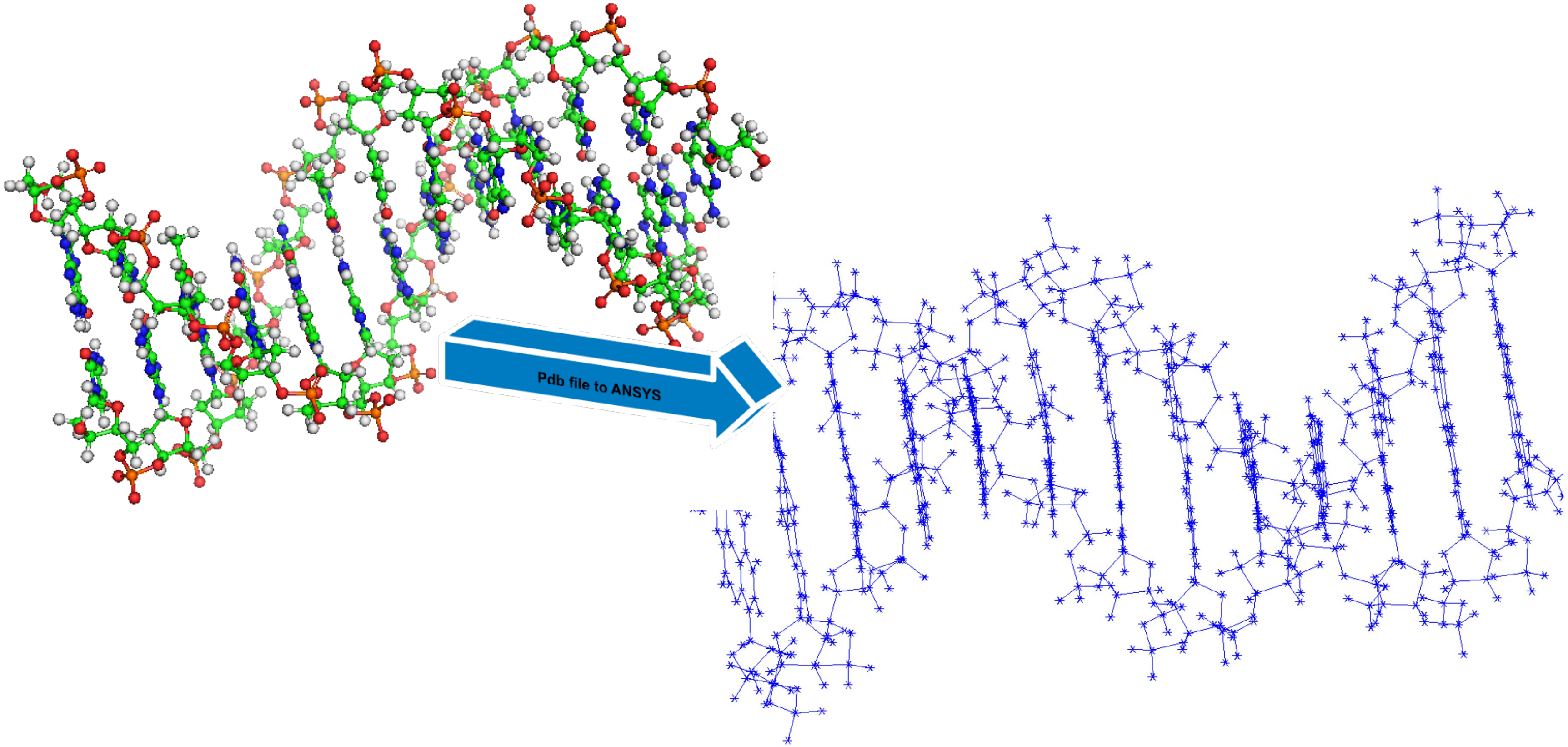
Example of armchair (4, 0) BN sheet. Boron atoms are in red, nitrogen atoms are in green.

Boldrin, L., Scarpa, F., Chowdhury, R., Adhikari, S. and Ruzzene, M., "Effective mechanical properties of hexagonal boron nitride nanosheets", Nanotechnology, 22[50] (2011), pp. 505702:1-7.

DNA Mechanics

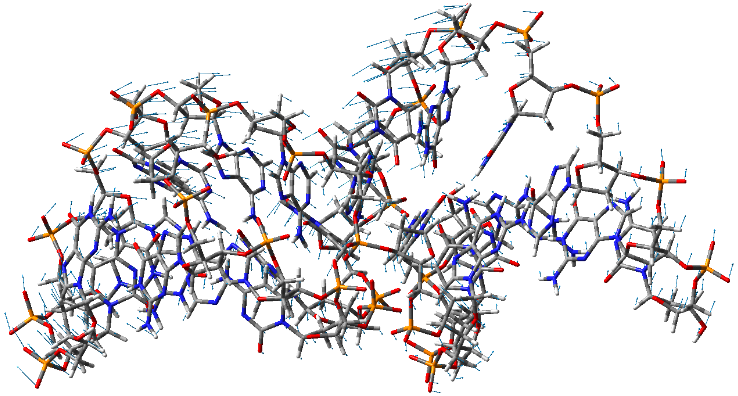
Atomistic FE of DNA

From protein data bank file to ANSYS input file – **a new code for automatic translation**

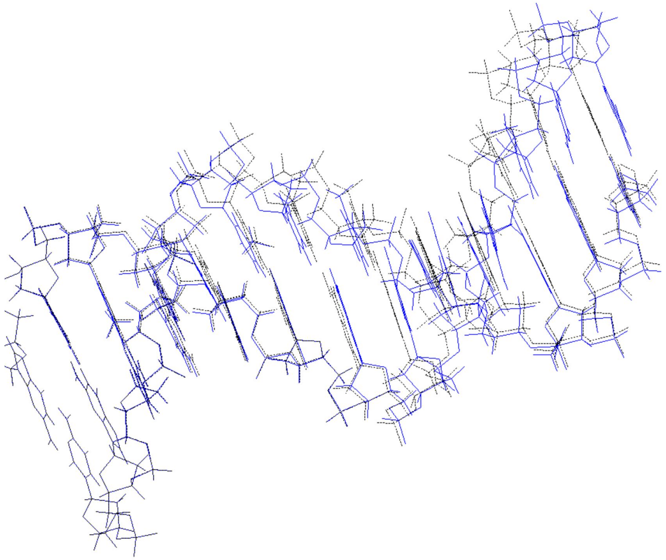


Atomistic FE of DNA

Material properties of the beams are obtained depending on the nature of the bonds



Mode 3 (MM:33.679; FE 38.768 GHz)



Mode 6 (MM:111.696; FE 112.71 GHz)

References

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2. Boldrin, L., Scarpa, F., Chowdhury, R., Adhikari, S. and Ruzzene, M., "Effective mechanical properties of hexagonal boron nitride nanosheets", *Nanotechnology*, 22[50] (2011), pp. 505702:1-7.
3. Murmu, T., Seinz, J., Adhikari, S. and Arnold, C., "Nonlocal buckling behaviour of bonded double-nanoplate-system", *Journal of Applied Physics*, 110[8] (2011), pp. 084316:1-8.
4. Flores, E. I. S., Adhikari, S., Friswell, M. I. and Scarpa, F., "Hyperelastic axial buckling of single wall carbon nanotubes", *Physica E: Low-dimensional Systems and Nanostructures*, 44[2] (2011), pp. 525-529.
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Conclusions: nanomechanics

- Atomistic finite element method is developed for general nanosalce structures:
  - Carbon nanotube
  - Fullerenes
  - Graphene
  - Nanoscale bio sensors
- Programs have been written to convert pdb files to Finite Element geometry file and material properties
- Encouraging results compared to MM simulation were obtained
- Future: nonlinearity, large-scale problems such as proteins & nanocomposites, molecular dynamic simulations, experimental validation