# Parallel Scientific Computing in C++ and MPI

A Seamless Approach to Parallel Algorithms and Their Implementation

George Em Karniadakis Robert M. Kirby II

CAMBRIDGE

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Frédéric Magoules, François-Xavier Roux, Guillaume Houzeaux

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how to use the bulk synchronous parallel BSP model and the freely available BSPlib communication library in parallel algorithm design and parallel programming Aimed at graduate students and researchers in mathematics physics and computer science the main topics treated in the book are core topics in the area of scientific computation and many additional topics are treated in numerous exercises An appendix on the message passing interface MPI discusses how to program using the MPI communication library MPI equivalents of all the programs are also presented The main topics treated in the book are core in the area of scientific computation solving dense linear systems by Gaussian elimination computing fast Fourier transforms and solving sparse linear systems by iterative methods Each topic is treated in depth starting from the problem formulation and a sequential algorithm through a parallel algorithm and its analysis to a complete parallel program written in C and BSPlib and experimental results obtained using this program on a parallel computer Additional topics treated in the exercises include data compression random number generation cryptography eigensystem solving 3D and Strassen matrix multiplication wavelets and image compression fast cosine transform decimals of pi simulated annealing and molecular dynamics The book contains five small but complete example programs written in BSPlib which illustrate the methods taught The appendix on MPI discusses how to program in a structured bulk synchronous parallel style using the MPI communication library It presents MPI equivalents of all the programs in the book The complete programs of the book and their driver programs are freely available online in the packages BSPedupack and MPIedupack of Parallel Scientific Computing Tobias Weinzierl, 2022-02-09 New insight in many scientific and engineering fields is unthinkable without the use of numerical simulations running efficiently on modern computers. The faster we get new results the bigger and accurate are the problems that we can solve It is the combination of mathematical ideas plus efficient programming that drives the progress in many disciplines Future champions in the area thus will have to be qualified in their application domain they will need a profound understanding of some mathematical ideas and they need the skills to deliver fast code The present textbook targets students which have programming skills already and do not shy away from mathematics though they might be educated in computer science or an application domain It introduces the basic concepts and ideas behind applied mathematics and parallel programming that we need to write numerical simulations for today s multicore workstations Our intention is not to dive into one particular application domain or to introduce a new programming language we lay the generic foundations for future courses and projects in the area The text is written in an accessible style which is easy to digest for students without years and years of mathematics education It values clarity and intuition over formalism and uses a simple N body simulation setup to illustrate basic ideas that are of relevance in various different subdomains of scientific computing Its primary goal is to make theoretical and paradigmatic ideas accessible to undergraduate students and to bring the fascination of the field across **Parallel Scientific Computing Frédéric** Magoules, François-Xavier Roux, Guillaume Houzeaux, 2016-01-26 Scientific computing has become an indispensable tool in

numerous fields such as physics mechanics biology finance and industry For example it enables us thanks to efficient algorithms adapted to current computers to simulate without the help of models or experimentations the deflection of beams in bending the sound level in a theater room or a fluid flowing around an aircraft wing This book presents the scientific computing techniques applied to parallel computing for the numerical simulation of large scale problems these problems result from systems modeled by partial differential equations Computing concepts will be tackled via examples Implementation and programming techniques resulting from the finite element method will be presented for direct solvers iterative solvers and domain decomposition methods along with an introduction to MPI and OpenMP Computation Rob H. Bisseling, 2020-09-30 Building upon the wide ranging success of the first edition Parallel Scientific Computation presents a single unified approach to using a range of parallel computers from a small desktop computer to a massively parallel computer The author explains how to use the bulk synchronous parallel BSP model to design and implement parallel algorithms in the areas of scientific computing and big data and provides a full treatment of core problems in these areas starting from a high level problem description via a sequential solution algorithm to a parallel solution algorithm and an actual parallel program written in BSPlib Every chapter of the book contains a theoretical section and a practical section presenting a parallel program and numerical experiments on a modern parallel computer to put the theoretical predictions and cost analysis to the test Every chapter also presents extensive bibliographical notes with additional discussions and pointers to relevant literature and numerous exercises which are suitable as graduate student projects The second edition provides new material relevant for big data science such as sorting and graph algorithms and it provides a BSP approach towards new hardware developments such as hierarchical architectures with both shared and distributed memory A single simple hybrid BSP system suffices to handle both types of parallelism efficiently and there is no need to master two systems as often happens in alternative approaches Furthermore the second edition brings all algorithms used up to date and it includes new material on high performance linear system solving by LU decomposition and improved data partitioning for sparse matrix computations The book is accompanied by a software package BSPedupack freely available online from the author's homepage which contains all programs of the book and a set of test driver programs This package written in C can be run using modern BSPlib implementations such as MulticoreBSP for C or BSPonMPI PAX **Computer** Tsutomu Hoshino, 1985 Environment and Tools for Parallel Scientific Computing J. Dongarra, 1997

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