Advanced Computational Fracture Mechanics

(191015L02), ONLINE mode

A short term course under the Global Initiative of Academic Network (GIAN) program of Government of India

15-19 January 2024

Organized by

School of Mechanical Sciences

Indian Institute of Technology

Bhubaneswar

About the course

Material behavior at small scales provide crucial information about the physical properties at higher scales, particularly with respect to material failure. For instance, macroscopic properties of materials, such as: toughness, strength, ductility, conductivity and chemical diffusion are strongly influenced by the presence of defects like cracks and dislocations, which evolve at nano scales. In this context, fracture simulations play a key role in devising new lighter, stronger and efficient materials for various applications. Study of fracture using computational methods has deep-reaching applications throughout science and engineering. Computational fracture analysis requires developing suitable analytical models, discretizing the resulting partial differential equations, and solving them numerically. Each of the above three steps poses its own difficulties, like: non-linear and non-homogeneous behavior around the crack tip. Variety of solutions have been proposed to tackle such issues, both academically and for practical applications, e.g., the bottom up approach.

The aim of this short course is to present the state-of-the-art and the most recent developments in computational methods for the analysis and simulation of fracture at multiple scales, such that the design of materials can be optimized. The course will be beneficial to students at all levels (B.Tech./ M.Sc./M.Tech./PhD), faculty members, academicians, researchers from research and development organizations and professionals from various public and private sectors, to get a kick-start in the areas related to computational modelling of fracture.

Objectives

The main objective of the proposed course is to introduce the advanced computational methods for fracture, which will help to develop better and efficient techniques to simulate and study fracture in various applications. The primary objectives are as follows:

1. Expose the participants to the fundamental aspects of computational fracture: strong and weak forms, partition of unity and its relation to completeness.
2. Building confidence and capability amongst the participants on computational methods to simulate moving interfaces and/or free surfaces with discontinuities, where the mesh is not required to conform to the free surface and the discontinuous quantities can be captured in the finite element interpolant with minimal smearing of the discontinuities. Introduction to extended finite element method, phantom node method, peri-dynamics, phase field method, to name a few.
3. Introduction to sub-scale analysis: molecular/ atomistic methods to simulate fracture at Nano/quantum scales, along with the relevant mathematical models and implementation aspects.
4. Multiscale methods by coupling the coarse and fine scales, to simulate the crack growth.
5. Applications of the discussed computational methods to engineering applications, particularly, for non-linear, multiscale and multi-field problems.
6. Introduction to data driven analysis for Engineering applications, especially: machine learning interatomic potentials, neural operators and PINNs.

Teaching faculty

Prof. Dr-Ing. Timon Rabczuk (TR),

Chair of Computational Mechanics, Vice President for Research and Projects,
Institute for Structural Mechanics, Bauhaus University Weimar, Germany.

Prof. Rabczuk is the chair of computational mechanics at Bauhaus Universität-Weimar, since 2009. He obtained his PhD from the University of Karlsruhe. He worked at the Fraunhofer-Institute (Ernst Mach), Freiburg before joining the computational mechanics group of Prof. Belytschko at Northwestern University in Evanston, USA, where he was working for 4 years as post-doctoral fellow. As a result, he has the experience of directly working with developers of advanced computational methods like XFEM. He has developed collaborations with several researchers across the globe. The main research focus of Prof. Rabczuk is computational solid mechanics with emphasis on method development for problems involving fracture and failure of solids and fluid-structure interaction. Therefore, he will be working in the areas related to: constitutive modelling, material instabilities, fracture, strain localization, numerical methods, machine learning, to name a few.

Prof. Rabczuk has secured funds from several prestigious agencies to perform research on cutting edge problems. As a result, he has published more than 600 articles in high quality ISI journals. His h-index is 121 with 53644 citations. He is identified as the highly cited researcher. He is the editor and editorial board member of several international journals. To summarize, Prof. Rabczuk is an expert in the areas of advanced computational fracture mechanics.

Dr. Pattabhi Ramaiah Budarapu (PRB),

Associate Professor,

School of Mechanical Sciences, IIT Bhubaneswar.

Dr. Budarapu currently working as Associate Professor in the School of Mechanical Sciences, IIT Bhubaneswar. He has held postdoctoral research fellowship positions in the IMT School for Advanced studies Lucca, Italy and Masdar Institute of Science and Technology at Abudhabi, UAE. He received his PhD degree from Bauhaus University of Weimar, Germany. His research interests are: Lithium-ion batteries; Photovoltaic Solar Cells; Cellular structures; Deep machine learning; Multiscale Multiphysics analysis; Computational Methods for Fracture. He has published over 50 peer-reviewed journal papers.

Dr. Budarapu serves as the Editorial board member of the International Journal of Computational Methods and Frontiers of Structural and Civil Engineering journals. He has also experience of hosting special issues in the Engineering Analysis with Boundary Elements, Theoretical and Applied Fracture Mechanics, International Journal of Computational Methods, and materials journals, as lead guest editor. He is an active reviewer of more than 30 international journals. He serves as organising committee member for several conferences, including WCCM, ICF, ICCM, to name a few apart from delivering several presentations/invited talks at international conferences and universities.

Schedule

The course is planned for **38 hours** in total, with **23 lecture** hours and **15 tutorial** hours. Day wise schedule of the lecture classes and tutorials is given below.

Day 1: 15.01.2024

L1: Introduction to computational methods for fracture
L2: XFEM: basic concepts, partition of unity and its relation to completeness
L3: Overview of meshfree methods
L4: XFEM: strong and weak discontinuities
L5: Introduction to LEFM
L6: Application of XFEM to problems in LEFM
T1: Estimation of global stiffness matrices in XFEM.

Day 2: 16.01.2024

L7: XFEM for non-linear and multi-field problems
L8: Numerical examples using XFEM
L9: The phantom node method (Hansbo-Hansbo XFEM)
L10: Extended meshfree methods.
T2: Computer implementation algorithms of XFEM and the phantom node method.

Day 3: 17.01.2024

T3: Computer implementation aspects, solution schemes of extended meshfree methods
L11: Computational methods based on Peridynamics and peridynamic operators
T4: Hands-on experience with numerical codes on meshfree methods and peridynamics
L12: Phase field models for fracture
L13: Phase field models for vesicles

Day 4: 18.01.2024

L14: Introduction to micro and nano-mechanics of failure, potential functions

L15: Implementation algorithms of molecular dynamics (LAMMPS) simulations for fracture
T5: Hands-on experience with molecular simulations using open source codes like LAMMPS.
T6: Practical applications of molecular dynamics simulations for materials design.
L16: Introduction to multiscale methods for fracture
L17: Multiscale methods for fracture by coupling coarse and fine scales

Day 5: 19.01.2024
T7: Implementation aspects of multiscale methods
L18: Introduction to data-driven analysis for engineering applications
L19: Machine Learning Interatomic Potentials
T8: Development of artificial neural network based models
L20: Physics informed neural networks (PINNs) and neural operators (NO)

Who can attend?

1. Faculty members, research scholars and students from academic and technical institutions.
2. Executives, engineers and researchers from manufacturing, service & government organizations including Research and Development laboratories.

About School of Mechanical Sciences

The School of Mechanical Sciences at IIT Bhubaneswar offers the following programs: B. Tech in Mech. Engg., and Dual degree - B. Tech in Mech. Engg. and M. Tech in MSD, TSE and ME; M. Tech in MSD, TSE and ME; and PhD. The total faculty strength is 25 and the student strength is around 700.

Date	08:00-08:55	09:00-09:55	10:00-10:55	11:15-12:10	12:15-13:10	14:30-15:25	15:30-16:25	16:40-17:55
15.01.2024	L1	L2	L3	L4	L5	L6	T1	
16.01.2024		L7	L8		L9	L10	T2	
17.01.2024	T3		L11	T4		L12	L13	
18.01.2024	L14	L15	T5		T6		L16	L17
19.01.2024	T7		L18	L19		T8	L20	
Legend	Lecture, TR		Tutorial, TR		Lecture, PRB		Tutorial, PRB	

Registration

The course will be delivered through online mode for which the registration can be confirmed by paying a non-refundable fee of **₹4000**, for employees, researchers including research scholars. Whereas, the student (B. Tech. and M. Tech.) participants can register by paying a registration fee of **₹2000**. The registration fee includes all study material. The registration has to be confirmed by submitting the filled in registration form. The meeting links for joining the online lectures will be provided in advance.

All the payments must be made in favour of CEP, IITBBS, Canara Bank: **A/C No: 24282010001960, IFSC: CNRB0017282**

Principal coordinator: Dr. Pattabhi Ramaiah Budarapu, School of Mechanical Sciences, IIT Bhubaneswar
Contact details: Dr. Pattabhi Ramaiah Budarapu, Email: acfm_gian2024@iitbbs.ac.in, Phone (O): +91-674-7137124

About IIT Bhubaneswar

Indian Institute of Technology Bhubaneswar (IITBBS) is a prominent institute among the eight new IITs initiated in 2008. The institute's vision is to be a highly respected institute in the world for its distinctive knowledge. Therefore, IITBBS is making strong strides to be among those which offer world class education. With an objective to create technologists and scientists of the highest caliber, the institute targets to provide its students with holistic education and opportunities to get empowered with the right academic preparation, analytical skills, creative skills and healthy mind. IIT Bhubaneswar offers programs like B. Tech, M. Tech, MS by research, M.Sc. and PhD in various disciplines. With a mission to shape ourselves into a learning community, we encourage interdisciplinary research, infuse excitement in students innovation and invention, design/creation and entrepreneurship, and strive for productive partnership between the industry and the Institute. The schools at IITBBS are equipped with state of the art equipment/facilities/laboratories and its faculty members are involved in a broad range of research areas and industrial consultancy.

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15-19 January 2024, School of Mechanical Sciences, IIT Bhubaneswar.

Registration Form

Registration information

Name: _____Gender: _____

Designation: _____

Department: _____

Address: _____

_____

City: _____ State _____ Pin Code _____

Phone (O): _____ Mobile: _____

Email: _____

Educational qualification: _____

Areas of research: _____

Registration fees:

	Registration	**Course fee** [$]
☐	Delegate*:	₹ 4000
☐	Student participant**:	₹ 2000

*Delegates: All participants, except student participants

**Student participants: B. Tech. and M. Tech. students only

[$]includes welcome kit, all study material, working lunch and taxes

Mode of Payment

Payment (by one of the methods listed below) must accompany the registration form. Please note that your registration will not be processed until payment is received in full.

A: Bank draft (payable at Bhubaneswar in favour of CEP, IIT Bhubaneswar) ☐

B: Bank transfer (in favour of CEP, IIT Bhubaneswar) ☐

C: UPI transfer (scan the bar code in the next page) ☐

Payment details

A: Draft no: _____ Date _____

Name of the bank _____

B: Date of transfer: _____ Name of the bank _____

Transaction reference no: _____

C: Date and mode/app for transfer: _____ Bank name _____

Transaction reference no: _____

Date:

Place:

Signature of the participant

Name with designation

( )

CEP IIT BHUBANESWAR

234391134001960@cnrb

Details for bank transfer:

Demand draft/Online transfer in favour of CEP, IIT Bhubaneswar,

Canara Bank, **A/C No.: 24282010001960, IFSC: CNRB0017282**.

All Correspondence must be addressed to:

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