

# Curriculum Vitae

## Aruna Prakash, Ph.D

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## Personal Details

- |                              |                                                                                                                                                                    |
|------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| • Date of Birth              | 21 October 1979                                                                                                                                                    |
| • Place of Birth             | Belur, Karnataka state, India                                                                                                                                      |
| • Nationality                | German                                                                                                                                                             |
| • Marital Status             | Married with two kids                                                                                                                                              |
| • Address                    | Am Wasserturm 9, 09603 Großschirma                                                                                                                                 |
| • Professional Qualification | Ph.D (Doctorate in Engineering)                                                                                                                                    |
| ▪ Current Position           | Senior Scientist,<br>Micro-Mechanics & Multiscale Materials Modelling (M <sup>5</sup> ),<br>Institute of Mechanics and Fluid Dynamics,<br>TU Bergakademie Freiberg |

## Research Areas

- Large scale atomistic simulations – Molecular dynamics and statics
- Machine learning using atomistic simulation data in materials science
- Multiscale materials modeling
- Small scale plasticity, nanomechanics
- Experimentally informed “realistic” atomistic and finite element simulations
- Finite element (FE) modelling and simulations
- Plasticity, damage and failure of metals
- Development of scale bridging methods to couple atomistic and continuum scales
- Crystal plasticity finite element simulations of deformation of lightweight metals (e.g. magnesium, aluminum)
- Development of computational models for severe plastic deformation processes like accumulative roll bonding (ARB) and equal channel angular pressing (ECAP)
- Atomistic simulations of plasticity and failure in nanocrystalline materials
- Modeling of dislocation – grain boundary interactions
- Atomistic simulations of dislocation processes in superalloys
- Development of analysis and visualization methods for atomistic simulations
- Open source software development for multiscale simulation frameworks
- Optimization of material properties
- Big Data in materials science – handling and analysis of large amounts of data (>100TB)

## Education

- Ph.D      2010      Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany  
Advisors: Prof. Hermann Riedel, Prof. Peter Gumbsch  
Thesis title: “*Computational micromechanics of polycrystals: Special emphasis on twinning and recrystallization in magnesium alloys and TWIP-steels*”
- M.S      2005      Universität Stuttgart, Stuttgart, Germany  
Computational Mechanics of Materials and Structures  
(COMMAS Master’s program)  
Thesis title: “*Parameter identification for material models from inhomogeneous experiments with three-dimensional surface matching*”
- B.E      2001      B.M.S. College of Engineering, Bangalore University, Bangalore, India  
Department of Mechanical Engineering  
Thesis title: “*Preliminary studies related to compact flexible bearing supports under restricted space situations*”

## Professional Experience

### 2018 to present:

Senior Scientist and Group Leader at the *Micro-Mechanics & Multiscale Materials Modelling (M<sup>5</sup>) Group*, TU Bergakademie Freiberg.

*Job responsibilities:* Teaching (8 SWS), supervision of thesis and project work of Master students, research broadly in the field of computational materials science, with particular focus on atomistic simulations, data science and informatics, machine learning using atomistic datasets, small-scale/nanoscale mechanics of metals and glasses, bridging of length scales using statistical machine learning

### 2011 to 2018:

Scientific assistant (*ger.* Wissenschaftlicher Assistant) at the *Institute-I, Materials Science and Engineering*, FAU Erlangen-Nürnberg, Erlangen, Germany

*Job responsibilities:* Teaching (5 SWS), Supervision of PhD, Bachelor’s and Master’s students, Coordination of Exams at the Institute, System administration of linux workstations.

### 2010 to 2011

Postdoctoral research associate at the Fraunhofer Institute for Mechanics of Materials, Freiburg, Germany. As a postdoctoral fellow, I worked primarily on industry related research projects.

My research was focused on two industry contract projects: In the first project for Salzgitter Mannesmann Forschung GmbH (SZMF), I developed a software called IdentiPy, which helps identify material parameters from finite element simulations with Abaqus. In the second project for Deutsche Edelstahlwerke (DEW), I worked on finite element computations investigating the evolution of porosity during hot rolling of large steel ingots.

### 2005 to 2009

Research scientist at the Fraunhofer Institute for Mechanics of Materials, Freiburg, Germany.

My Ph.D research was focused on the formability of magnesium alloys, in a project under the framework of the magnesium priority program (SPP 1168) of the DFG. Additionally, I also worked on a project under the framework of the Fraunhofer-Max Planck cooperation.

The PhD thesis was supervised by Prof. H. Riedel (winner of the Leibniz prize in 1991) and co-supervised by Prof. P. Gumbsch (winner of the Leibniz prize in 2007). The PhD defense was carried out at the Karlsruhe Institute of Technology (KIT).

### 2002 to 2003

Programmer Analyst at Cognizant Technology Solutions India Pvt. Ltd.,  
Bangalore, India

Worked as a part of a Team and helped execute two projects for General Motors Inc., USA.

I was awarded an employee appreciation award in appreciation of the effort towards the GO<sup>2</sup> project

## Publications (Total: 40, Citations: > 900, H-index: 16)

### Peer-reviewed Journal Articles

- [A. Prakash](#) [2023], Atomistic modeling of idealized equal channel angular pressing process, **Journal of Materials Science**, *Under Review*
- S. Ganisetti, A. Atila, J. Guérolé, [A. Prakash](#), J. Horbach, L. Wondraczek, E. Bitzek [2023], The origin of deformation induced topological anisotropy in silica glass, **Acta Materialia**, **257**, 119108
- [A. Prakash](#), S. Sandfeld [2022], Automated analysis of continuum fields from atomistic simulations using statistical machine learning, **Advanced Engineering Materials**, **24**, 2200574
- S. Roy, [A. Prakash](#), S. Sandfeld [2022], Sintering of alumina nanoparticles: comparison of interatomic potentials, molecular dynamics simulations, and data analysis, **Modelling and Simulation in Materials Science and Engineering**, **30**, 065009
- B. Diepold, C. Schunk, F. Kümmel, T. Fey, [A. Prakash](#), H.W. Höppel, M. Göken [2022], Fatigue Life Optimized Layer Architecture of Ultrafine-Grained Al–Ti Laminates Under Bending Stresses, **Advanced Engineering Materials**, **24**, 2101143
- M. Vimal, S. Sandfeld, [A. Prakash](#) [2022], Grain segmentation in atomistic simulations using orientation based iterative self-organizing data analysis, **Materialia**, **21**, 101314
- D. Bayer-Buhr, M. Vimal, [A. Prakash](#), U. Gross, T. Fieback [2022], Determination of thermal accommodation coefficients on CaSiO<sub>3</sub> and SiO<sub>2</sub> using molecular dynamics and experiments, **International Journal of Heat and Mass Transfer**, **183**, 122219
- P.H. Serrao, S. Sandfeld, [A. Prakash](#) [2021], *OptiMic: A tool to generate optimized polycrystalline microstructures for materials simulations*, **SoftwareX**, **15**, 100708
- S. Lee, A. Vaid, J. Im, B. Kim, [A. Prakash](#), J. Guérolé, D. Kiener, E. Bitzek, S. H. Oh [2020], *In-situ observation of the initiation of plasticity by nucleation of prismatic dislocation loops*, **Nature Communications**, **11**, 2367
- J. Guérolé, W.G. Nöhring, A. Vaid, F. Houllé, Z. Xie, [A. Prakash](#), E. Bitzek [2020], *Assessment and optimization of the fast inertial relaxation engine (FIRE) for energy minimization in atomistic simulations and its implementation in LAMMPS*, **Computational Materials Science**, **175**, 109584
- Z. Xie, J. Shin, J. Renner, [A. Prakash](#), D. S. Gianola and E. Bitzek [2020], *Origins of strengthening and failure in twinned Au nanowires: Insights from in-situ experiments and atomistic simulations*, **Acta Materialia**, **187**, 166-175
- A. Vaid, J. Guérolé, [A. Prakash](#), S. Korte-Kerzel, E. Bitzek [2019], *Atomistic simulations of basal dislocations in Mg interacting with Mg<sub>17</sub>Al<sub>12</sub> precipitates*, **Materialia**, **7**, 100355
- K. Frydrych, K. Kowalczyk-Gajewska, [A. Prakash](#) [2019], *On solution mapping and remeshing in crystal plasticity finite element simulations: Application to equal channel angular pressing*, **Modelling and Simulation in Materials Science and Engineering**, **27**, 075001
- F. Kümmel, B. Diepold, K.F. Sauer, C. Schunk, [A. Prakash](#), H.W. Höppel, M. Göken [2019], *High lightweight potential of ultrafine-grained aluminum/steel laminated metal composites produced by accumulative roll bonding*, **Advanced Engineering Materials**, **21**, 1800286

- A. Prakash, S. Sandfeld [2018], *Chances and challenges in fusing data science with materials science*, **Practical Metallography**, **55**, 493-514
- F. Houllé, F. Walsh, A. Prakash, E. Bitzek [2018], *Atomistic simulations of compression tests on  $\gamma$  precipitate containing  $Ni_3Al$  nanocubes*, **Metallurgical and Materials Transactions A**, **49**, 4158-4166
- F. Kümmel, B. Diepold, A. Prakash, H.W. Höppel, M. Göken [2018], *Enhanced monotonic and cyclic mechanical properties of ultrafine-grained laminated metal composites with strong and stiff interlayers*, **International Journal of Fatigue**, **116**, 379-387
- S. Sandfeld, A. Prakash et al. [2018], *Digitale Transformation in der Materialwissenschaft und Werkstofftechnik*, **Strategy Paper of the German Materials Society (DGM)**
- A. Prakash, D. Weygand, E. Bitzek [2017], *Influence of grain boundary topology and structure on the deformation behavior of nanocrystalline aluminum*, **International Journal of Plasticity**, **97**, 107-125
- J. Guénolé, A. Prakash, E. Bitzek [2017], *Atomistic simulations of focused ion beam machining of strained silicon*, **Applied Surface Science**, **416**, 86-95
- A. Prakash, E. Bitzek [2017], *Idealized vs. realistic microstructures: Influence of eigen-stresses on the activity of dislocation loops in  $\gamma/\gamma'$  microstructures*, **Materials**, **10**, 88
- J. Guénolé, A. Prakash, E. Bitzek [2016], *Influence of intrinsic strain on irradiation induced damage: the role of threshold displacement and surface binding energies*, **Materials and Design**, **111**, 405-413
- A. Korsunsky, J. Guénolé, E. Salvati, T. Sui, M. Mousavi, A. Prakash, E. Bitzek [2016], *Quantifying eigenstrain distributions induced by focused ion beam damage in silicon*, **Materials Letters**, **185**, 47-49
- A. Prakash, M. Hummel, S. Schmauder, E. Bitzek [2016], *NanoSCULPT: A methodology for generating complex realistic structures for atomistic simulations*, **MethodsX**, **3**, 219-230
- A. Prakash, J. Guénolé, J. Wang, J. Müller, E. Spiecker, M.J. Mills, I. Povstugar, P. Choi, D. Raabe, E. Bitzek [2015], *Atom probe informed simulations reveal the importance of local interface curvature*, **Acta Materialia**, **92**, 33-45  
→ Featured in a report in the August edition of the MRS (Materials Research Society) Bulletin.  
→ This paper is also among the Top 25 papers of the journal for the period April-June 2015.
- A. Prakash, W. Nöhring, R. A. Lebensohn, H. W. Höppel, E. Bitzek [2015], *A multiscale simulation framework of the accumulative roll bonding process accounting for texture evolution*, **Materials Science & Engineering A**, **631**, 104-119
- W. J. He, S. H. Zhang, A. Prakash, D. Helm [2014], *A hierarchical multi-scale model for hexagonal materials taking into account texture evolution during forming simulation*, **Computational Materials Science**, **82**, 464-475
- J. J. Möller, A. Prakash, E. Bitzek [2013], *FE2AT: finite element informed atomistic simulations*, **Modelling and Simulation in Materials Science and Engineering** **21**, 055011
- A. Prakash, R. A. Lebensohn [2009], *Simulation of micromechanical behavior of polycrystals: finite elements versus fast Fourier transforms*, **Modeling and Simulation in Materials Science and Engineering**, **17**, 064010  
→ Featured as the highlight paper of the year 2009 of the journal
- A. Prakash, S.M. Weygand, H. Riedel [2009], *Modeling the evolution of texture and grain shape in Mg alloy AZ31 using the crystal plasticity finite element method*, **Computational Materials Science**, **45**, 744-750

- A. Prakash, T. Hochrainer, E. Reisacher, H. Riedel [2008], *Twinning Models in Self-Consistent Texture Simulations of TWIP Steels*, **Steel Research International**, **79**, 645-652  
→ Awarded the best paper of the journal for the year 2008
- D. Helm, T. Hochrainer, A. Prakash [2008], *Modellierung und Simulation hoher- und höchstfester-Stähle*, **Konstruktion**, **60**, IW9
- C. Schmidt, R. Kawalla, T. Walde, H. Riedel, A. Prakash, C. Poizat [2007], *Experimental and numerical investigation of texture development during hot rolling of magnesium alloy AZ31*, **Materials Science Forum**, **539-543**, 3448-3453

#### Articles under preparation

- A. Prakash, B. Merle, S. Sandfeld, E. Bitzek, Nanoscale mechanisms govern the deformation behavior of notched ultra-thin films, Manuscript being reviewed by co-authors
- J. Guénolé, A. Prakash, K. Eifantis, E. Bitzek, On the quantification of edge and mixed dislocations absorbed in high-angle twist grain boundaries, In Preparation
- Z. Xie, A. Prakash, J. Guénolé, B. Winter, T. Przybilla, E. Spiecker, E. Bitzek, Atomistic simulations of nanoporous gold, In Preparation
- J. Guénolé, A. Prakash, E. Bitzek, Topological aspects on dislocation–grain boundary interaction, In Preparation

#### Peer-reviewed Book Chapters

- Z. Xie, J. Guénolé, A. Prakash, T. Przybilla, E. Spiecker [2018], Experimentally-Informed Large-Scale Atomistic Simulations of Nanoporous Gold, In: High Performance Computing in Science and Engineering, Bayerische Akademie der Wissenschaften, Leibniz-Rechenzentrum (LRZ)
- J. J. Möller, A. Prakash, E. Bitzek [2016], in S. Schmauder (Ed.), Multiscale Materials Modelling: Approaches to Full Multiscaling, De Gruyter Publishers
- A. Prakash, Ch. Schmidt, H. Riedel & R. Kawalla [2009], Experimental and numerical investigation of the activation of pyramidal slip during deformation of magnesium alloy AZ31, In K.U. Kainer (ed.) Proc. 8th Intl. Conf. Mg alloys and their applications, Weimar, Germany, pages 1276-1281
- R. Kawalla, C. Schmidt, H. Riedel, & A. Prakash [2006], Experimental and numerical investigation of texture development during hot rolling of magnesium alloys, In K.U. Kainer (ed.) Proc. of the 7th intl. conf. on magnesium alloys and their applications, Dresden Germany

#### Conference Proceedings

- J.-S. Klung, A. Prakash & D. Helm [2012], Simulation of the void fraction evolution during hot rolling of a plastic mould steel ingot, Proc. of Intl. Conf. Ingot Casting, Rolling and Forging, Aachen Germany
- J. Kadkhodapour, A. Butz, A. Prakash, & S. Ziaei Rad [2009], Finite element modeling of martensite grain size effect on localized deformation in dual phase steels, In E. Onate & D. J. R. Owen, eds., Proceedings of COMPLAS X, Barcelona, Spain
- A. Prakash, T. Hochrainer, E. Reisacher & H. Riedel [2007], Twinning models in self-consistent simulations of TWIP steels, In Proc. of 2nd SteelSim Conf., Graz/Seggau, Austria, pages 355-361

## Supervised works

- M. Vimal, "Understanding the deformation behavior of Cu-Zr based metallic glasses via atomistic simulations and machine learning", Master Thesis, 2022, TU Bergakademie Freiberg
- S. K. Vemuri, "Solving differential equations using neural networks", Programming Project, 2021, TU Bergakademie Freiberg
- D. K. Venkatesh, "Image driven machine learning for microstructure classification and segmentation", Programming Project, 2020, TU Bergakademie Freiberg
- A. H. Omranpoor, "Atomistic investigation of the interaction of dislocations with  $\Sigma 3$  grain boundaries in fcc metals", Master Thesis, 2020, TU Bergakademie Freiberg
- V. Muthusamy, "Atomic stress calculation in fcc metals", Programming Project, 2020, TU Bergakademie Freiberg
- P.H. Serrao, "Optimization of Voronoi tessellations in 2D and 3D based on user requirements", Programming Project, 2020, TU Bergakademie Freiberg
- H.V. Pawase, "Generation of voxelized and tetrahedral grids of atomistic samples for crystal plasticity finite element simulations", Programming Project, 2020, TU Bergakademie Freiberg
- P.P.C. Vundurthy, "Big-data visualization of large and ultra-large scale atomistic simulation datasets", Programming Project, 2019, TU Bergakademie Freiberg
- M.S.R. Erri, "Synthetic microstructure generation", Programming Project, 2019, TU Bergakademie Freiberg
- F. Walther, "Mehrskalenmodellierung des kumulativen Walzprozesses mittels Finite-Elemente-Simulationen und Experimenten", Master Thesis, 2018, FAU Erlangen-Nürnberg
- G. Weinländer, "A Crystal Plasticity Finite Element Study of Damage Evolution and Lifetime Prediction During Cyclic Loading", Master Thesis, 2017, FAU Erlangen-Nürnberg
- A. Vaid, "Role of Curvature in the Nucleation of Deformation Twins: An Atomistic Simulation Case Study", Mini Project for the MAP Master's Study Program, 2015, FAU Erlangen-Nürnberg
- D. Czajkowski, "An Atomistic Simulation Study on the Effect of Curvature on the Formation of Deformation Twins in Nanocrystalline Aluminum", Mini Project for the MAP Master's Study Program, 2015, FAU Erlangen-Nürnberg
- W.G. Nöhring, "Towards a Finite Element Multiscale Model of the Accumulative Roll Bonding Process", Master Thesis, 2013, FAU Erlangen- Nürnberg
- M. Al-Siraj, "Finite Element Based Investigation of the Effect of Lattice Misfit on the High Temperature Behavior of Cobalt and Nickel Based Superalloys", Master Thesis, 2013, FAU Erlangen-Nürnberg
- K.S.J. Prabhu, "Parameter Identification for Crystal Plasticity Based Homogenization Simulations", Master Thesis, 2010, Universität Stuttgart, Work carried out at the Fraunhofer IWM, Freiburg

## Awards

- 2017 – Best Poster award at the International CAE conference "Simulation: The Soul of Industry 4.0", Vicenza, Italy. Title of poster: *A multiscale simulation framework of the accumulative roll bonding process accounting for texture evolution*
- 2016 – Teaching award for the course "Übungen zu Computational Nanoscience" from the Faculty of Engineering, FAU Erlangen-Nürnberg. Award shared together with Prof. Erik Bitzek
- 2010 – Werkstoffmechanik Prize of the Plansee Group, 2nd place

- 2009 – Best paper award of the Journal *"Steel Research International"*
- 2003 – Employee appreciation award from Cognizant Technology Solutions India Pvt Ltd.

## Participation in acquisition of 3<sup>rd</sup> party funding

- DFG Sachbeihilfe / DFG Travel grant for travel to the workshop "Advances in Constitutive Relations Applied in Computer Codes" held in Udine/Italien, 2007
- DFG SPP 1168, project titled "Gekoppelte Simulation der Verformungs- und Rekristallisations-texturentwicklung bei der Halbwarmumformung von Magnesiumlegierungen", 2007
- Fraunhofer Gesellschaft – Max-Planck Gesellschaft Cooperation 2<sup>nd</sup> phase, "Simulation of the Mechanics of Polycrystals (CMCn)", 2008
- EU Research Fund for Coal and Steel (RFCS) project TWIP4EU, 2011
- DFG SFB-TR/103 Superalloy Single Crystals, Project C3, 2<sup>nd</sup> phase, 2015
- DFG GRK 1896, project B6 "Atomistic simulations of mechanical properties of nanostructures and interfaces", 2016

## Teaching (currently at TU Bergakademie Freiberg)

- Software Tools for Computational Materials Science – V+Ü (2 SWS)
- Crystal Plasticity: Texture and Anisotropy – V+Ü (3 SWS)
- Atomistic simulations methods – V+Ü (4 SWS)
- Theory, Modelling and Simulation of Microstructures – V+Ü (4 SWS)
- Mechanics of Materials – V+Ü (4 SWS)
- Journal club and research seminar – V (1,5 SWS)
- Personal programming project – Administration (7 SWS)

## Teaching (previously at FAU Erlangen-Nürnberg)

- Angewandte Grundlagen der Werkstoffwissenschaften – V+Ü (4 SWS), together with Prof. E. Bitzek and Dr. S. Neumeier
- Materials Properties – V (2 SWS)
- Introduction to the Finite Element Method – V (2 SWS)
- Rechneranwendungen in der Werkstoffwissenschaften – V+Ü (4 SWS), together with Prof. E. Bitzek and Dr. T. Fey
- Computational Nanoscience – Ü (2 SWS)
- Hauptseminar in englischer Sprache (2 SWS), together with Prof. P. Felber

## Invited Talks

- NanoSPD8, 2023, Bengaluru, India
- MRS Spring Meeting, 2017, Phoenix, USA
- Department of Materials Science and Engineering, Indian Institute of Science, 2017, Bengaluru, India
- Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, 2017, Mumbai, India
- Université de Lorraine – Metz, Laboratory of Microstructure Studies and Mechanics of Materials, 2016, Metz, France

- DGM Arbeitskreissitzung Mikrostrukturemechanik, 2015, Karlsruhe Institute of Technology, Karlsruhe, Germany
- Institute of Materials Simulation, 2015, FAU Erlangen-Nürnberg
- CECAM Workshop on Particle-based Simulations for Hard and Soft Matter, 2014, Stuttgart, Germany
- Indian Institute of Science (IISc), 2011, Bangalore, India
- 21<sup>st</sup> Composite Workshop, Dec 2008, Bad Herrenalb, Germany

## Invited tutorials

- *Atomistic simulations of dislocation properties*, Modeling and Simulation of Superalloys, Bochum, 2017
- *Finite element simulations for experiments*, Graduate Research School *In situ Microscopy with Electrons, X-rays and Scanning Probes*, FAU Erlangen-Nürnberg, 2016
- *Atomistic simulations with IMD: Stretching, Bending and Indentation*, CECAM Workshop on Particle-based Simulations for Hard and Soft Matter, Stuttgart, 2014

## Symposia (co)organized

- 4<sup>th</sup> Schöntal Symposium on Dislocation-based Plasticity, March 1<sup>st</sup> – 6<sup>th</sup> 2020, Bad Schöntal, Germany
- 1<sup>st</sup> International Workshop on Atom Probe Tomography, 12<sup>th</sup> – 15<sup>th</sup> September 2016 (<http://www.eam.fau.de/aptschool>)
- 50 years of Materials Research at Erlangen: International Symposium on Microstructure and Mechanical Properties of Advanced Metallic Materials, 29<sup>th</sup> – 30<sup>th</sup> October 2015 (<http://www.gmp.wm.uni-erlangen.de/50years.php>)
- DGM symposium “Atoms Defects and Microstructure: Atomistic and Mesoscale Simulations of Mechanical Properties”, as part of the Arbeitskreissitzung Mikrostrukturmechanik, 23 June 2014 (<http://www.eam.fau.de/microstructuremeeting>)

## University service

- Elite International Master's Program MAP – I was a member of the governing council (Studienkommission) of the Master's program "Advanced Materials and Processes" (MAP). I was also a member of the selection committee that conducts interviews to select prospective candidates for the program
- Exam coordination – As a scientific assistant at MSE I, FAU Erlangen-Nürnberg, I was responsible for organizing and coordinating multiple exams every semester for more than 300 candidates
- System administration – At the FAU Erlangen-Nürnberg, I was part of a team that was responsible for managing, installing and troubleshooting workstations and servers under the Linux operating system network



## Service to profession

### Open-source software

I am a co-author of multiple software packages that are now made available open-source to the scientific community. Only a brief overview is provided here.

#### OptiMic:

OptiMic is a software tool written in Python that enables the generation of optimized microstructures for both finite element as well as atomistic simulations. Using Voronoi tessellations, the tool generates both mono-dispersive as well as irregular grains. A key feature of the tool is that it gives the user extensive control on the optimization process via customizable cost functions, thus allowing one to tailor statistics of certain topological entities in the desired microstructure.

OptiMic is open-source and is hosted as a git repository on GitLab (<https://gitlab.com/arun.prakash.mimm/optimic>)

#### nanoSCULPT:

nanoSCULPT refers to a methodology and software tool to create complex and realistic structures for large scale atomistic simulations from arbitrarily shaped 3D datasets. The dataset defining an enclosed volume may come from different sources, viz. CAD drawings, simulated microstructures (snapshots of grain-growth or phase field simulations), digitization of experimental micrographs and tomography data.

nanoSCULPT is open-source and is hosted as a git repository on bitbucket (<http://bitbucket.org/arunpksh/nanosculpt>). Please visit the nanoSCULPT wiki (<http://bitbucket.org/arunpksh/nanosculpt/wiki>) for more details on the tool.

#### FE2AT

FE2AT stands for Finite Elements 2 ATomistics and is essentially used to perform finite element informed atomistic simulations. It is a simple but versatile open source tool that uses finite element calculations to provide appropriate initial and boundary conditions for atomistic simulations. FE2AT thus allows to forgo the simulation of large parts of the elastic loading process, even in the case of complex sample geometries and loading conditions.

FE2AT is open-source and is hosted as a git repository on bitbucket (<http://bitbucket.org/arunpksh/fe2at>). Please visit the FE2AT wiki (<http://bitbucket.org/arunpksh/fe2at/wiki>) for more details on the tool.

#### IdentiPy

IdentiPy is a software tool that enables the identification of material parameters for constitutive models from finite element simulations. It has been primarily programmed for optimizing parameters using simulations with the finite element software Abaqus, and is programmed using the Python programming language. IdentiPy is open source and is made available upon request. It is currently hosted as a git repository on bitbucket (<http://bitbucket.org/arunpksh/identipy>)

#### ParIdent-VPSC

ParIdent-VPSC stands for PARAmeter IDENTification for VPSC (Visco-plastic selfconsistent). Essentially, it is a software program that helps optimize material parameters for homogenization texture models like VPSC, Taylor, Relaxed Constraints, GIA etc. ParIdent-VPSC is open source and is made available upon request. It is currently hosted as a git repository on bitbucket (<http://bitbucket.org/arunpksh/ParIdentVPSC>)

### Journal referee

- Nature Communications
- Materials Science & Engineering A
- Modelling and Simulation in Materials Science and Engineering
- Metallurgical and Materials Transactions A
- Computational Materials Science
- Acta Materialia
- JoM – The Journal of The Minerals, Metals and Materials Society (TMS)

## Membership in Societies

- DGM – Deutsche Gesellschaft der Materialkunde
- VDI – Verein Deutscher Ingenieure
- DHV – Deutsche Hochschulverband
- MRS – Materials Research Society, USA

## Software skills

- Finite element software – Abaqus, Ansys
- Atomistic (molecular dynamics/statics) simulation software – IMD, LAMMPS
- Unix/Linux including system administration
- Programming languages: C, Fortran, Python, Matlab, R, AWK
- Data Science / Machine Learning: Scikit-learn, Pandas, ISODATA
- LaTeX, Microsoft office

## Languages

Languages	Reading	Speaking	Writing
<b>Kannada</b>	<i>mother tongue</i>	<i>mother tongue</i>	<i>mother tongue</i>
<b>English</b>	<i>Native</i>	<i>Native</i>	<i>Native</i>
<b>German</b>	<i>Excellent</i>	<i>Excellent</i>	<i>Excellent</i>
<b>Hindi</b>	<i>Excellent</i>	<i>Excellent</i>	<i>Excellent</i>

## References

Prof. Dr. Dierk Raabe Director, Max-Planck-Institute for Iron Research (MPIE) Email: <a href="mailto:raabe@mpie.de">raabe@mpie.de</a>	Prof. Dr. Siegfried Schmauder Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre (IMWF) Universität Stuttgart Email: <a href="mailto:Siegfried.schmauder@imwf.uni-stuttgart.de">Siegfried.schmauder@imwf.uni-stuttgart.de</a>
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