

# Writing Scientific Software

A GUIDE TO  
GOOD STYLE

SUELY OLIVEIRA & DAVID STEWART

# Writing Scientific Software A Guide To Good Style

**Harry Henderson**



## **Writing Scientific Software A Guide To Good Style:**

*Writing Scientific Software* Suely Oliveira, 2006 This manual of scientific computing style will prove to be an essential addition to the bookshelf and lab of everyone who writes numerical software Scientists engineers and computer scientists who follow its advice will learn how to write good software and how to test it for bugs accuracy and performance Writing Scientific Software Suely Oliveira, David E. Stewart, 2006-09-07 The core of scientific computing is designing writing testing debugging and modifying numerical software for application to a vast range of areas from graphics meteorology and chemistry to engineering biology and finance Scientists engineers and computer scientists need to write good code for speed clarity flexibility and ease of re use Oliveira and Stewart s style guide for numerical software points out good practices to follow and pitfalls to avoid By following their advice readers will learn how to write efficient software and how to test it for bugs accuracy and performance Techniques are explained with a variety of programming languages and illustrated with two extensive design examples one in Fortran 90 and one in C other examples in C C Fortran 90 and Java are scattered throughout the book This manual of scientific computing style will be an essential addition to the bookshelf and lab of everyone who writes numerical software **Writing Scientific Software** Suely Oliveira, David Stewart, 2006 A manual and guide to good scientific computing style explaining how to write good software and how to test it for bugs accuracy and performance **Scientific Software Design** Damian Rouson, Jim Xia, Xiaofeng Xu, 2011-04-29 The authors analyze how the structure of a package determines its developmental complexity according to such measures as bug search times and documentation information content The work presents arguments for why these issues impact solution cost and time more than does scalable performance The final chapter explores the question of scalable execution and shows how scalable design relates to scalable execution The book s focus is on program organization which has received considerable attention in the broader software engineering community where graphical description standards for modeling software structure and behavior have been developed by computer scientists These discussions might be enriched by engineers who write scientific codes This book aims to bring such scientific programmers into discussion with computer scientists The authors do so by introducing object oriented software design patterns in the context of scientific simulation Software Engineering for Science Jeffrey C. Carver, Neil P. Chue Hong, George K. Thiruvathukal, 2016-11-03 Software Engineering for Science provides an in depth collection of peer reviewed chapters that describe experiences with applying software engineering practices to the development of scientific software It provides a better understanding of how software engineering is and should be practiced and which software engineering practices are effective for scientific software The book starts with a detailed overview of the Scientific Software Lifecycle and a general overview of the scientific software development process It highlights key issues commonly arising during scientific software development as well as solutions to these problems The second part of the book provides examples of the use of testing in scientific software development including key issues and

challenges The chapters then describe solutions and case studies aimed at applying testing to scientific software development efforts The final part of the book provides examples of applying software engineering techniques to scientific software including not only computational modeling but also software for data management and analysis The authors describe their experiences and lessons learned from developing complex scientific software in different domains About the Editors Jeffrey Carver is an Associate Professor in the Department of Computer Science at the University of Alabama He is one of the primary organizers of the workshop series on Software Engineering for Science <http://www.SE4Science.org> workshops Neil P Chue Hong is Director of the Software Sustainability Institute at the University of Edinburgh His research interests include barriers and incentives in research software ecosystems and the role of software as a research object George K Thiruvathukal is Professor of Computer Science at Loyola University Chicago and Visiting Faculty at Argonne National Laboratory His current research is focused on software metrics in open source mathematical and scientific software

**Encyclopedia of Computer Science and Technology** Harry Henderson, 2009 Presents an illustrated A Z encyclopedia containing approximately 600 entries on computer and technology related topics

**Scientific Computing with Case Studies** Dianne P. O'Leary, 2009-01-01 This book is a practical guide to the numerical solution of linear and nonlinear equations differential equations optimization problems and eigenvalue problems It treats standard problems and introduces important variants such as sparse systems differential algebraic equations constrained optimization Monte Carlo simulations and parametric studies Stability and error analysis are emphasized and the Matlab algorithms are grounded in sound principles of software design and understanding of machine arithmetic and memory management Nineteen case studies provide experience in mathematical modeling and algorithm design motivated by problems in physics engineering epidemiology chemistry and biology The topics included go well beyond the standard first course syllabus introducing important problems such as differential algebraic equations and conic optimization problems and important solution techniques such as continuation methods The case studies cover a wide variety of fascinating applications from modeling the spread of an epidemic to determining truss configurations

**21st Century C** Ben Klemens, 2012-10-15 Throw out your old ideas about C and get to know a programming language that s substantially outgrown its origins With this revised edition of 21st Century C you ll discover up to date techniques missing from other C tutorials whether you re new to the language or just getting reacquainted C isn t just the foundation of modern programming languages it is a modern language ideal for writing efficient state of the art applications Get past idioms that made sense on mainframes and learn the tools you need to work with this evolved and aggressively simple language No matter what programming language you currently favor you ll quickly see that 21st century C rocks Set up a C programming environment with shell facilities makefiles text editors debuggers and memory checkers Use Autotools C s de facto cross platform package manager Learn about the problematic C concepts too useful to discard Solve C s string building problems with C standard functions Use modern syntactic features

for functions that take structured inputs Build high level object based libraries and programs Perform advanced math talk to internet servers and run databases with existing C libraries This edition also includes new material on concurrent threads virtual tables C99 numeric types and other features      Scientific Computing Michael T. Heath, 2018-11-14 This book differs from traditional numerical analysis texts in that it focuses on the motivation and ideas behind the algorithms presented rather than on detailed analyses of them It presents a broad overview of methods and software for solving mathematical problems arising in computational modeling and data analysis including proper problem formulation selection of effective solution algorithms and interpretation of results In the 20 years since its original publication the modern fundamental perspective of this book has aged well and it continues to be used in the classroom This Classics edition has been updated to include pointers to Python software and the Chebfun package expansions on barycentric formulation for Lagrange polynomial interpretation and stochastic methods and the availability of about 100 interactive educational modules that dynamically illustrate the concepts and algorithms in the book Scientific Computing An Introductory Survey Second Edition is intended as both a textbook and a reference for computationally oriented disciplines that need to solve mathematical problems      *Learning Scientific Programming with Python* Christian Hill, 2020-11-12 Learn to master basic programming tasks from scratch with real life scientifically relevant examples and solutions drawn from both science and engineering Students and researchers at all levels are increasingly turning to the powerful Python programming language as an alternative to commercial packages and this fast paced introduction moves from the basics to advanced concepts in one complete volume enabling readers to gain proficiency quickly Beginning with general programming concepts such as loops and functions within the core Python 3 language and moving on to the NumPy SciPy and Matplotlib libraries for numerical programming and data visualization this textbook also discusses the use of Jupyter Notebooks to build rich media shareable documents for scientific analysis The second edition features a new chapter on data analysis with the pandas library and comprehensive updates and new exercises and examples A final chapter introduces more advanced topics such as floating point precision and algorithm stability and extensive online resources support further study This textbook represents a targeted package for students requiring a solid foundation in Python programming      **Methodologies and Applications of Computational Statistics for Machine Intelligence** Samanta, Debabrata, Rao Althar, Raghavendra, Pramanik, Sabyasachi, Dutta, Soumi, 2021-06-25 With the field of computational statistics growing rapidly there is a need for capturing the advances and assessing their impact Advances in simulation and graphical analysis also add to the pace of the statistical analytics field Computational statistics play a key role in financial applications particularly risk management and derivative pricing biological applications including bioinformatics and computational biology and computer network security applications that touch the lives of people With high impacting areas such as these it becomes important to dig deeper into the subject and explore the key areas and their progress in the recent past Methodologies and Applications of Computational

Statistics for Machine Intelligence serves as a guide to the applications of new advances in computational statistics. This text holds an accumulation of the thoughts of multiple experts together, keeping the focus on core computational statistics that apply to all domains. Covering topics including artificial intelligence, deep learning, and trend analysis, this book is an ideal resource for statisticians, computer scientists, mathematicians, lecturers, tutors, researchers, academic and corporate libraries, practitioners, professionals, students, and academicians.

*Higher Mathematics for Science, Technology and Engineering* S. G. Ahmed, 2016-01-07 Higher Mathematics for Science Technology and Engineering is a textbook for undergraduate and postgraduate students undertaking science, technology, engineering, and mathematics STEM courses. The book begins with an introduction to one variable functions, followed by chapters covering functional derivatives, partial differentiation, integrals, matrices, and determinant theory, partial fractions, and much more. Key features of this textbook include simple, easy-to-understand explanations of relevant concepts, a wide range of simple and complex examples, several figures where appropriate.

*Numerical Analysis: A Graduate Course* David E. Stewart, 2022-12-01 This book aims to introduce graduate students to the many applications of numerical computation, explaining in detail both how and why the included methods work in practice. The text addresses numerical analysis as a middle ground between practice and theory, addressing both the abstract mathematical analysis and applied computation and programming models instrumental to the field. While the text uses pseudocode, Matlab and Julia codes are available online for students to use and to demonstrate implementation techniques. The textbook also emphasizes multivariate problems alongside single variable problems and deals with topics in randomness, including stochastic differential equations and randomized algorithms, and topics in optimization and approximation relevant to machine learning. Ultimately, it seeks to clarify issues in numerical analysis in the context of applications and presenting accessible methods to students in mathematics and data science.

**Environmental Literacy in Science and Society** Roland W. Scholz, Claudia R. Binder, 2011-07-21 In an era where humans affect virtually all of the earth's processes, questions arise about whether we have sufficient knowledge of human environment interactions. How can we sustain the Earth's ecosystems to prevent collapses, and what roles should practitioners and scientists play in this process? These are the issues central to the concept of environmental literacy. This unique book provides a comprehensive review and analysis of environmental literacy within the context of environmental science and sustainable development. Approaching the topic from multiple perspectives, it explores the development of human understanding of the environment and human environment interactions in the fields of biology, psychology, sociology, economics, and industrial ecology. The discussion emphasises the importance of knowledge integration and transdisciplinary processes as key strategies for understanding complex human environment systems. HES. In addition, the author defines the HES framework as a template for investigating sustainably coupled human environment systems in the 21st century.

**Introduction to Tensor Network Methods** Simone Montangero, 2018-11-28 This volume of lecture notes briefly introduces the basic concepts needed in any

computational physics course software and hardware programming skills linear algebra and differential calculus It then presents more advanced numerical methods to tackle the quantum many body problem it reviews the numerical renormalization group and then focuses on tensor network methods from basic concepts to gauge invariant ones Finally in the last part the author presents some applications of tensor network methods to equilibrium and out of equilibrium correlated quantum matter The book can be used for a graduate computational physics course After successfully completing such a course a student should be able to write a tensor network program and can begin to explore the physics of many body quantum systems The book can also serve as a reference for researchers working or starting out in the field **Scientific**

**Writing: A Complete Guide** Mitchell P. Jones, 2022-04-24 Be it academia or industry if you're destined for a career in science and technology scientific writing is an essential skill that can make your competence shine or cloud it completely Consolidate your knowledge with this complete guide Mitchell P Jones Scientific Writing A Complete Guide is an essential overview of scientific writing for theses journal articles conference papers and book chapters In clear concise and precise language Jones lays out the basic steps for compiling a highly scoped and impactful manuscript Comprehensive and firmly instructional this guide features step by step directions content and structure suggestions with useful examples tips on how to set up and caption effective tables graphs and schematics and equation and unit formatting principles It also introduces and contrasts each publication type provides shortcuts for efficient referencing titling and editing and details what to expect during the thesis examination and publishing processes This guide contains all content in the Scientific Writing for Beginners series including bachelor's master's and Ph.D theses journal articles conference papers and book chapters It is intended for the intermediate reader seeking an overview of all content Beginners are directed to the specifically formatted sub guides available for each document type **A Guide to the Scientific Career** Mohammadali M. Shoja, Anastasia

Arynchyna, Marios Loukas, Anthony V. D'Antoni, Sandra M. Buerger, Marion Karl, R. Shane Tubbs, 2020-01-09 A concise easy to read source of essential tips and skills for writing research papers and career management In order to be truly successful in the biomedical professions one must have excellent communication skills and networking abilities Of equal importance is the possession of sufficient clinical knowledge as well as a proficiency in conducting research and writing scientific papers This unique and important book provides medical students and residents with the most commonly encountered topics in the academic and professional lifestyle teaching them all of the practical nuances that are often only learned through experience Written by a team of experienced professionals to help guide younger researchers A Guide to the Scientific Career Virtues Communication Research and Academic Writing features ten sections composed of seventy four chapters that cover qualities of research scientists career satisfaction and its determinants publishing in academic medicine assessing a researcher's scientific productivity and scholarly impact manners in academics communication skills essence of collaborative research dealing with manipulative people writing and scientific misconduct ethical and legal aspects plagiarism research regulations

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**A Practical Guide to Scientific Writing in Chemistry** Andrew Terhemen Tyowua,2023-03-31 Successful completion of postgraduate studies especially PhD and career advancement in academia strongly depend on the ability to publish scientific papers or books and attract research grants However many chemical scientists find preparing scientific papers and research grant and book proposals difficult partly because of insufficient training in writing and partly because there are few practical books to enable them to learn the art This step by step practical guide is intended mainly for postgraduate students and early career researchers in chemical science and the libraries that serve them but will also be useful to other scientists Key Features Improves the reader s chances of getting their manuscript published in chemistry journals Increases the likelihood of winning research grants in chemistry Takes a lead by the hand approach Contains chapters on the preparation of graphical abstracts and research highlights Uses sketches and other illustration styles to aid mental visualization of concepts Contains practical examples taken from published papers and successful research grant proposals *Applied Computer Science for GGOS Observatories* Alexander N.J. Neidhardt,2017-08-08 This book combines elementary theory from computer science with real world challenges in global geodetic observation based on examples from the Geodetic Observatory Wettzell Germany It starts with a step by step introduction to developing stable and safe scientific software to run successful software projects The use of software toolboxes is another essential aspect that leads to the application of generative programming An example is a generative network middleware that simplifies communication One of the book s main focuses is on explaining a potential strategy involving autonomous production cells for space geodetic techniques The complete software design of a satellite laser ranging system is taken as an example Such automated systems are then combined for global interaction using secure communication tunnels for remote access The network of radio telescopes is used as a reference Combined observatories form coordinated multi agent systems and offer solutions for operational aspects of the Global Geodetic Observing System GGOS with regard to Industry 4 0 *Writing Scientific Research in Communication Sciences and Disorders* Robert H. Brookshire,Shelley B. Brundage,2015-11-02 Writing Scientific Research in Communication Sciences and Disorders is a comprehensive guide to the preparation and publication of research papers for researchers in communication

sciences and disorders Individual chapters address the structure content and style of the introduction method results and discussion sections of a research paper The balance of the text examines the writing process including the nuts and bolts of preparing tables and graphs reviewing different voices and grammar issues editing your own work working with editors and peer reviewers and getting started toward becoming a productive writer Each topic is illustrated with informative examples with clear direct and often humorous discussion of what makes the examples good or bad Writing is essential in nearly every profession and particularly in communication sciences and disorders where researchers must be able to express complex ideas to a variety of audiences from colleagues to members of health care teams to clients and family members Therefore competency in written expression is required for certification and entry into clinical practice in communication sciences and disorders Writing Scientific Research in Communication Sciences and Disorders will be a valuable supplementary text for undergraduate and graduate students in courses that include writing assignments and critical assessment of research literature such as research methods and evidence based clinical methods courses as well as in thesis and dissertation preparation Researchers looking for a guide to help improve their own writing will also find this text to be an invaluable resource that answers the big and little questions that arise in preparing manuscripts

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