FRASCALs mini lecture programme consists of four pillars addressing **(A) Mathematical Skills, (B) Modelling Approaches, (C) Computational Methods**, as well as **(D) Material Sciences Background**. It thus covers the most important techniques and tools to be employed in the doctoral projects and ensures profound interdisciplinary education. Table 1 is an excerpt of Table 2 and gathers representative mini lectures to be given by the PAs and external experts. In the sequel, the profiles of these mini lectures are detailed.

Table 1: Overview of representative mini lectures given by the PAs and external partners

	Title	Acronym	Page
(A) Maths Skills	Tensor Calculus	ITENS	19
	Partial Differential Equations Optimisation	IPDEO	21
	Mathematical Optimisation	IOPTI	20
	Numerics	INUMS	7
(B) Modelling Approaches	Statistical Mechanics of Fracture	ISTAT	14
	Continuum Mechanics	ICOME	18
	Mesoscopic Modelling	IMEMO	15
	Material Modelling	IMAMO	8
	Sequential Multiscale Modelling	ISEMO	23
	Concurrent Modelling	ICOMO	16
	Homogenisation	IHOMO	9
	Elastoplastic Fracture Mechanics	IPLAS	10
(C) Computational Methods	Density Functional Theory	IDFT	12
	Accelerated MD and Free Energies	IACC	13
	Atomistic Simulation Methods	IATOM	3
	Finite Element Method	IFEM	17
	Geometric Time Integration	IGETI	6
(D) Materials Science	Polymers and Polymer-Based Composites	IPOLY	22
	Composites	ICOMP	24
	Deformation and Fracture Mechanisms	IMECH	4
(E) Ext.	Elastic Fracture Mechanics	IFRAC	5
	Structural Optimisation	ISTOP	11

Classification
General Background
Discrete Approaches
Continuum Approaches
Multiscale Approaches

Table 2: Representative courses specific to the RTG: type (T) [lecture (L), seminar (S), key skills training course (KS), lab training (LT), workshop (WS)], duration (D) in 45' blocks, frequency (F) in years, target group (TG) [RTG cohort (C), FAU students (S)], credit points (CP), compulsory course (Cmp) [compulsory course (CC), elective course (EC), optional course (OC)]

	Title	T	D in 45'	F in a	Contents	TG	Prospective Instructor	Cmp	CP
(A) Maths Skills	Tensor Calculus	L	7	1.5	tensor representation, tensor algebra, tensor analysis, integral theorems	C	Steinmann	EC	1
	Partial Differential Equations Optimisation	L	7	1.5	PDE constrained optimisation, existence of solutions, discretisation, num. solution	C	Stingl	EC	1
	Mathematical Optimisation	L	7	1.5	optimisation problems, optimality conditions, descent methods, programming	C	Stingl	EC	1
	Numerics	L	7	1.5	(non)linear equation systems, eigenvalue problems, modal reduction, autom. differentiation	C	Leyendecker	EC	1
(B) Modelling Approaches	Statistical Mechanics of Fracture	L	7	1.5	defects and fluctuations, crack growth, fibre bundle and network models, failure criteria	C	Moretti	EC	1
	Continuum Mechanics	L	7	1.5	kinematics, stresses, balance laws, constitutive laws	C	Steinmann	EC	1
	Mesoscopic Modelling	L	7	1.5	basic concepts, model construction, fracture modelling and failure criteria, kinetic MC	C	Moretti	EC	1
	Material Modelling	L	7	1.5	modelling of elasticity, elastoplasticity, viscoplasticity, viscoelasticity	C	Mergheim	EC	1
	Sequential Multiscale Modelling	L	7	1.5	basics, parameter identification, local parameters, statistical averaging, reverse modelling	C	Zaiser	EC	1
	Concurrent Modelling	L	7	1.5	atomistic and continuum approaches, coupling techniques	C	Pfaller	EC	1
	Homogenisation	L	7	1.5	analytical homogenisation, RVE, effective properties, bounds	C	Mergheim	EC	1
	Elastoplastic Fracture Mechanics	L	7	1.5	fracture mechanisms, small/large scale yielding, CTOD, J-integral	C	Mergheim	EC	1
(C) Computational Methods	RTG Software Platform	LT	3x7	3	introduction to RTG's software platform (ESPRESSO / LAMMPS-LIGGGHTS / deal.II)	C	PAs	CC	3x1
	Density Functional Theory	L	7	1.5	basic concepts of DFT, functionals, implementation of DFT, boundary conditions	C	Meyer	EC	1
	Accelerated MD and Free Energies	L	7	1.5	simulating rare events, constrained/steered/targeted MD, free energy surface reconstruction	C	Meyer	EC	1
	Atomistic Simulation Methods	L	7	1.5	interaction potentials, boundary conditions, solution algorithms, advanced analysis	C	Bitzek	EC	1
	Finite Element Method	L	7	1.5	weak form, discretisation and shape functions, quadrature rules, solution	C	Pfaller	EC	1
	Geometric Time Integration	L	7	1.5	structure preserving integration of ODEs, symplecticity, invariants	C	Leyendecker	EC	1
(D) Materials Science	Introduction to Testing & Characterisation	LT	7	3	introduction to materials testing and characterisation procedures with focus on fracture	C	PAs	CC	1
	Polymers and Polymer-Based Composites	L	7	1.5	modelling concepts, molecular mechanics, coarse-graining, multiscale simulation	C	Zahn	EC	1
	Composites	L	7	1.5	composite mechanics, failure mechanisms, scale effects	C	Zaiser	EC	1
	Deformation and Fracture Mechanisms	L	7	1.5	microstructure and defects, crack propagation, stress corrosion cracking, fatigue	C	Bitzek	EC	1
(E) External	Elastic Fracture Mechanics	L	7	3	stress/strain concentrations/singularities, crack propagation due to static and dynamic loads	C	Kolk	EC	1
	Structural Optimisation	L	7	3	basics of structural optimisation, mathematical aspects, shape and topology optimisation	C	Meske	EC	1
					further mini lectures to be proposed by the mentoring teams	C	externals		
(F) Key Skills	Introduction to Research at FAU	KS	7	3	introduction to basic aspects (gender equality, German system of science, career planning)	C	Graduate Ctr	CC	1
	Good Scientific Practice (GSP)	KS	7	3	good scientific practice, authorship, avoiding plagiarisms and misbehaviour	C	Graduate Ctr	CC	1
	Gender Equality in Research	KS	7	3	advanced course on gender equality (gender awareness, gender bias, measures, etc.)	C	external	CC	1
	Presentation Skills	KS	14	3	principles of communication, producing and performing presentations	C	external	EC	2
	Career Planning	KS	7	3	advanced course on career planning	C	Graduate Ctr	EC	1
	Scientific Writing	KS	7	3	introduction to scientific writing in English	C	external	EC	1
	Time Management for Doctoral Researchers	KS	7	3	principles in time management during a doctorate	C	external	EC	1
	Research Data Management Course	KS	7	3	introduction to managing research data	C	Graduate Ctr	EC	1
(G) RTG Events	RTG Seminar	S	7	0.5		C		CC	1
	Alumni & Visitor Workshop	WS	7	1		C		CC	1
	RTG Retreats	S	7	1.5		C		CC	1

Classification	General Background	Discrete Approaches	Continuum Approaches	Multiscale Approaches	Key Skills	RTG Events

Introduction to Atomistic Simulation Methods (IATOM)

Classification: Computational methods (C), discrete approaches

Lecturer: Erik Bitzek

Language: English

Contents:

- Atomic interaction potentials for metals, ceramics and polymers
- Sample generation and boundary conditions
- Molecular dynamic integration algorithms for different Thermodynamic ensembles
- Energy minimization algorithms and structure optimization
- Modelling of thermally activated processes, NEB, kMC
- Advanced analysis and visualization methods

Objectives:

The students

- are familiar with the basic concepts of atomistic simulation methods and can discuss them in the context of a multiscale modelling framework
- are able to choose the best potential for a given material and problem
- can choose the most adequate atomistic simulation method for a given problem and given resources
- can compare and discuss different algorithmic realizations for molecular dynamics and energy minimization
- can discuss the choice of simulation parameters and boundary conditions
- can critically assess the atomic simulation results presented by their colleagues or in publications

Introduction to Deformation&Fracture Mechanisms in Crystalline&Amorphous Materials (IMECH)

Classification: Materials science (D), general background

Lecturer: Erik Bitzek

Language: English

Contents:

- Microstructure and defects in crystals: vacancies, dislocations, grain boundaries
- Characterization of and defects in amorphous materials
- Brittle crack propagation in crystals (metals, ceramics) and amorphous materials (metallic and inorganic glasses, polymers)
- Ductile fracture in metals
- Fracture in polymers
- Stress corrosion cracking
- Nucleation and propagation of fatigue cracks

Objectives:

The students

- can describe and characterize the microstructure and defects in various classes of materials and are familiar with the properties of different types of defects
- can classify materials according to their intrinsic, theoretical ductility/brittleness
- are familiar with the concept of lattice or bond trapping and kink mobility
- can describe the atomic- and meso-scale deformation mechanisms in crystals, metallic and inorganic glasses and polymers (e.g., dislocations, shear transformation zones, shear bands, void formation, crazing,…)
- know the processes during stress corrosion cracking and can model subcritical crack growth
- can describe the mechanisms leading to crack nucleation and growth during fatigue of metals, ceramics, engineering plastics and composites

Introduction to Elastic Fracture Mechanics (IFRAC)

Classification: External (E), continuum approaches

Lecturer: Karsten Kolk (member of external advisory board)

Language: English

Contents:

- Overview on fracture mechanics
- Stress/strain concentrations and singularities at notches and crack tips
- Crack propagation due to static loads
- Fatigue cracks
- Crack propagation due to dynamic loads
- Fracture properties
- Finite Elements (FE) in elastic fracture mechanics

Objectives:

The students

- possess an overview on fracture mechanics
- are able to assess the stress/strain state at notches and crack tips
- are familiar with fracture criteria
- are familiar with concepts of fatigue fracture
- know how to determine fracture properties
- are able to apply the FE method to fracture problems

Introduction to Geometric Time Integration (IGETI)

Classification: Computational methods (C), continuum approaches

Lecturer: Sigrid Leyendecker

Language: English

Contents:

- Numerical integration of ordinary differential equations
- Conservation of first integrals (linear and quadratic invariants, Noether theorem)
- Symmetric integration
- Symplectic integration of Hamiltonian systems
- Variational integrators
- Error analysis

Objectives:

The students

- are familiar with standard schemes for the numerical integration of ODEs
- understand the concept of convergence
- understand the structure and conservation properties of analytical solutions of ODEs
- can derive numerical schemes that conserve the characteristic properties of a given ODE
- can analyse the convergence and conservation properties in their own implementations

Introduction to Numerics (INUMS)

Classification: Mathematical skills (A), general background

Lecturer: Sigrid Leyendecker

Language: English

Contents:

- Linear systems of equations, minimisation of potential energy, linear dynamical systems, dynamics in frequency domain
- Eigenvalue problems, modal analysis, decoupling of linear dynamical systems, modal reduction
- Nonlinear systems of equations, incremental elastostatics, minimisation of potential energy
- Automatic differentiation, tool for model generation, linearization of nonlinear mechanical systems

Objectives:

The students

- know standard numerical schemes in mechanics
- understand which numerical method is appropriate for the solution of a given mechanical problem
- are able to analyse mathematical-mechanical interrelationships in numerics
- are able to validate the successful operations of a numerical method
- are able to analyse, which errors occur due to mathematical modelling, a numerical method or implementation errors

Introduction to Material Modelling (IMAMO)

Classification: Modelling approaches (B), continuum approaches

Lecturer: Julia Mergheim

Language: English

Contents:

- Material behaviour and testing
- Basics of continuum mechanics
- Elasticity
- Elastoplasticity
- Viscoplasticity
- Viscoelasticity
- Models in 1D and 3D
- Algorithms in 1D and 3D

Objectives:

The students

- are familiar with the general microstructure of metals and polymers
- are familiar with the general material behaviour of metals and polymers
- are able to classify experimental observations of uniaxial tensile tests
- know the characteristics of elastic, elastoplastic, viscoplastic and viscoelastic behaviour
- can formulate thermodynamic consistent models in elasticity, elastoplasticity, viscoplasticity and viscoelasticity
- know suitable algorithms to implement the models in a numeric framework (e.g. Finite Elements)

Introduction to Homogenisation (IHOMO)

Classification: Modelling approaches (B), multiscale approaches

Lecturer: Julia Mergheim

Language: English

Contents:

- Basics of linear elasticity, anisotropy
- Scale transition
- Representative Volume Element
- Effective properties
- Hill-Mandel condition
- Eshelby solution
- Mori-Tanaka, self-consistent scheme
- Bounds

Objectives:

The students

- are familiar with the basic assumptions of homogenisation methods
- know the Hill-Mandel condition, the properties of a Representative Volume Element
- know various analytical homogenisation methods
- can derive approximations of effective properties for simple linear elastic microstructures
- can derive bounds for the effective properties
- know the limits of the analytical homogenisation methods

Introduction to Elastoplastic Fracture Mechanics (IPLAS)

Classification: Modelling approaches (B), continuum approaches

Lecturer: Julia Mergheim

Language: English

Contents:

- Mechanisms of elastoplastic fracture
- Experiments in elastoplastic fracture mechanics
- Small/large scale yielding
- Dugdale model
- Crack-tip opening displacement (CTOD)
- Crack-tip fields
- J-integral concept
- Crack-growth resistance curves
- Finite Elements (FE) in elastoplastic fracture mechanics

Objectives:

The students

- know basic mechanisms of elastoplastic fracture
- can name experiments to measure fracture toughness
- know the differences between small and large scale yielding
- know the Dugdale model, the CTOD approach, the J-integral concept
- can derive crack-tip fields for perfect plasticity
- are able to understand crack-resistance curves
- can apply the FE method to derive the J-integral for a stationary crack

Introduction to Structural Optimisation (ISTOP)

Classification: External (E), continuum approaches

Lecturer: Ralf Meske (member of external advisory board)

Language: English

Contents:

- Introduction to structural optimisation
- Mathematical foundations
- Determination of system responses and sensitivities
- Optimisation with Excel
- Parameter optimisation with gradient-based algorithms
- Shape optimisation
- Topology optimisation
- Global approximation methods
- Global optimisation algorithms

Objectives:

The students

- know different optimisation methods
- understand mathematical foundations of optimisation
- know how to define an optimisation problem
- are able to consider restrictions from manufacturing by appropriate manufacturing constraints
- understand the scope and restrictions of different optimisation procedures
- are able to identify the best suited optimisation procedure based on the given problem
- are able to compare results of different optimisation procedures as well as to evaluate the influence of the chosen optimisation strategy, the quality of result and its feasibility

Introduction to Density Functional Theory (IDFT)

Classification: Computational methods (C), discrete approaches

Lecturer: Bernd Meyer

Language: English

Contents:

- Introduction to the basic concept of density functional theory (DFT)
- Overview of available functionals, discussion of their advantages and disadvantages
- Different implementations of DFT in computer codes
- Basis sets, k-point sampling, Brillouin zone integrations
- Boundary conditions: periodic versus finite cluster calculations

Objectives:

The students

- have a basic understanding of what is done in a DFT calculation
- can choose the best DFT code for a given problem
- are able to run first simple calculations
- are familiar with the pro and cons of different families of functionals
- can critically assess the results of DFT calculations in publications

Introduction to Accelerated MD and Free Energies (IACC)

Classification: Computational methods (C), discrete approaches

Lecturer: Bernd Meyer

Language: English

Contents:

- How to simulate rare events (thermally activated processes) in molecular dynamics (MD)
- Constrained MD, steered MD, targeted MD, umbrella sampling, replica exchange, metadynamics, multiple walker, particle insertion methods
- How to reconstruct the free energy surface
- Thermodynamic integration, weighted histogram analysis, metadynamics

Objectives:

The students

- understand the problems associated with the limited simulation time in MD
- are familiar with the basic concepts of accelerated MD techniques
- can choose an appropriate rare event method for solving a given problem
- are able to determine free energy changes and free energy barriers from the results of their MD simulations
- can critically assess MD simulation results in publications

Introduction to Statistical Mechanics of Fracture (ISTAT)

Classification: Modelling approaches (B), discrete approaches

Lecturer: Paolo Moretti

Language: English

Contents:

- Defects and fluctuations in fracture
- Fracture and damage percolation
- Extreme value statistics for independent cracks
- Slow crack growth, stress redistribution, and stress localization
- Fibre bundle models for fracture and load sharing schemes
- Network models for fracture: fuse and beam models
- Failure criteria in statistical models of fracture

Objectives:

The students

- understand the role of fluctuations in fracture mechanics
- can identify realistic sources of fluctuations and heterogeneity
- understand the difference between quasi-static and dynamic methods
- know the concept of percolation and its application to material failure
- can use simple arguments of extreme statistics in fracture problems
- can map fibre bundle and fibre network models to problems in biological materials
- understand the role of stress redistribution in the fault tolerance of materials

Introduction to Mesoscopic Modelling (IMEMO)

Classification: Modelling approaches (B), continuum approaches

Lecturer: Paolo Moretti

Language: English

Contents:

- Basic concepts of mesoscopic modelling and coarse-graining
- From the micro- to the mesoscale: Construction of mesoscale models
- Basic concepts of mesoscopic modelling in fracture
- Failure criteria at the mesoscopic scale
- Cellular automata
- Kinetic Monte Carlo method
- Heterogeneous contact patterns and network models

Objectives:

The students

- understand the advantages offered by mesoscopic modelling
- learn its scope and limitations as opposed to atomistic modelling
- can use atomistic simulation results for construction and parametrization of mesoscopic models
- can name simple examples of fracture problems that can be modelled at the mesoscale
- can identify time- and length-scales that can be dealt with using mesoscopic models
- get an overview of simple simulation protocols of relevance at the mesoscale

Introduction to Concurrent Modelling (ICOMO)

Classification: Modelling approaches (B), multiscale approaches

Lecturer: Sebastian Pfaller

Language: English

Contents:

- Basics of atomistic and continuum modelling
- Hierarchical concurrent modelling approaches
- Partitioned-domain concurrent modelling approaches
- Comparison and assessment of concurrent approaches

Objectives:

The students

- are familiar with the basic ideas of atomistic and continuum modelling
- know hierarchical concurrent modelling approaches
- know partitioned-domain concurrent modelling approaches
- can discuss the choice of coupling approaches
- are able to choose appropriate strategies based on specific problems

Introduction to the Finite Element Method (IFEM)

Classification: Computational methods (C), continuum approaches

Lecturer: Sebastian Pfaller

Language: English

Contents:

- Basic concept of the Finite Element Method
- Weak form
- Discretisation and shape functions
- Quadrature rules
- Finite elements in two- and three-dimensional elasticity

Objectives:

The students

- are familiar with the basic concept of the finite element method
- are able to model linear problems in elasticity
- are familiar with the isoparametric concept
- know different methods for numerical integration
- know how to discretize and solve problems in continuum mechanics
- can derive weak and discrete representations of boundary value problems

Introduction to Continuum Mechanics (ICOME)

Classification: Modelling approaches (B), continuum approaches

Lecturer: Paul Steinmann

Language: English

Contents:

- Placement, configurations, motion, deformation map
- Deformation gradient, strain measures, polar and spectral decomposition
- Stress measures, balance equations
- Velocity, velocity gradient, rates of stress and strain
- Variation, weak form, linearization
- Exploitation of dissipation inequality, constitutive models

Objectives:

The students

- are familiar with the Lagrangian and Eulerian description of motion
- are familiar with the concept and analysis of strain
- are familiar with the concept and analysis of stress
- are familiar with various rates of stress and strain
- know how to formulate and linearize the weak form
- know how to model elementary constitutive behaviour

Introduction to Tensor Calculus (ITENS)

Classification: Mathematical skills (A), general background

Lecturer: Paul Steinmann

Language: English

Contents:

- Index versus symbolic notation, coordinate representation
- Vector and tensor products
- Eigenvalue problem, invariants, spectral representation, Cayley-Hamilton theorem
- Isotropic tensor functions, representation theorems
- Gradient, divergence, rotation of tensor fields
- Integral theorems (Gauss, Stokes)

Objectives:

The students

- are familiar with the notation and coordinate representation of tensors
- are able to compute various vector and tensor products
- are familiar with the spectral representation and its consequences
- know how to compute isotropic tensor functions
- know how to compute the gradient, divergence or rotation of a tensor field
- are familiar with the relevant integral theorems

Introduction to Mathematical Optimization (IOPTI)

Classification: Mathematical skills (A), general background

Lecturer: Michael Stingl

Language: English

Contents:

- Unconstrained and Constrained Optimisation problems
- Necessary and sufficient Optimality conditions
- Descent methods – generic framework and Newton's method
- Lagrange-Duality and Karush-Kuhn-Tucker (KKT) conditions
- Lagrange-Newton method for equality constrained optimization
- Basics of interior point (IP) as well as sequential quadratic programming (SQP) idea

Objectives:

The students

- are to model and classify finite dimensional optimization problems
- to derive optimality conditions for various classes of optimization problems
- to apply and implement descent-based solution strategies including Newton's method for unconstrained optimization
- calculate solutions of constrained optimization problems based on KKT conditions
- know to apply advanced optimization techniques like IP or SQP to the local solution of constrained smooth non-linear optimization problems

Introduction to Optimization with Partial Differential Equations (IPDEO)

Classification: Mathematical skills (A), general background

Lecturer: Michael Stingl

Language: English

Contents:

- Prototypical PDE constrained optimization problems with control in right hand side
- Existence of Solutions
- Discretization schemes and convergence
- Algebraic form and numerical solution
- Extension to shape and material optimization

Objectives:

The students

- are able to formulate well-posed PDE constrained optimization problems
- know appropriate discretization schemes
- are able to convert variational problems into algebraic form
- are familiar with numerical solution concepts based on the algebraic formulations
- know examples of shape and material optimization problems and how to compute approximate solutions numerically

Introduction to Polymers and Polymer-Based Composites (IPOLY)

Classification: Materials science (D), general background

Lecturer: Dirk Zahn

Language: English

Contents:

- Basic concept of modelling polymers
- Application of molecular mechanics models for the analysis of folding and unfolding
- Application of molecular mechanics models for the analysis of polymer-particle interactions
- Up-scaling to coarse-grained models
- Multiscale simulations of polymer-metaloxide composites

Objectives:

The students

- are familiar with the basic concept of molecular mechanics of polymer models
- are familiar with the basic concept of molecular dynamics simulations
- know scale-bridging methods for composite simulations
- know how to rationalize fracture processes at different length scales

Introduction to Sequential Multiscale Modelling (ISEMO)

Classification: Modelling approaches (B), multiscale approaches

Lecturer: Michael Zaiser

Language: English

Contents:

- Sequential and concurrent multiscale modelling
- Parameter Identification: Statistical coarse-graining vs. phenomenology
- Direct computation of local parameters
- Parameter passing by statistical averaging
- Parameter passing by reverse modelling (Parameter fitting)
- Equation-free methods

Objectives:

The students

- can devise problem-matched modelling strategies (sequential/concurrent/hybrid)
- can use bottom-up and top-down methods for parameter identification
- distinguish parameters representing local and collective (emergent) properties
- can evaluate local parameters by direct computation
- can evaluate collective parameters by statistical averaging (bottom-up) or reverse modelling (top-down)
- understand the ideas and conceptual problems involved in equation-free multiscale modelling

Introduction to Composites (ICOMP)

Classification: Materials science (D), general background

Lecturer: Michael Zaiser

Language: English

Contents:

- Basic concepts of composite mechanics
- Fibre reinforced composites
- Laminated structures
- Failure mechanisms and failure modelling
- Scale effects: From macro- to nanocomposites

Objectives:

The students

- understand the ideas behind the use of composite materials
- can evaluate properties of random and directed fibre composites
- can calculate stress and strain states in laminated plates
- understand different failure mechanisms in composite structures
- know the parameters controlling composite failure
- know the physical origins of scale dependent behaviour in nanocomposites
- can model scale dependent behaviour using scale dependent constitutive models