

# Contents

## Part I Basics

<b>1</b>	<b>Parallel Programming Paradigms</b> . . . . .	3
1.1	Computational Models . . . . .	3
1.1.1	Performance Metrics . . . . .	3
1.1.2	Single Instruction Multiple Data Architectures and Pipelining . . . . .	5
1.1.3	Multiple Instruction Multiple Data Architectures . . . . .	9
1.1.4	Hierarchical Architectures . . . . .	10
1.2	Principles of Parallel Programming . . . . .	11
1.2.1	From Amdahl’s Law to Scalability . . . . .	12
	References. . . . .	14
<b>2</b>	<b>Fundamental Kernels</b> . . . . .	17
2.1	Vector Operations . . . . .	17
2.2	Higher Level BLAS . . . . .	19
2.2.1	Dense Matrix Multiplication . . . . .	20
2.2.2	Lowering Complexity via the Strassen Algorithm . . . . .	22
2.2.3	Accelerating the Multiplication of Complex Matrices . . . . .	24
2.3	General Organization for Dense Matrix Factorizations . . . . .	25
2.3.1	Fan-Out and Fan-In Versions . . . . .	25
2.3.2	Parallelism in the Fan-Out Version . . . . .	26
2.3.3	Data Allocation for Distributed Memory . . . . .	28
2.3.4	Block Versions and Numerical Libraries . . . . .	29
2.4	Sparse Matrix Computations . . . . .	30
2.4.1	Sparse Matrix Storage and Matrix-Vector Multiplication Schemes . . . . .	31
2.4.2	Matrix Reordering Schemes . . . . .	36
	References. . . . .	43

**Part II Dense and Special Matrix Computations**

- 3 Recurrences and Triangular Systems . . . . . 49**
  - 3.1 Definitions and Examples . . . . . 49
  - 3.2 Linear Recurrences . . . . . 51
    - 3.2.1 Dense Triangular Systems . . . . . 52
    - 3.2.2 Banded Triangular Systems . . . . . 57
    - 3.2.3 Stability of Triangular System Solvers . . . . . 59
    - 3.2.4 Toeplitz Triangular Systems . . . . . 61
  - 3.3 Implementations for a Given Number of Processors . . . . . 66
  - 3.4 Nonlinear Recurrences . . . . . 72
  - References. . . . . 78
  
- 4 General Linear Systems . . . . . 79**
  - 4.1 Gaussian Elimination. . . . . 80
  - 4.2 Pairwise Pivoting . . . . . 82
  - 4.3 Block LU Factorization . . . . . 84
    - 4.3.1 Approximate Block Factorization . . . . . 85
  - 4.4 Remarks . . . . . 87
  - References. . . . . 88
  
- 5 Banded Linear Systems . . . . . 91**
  - 5.1 LU-based Schemes with Partial Pivoting . . . . . 91
  - 5.2 The Spike Family of Algorithms. . . . . 94
    - 5.2.1 The Spike Algorithm. . . . . 95
    - 5.2.2 Spike: A Polyalgorithm . . . . . 99
    - 5.2.3 The Non-diagonally Dominant Case . . . . . 100
    - 5.2.4 The Diagonally Dominant Case . . . . . 104
  - 5.3 The Spike-Balance Scheme . . . . . 105
  - 5.4 A Tearing-Based Banded Solver . . . . . 115
    - 5.4.1 Introduction . . . . . 115
    - 5.4.2 Partitioning . . . . . 115
    - 5.4.3 The Balance System . . . . . 118
    - 5.4.4 The Hybrid Solver of the Balance System . . . . . 124
  - 5.5 Tridiagonal Systems . . . . . 126
    - 5.5.1 Solving by Marching . . . . . 128
    - 5.5.2 Cyclic Reduction and Parallel Cyclic Reduction . . . . . 130
    - 5.5.3 LDU Factorization by Recurrence Linearization . . . . . 139
    - 5.5.4 Recursive Doubling . . . . . 143
    - 5.5.5 Solving by Givens Rotations . . . . . 144
    - 5.5.6 Partitioning and Hybrids . . . . . 149
    - 5.5.7 Using Determinants and Other Special Forms. . . . . 155
  - References. . . . . 159

<b>6</b>	<b>Special Linear Systems</b>	165
6.1	Vandermonde Solvers	166
6.1.1	Vandermonde Matrix Inversion	170
6.1.2	Solving Vandermonde Systems and Parallel Prefix	172
6.1.3	A Brief Excursion into Parallel Prefix	174
6.2	Banded Toeplitz Linear Systems Solvers	176
6.2.1	Introduction	176
6.2.2	Computational Schemes	182
6.3	Symmetric and Antisymmetric Decomposition (SAS)	192
6.3.1	Reflexive Matrices as Preconditioners	194
6.3.2	Eigenvalue Problems	196
6.4	Rapid Elliptic Solvers	197
6.4.1	Preliminaries	198
6.4.2	Mathematical and Algorithmic Infrastructure	199
6.4.3	Matrix Decomposition	201
6.4.4	Complete Fourier Transform	203
6.4.5	Block Cyclic Reduction	205
6.4.6	Fourier Analysis-Cyclic Reduction	210
6.4.7	Sparse Selection and Marching	211
6.4.8	Poisson Inverse in Partial Fraction Representation	214
6.4.9	Notes	218
	References	220
<b>7</b>	<b>Orthogonal Factorization and Linear Least Squares Problems</b>	227
7.1	Definitions	227
7.2	QR Factorization via Givens Rotations	228
7.3	QR Factorization via Householder Reductions	232
7.4	Gram-Schmidt Orthogonalization	233
7.5	Normal Equations Versus Orthogonal Reductions	235
7.6	Hybrid Algorithms When $m \gg n$	236
7.7	Orthogonal Factorization of Block Angular Matrices	237
7.8	Rank-Deficient Linear Least Squares Problems	242
	References	246
<b>8</b>	<b>The Symmetric Eigenvalue and Singular-Value Problems</b>	249
8.1	The Jacobi Algorithms	251
8.1.1	The Two-Sided Jacobi Scheme for the Symmetric Standard Eigenvalue Problem	251
8.1.2	The One-Sided Jacobi Scheme for the Singular Value Problem	254
8.1.3	The Householder-Jacobi Scheme	259
8.1.4	Block Jacobi Algorithms	261
8.1.5	Efficiency of Parallel Jacobi Methods	262

- 8.2 Tridiagonalization-Based Schemes. . . . . 263
  - 8.2.1 Tridiagonalization of a Symmetric Matrix . . . . . 264
  - 8.2.2 The QR Algorithm: A Divide-and-Conquer Approach. . . . . 265
  - 8.2.3 Sturm Sequences: A Multisectioning Approach. . . . . 267
- 8.3 Bidiagonalization via Householder Reduction. . . . . 272
- References. . . . . 273

**Part III Sparse Matrix Computations**

- 9 Iterative Schemes for Large Linear Systems . . . . . 277**
  - 9.1 An Example. . . . . 278
  - 9.2 Classical Splitting Methods . . . . . 280
    - 9.2.1 Point Jacobi . . . . . 281
    - 9.2.2 Point Gauss-Seidel . . . . . 282
    - 9.2.3 Line Jacobi . . . . . 283
    - 9.2.4 Line Gauss-Seidel . . . . . 286
    - 9.2.5 The Symmetric Positive Definite Case. . . . . 287
  - 9.3 Polynomial Methods . . . . . 294
    - 9.3.1 Chebyshev Acceleration. . . . . 294
    - 9.3.2 Krylov Methods . . . . . 299
  - References. . . . . 309
- 10 Preconditioners . . . . . 311**
  - 10.1 A Tearing-Based Solver for Generalized Banded Preconditioners . . . . . 312
  - 10.2 Row Projection Methods for Large Nonsymmetric Linear Systems. . . . . 312
    - 10.2.1 The Kaczmarz Scheme . . . . . 313
    - 10.2.2 The Cimmino Scheme . . . . . 319
    - 10.2.3 Connection Between RP Systems and the Normal Equations . . . . . 319
    - 10.2.4 CG Acceleration . . . . . 320
    - 10.2.5 The 2-Partitions Case . . . . . 321
    - 10.2.6 Row Partitioning Goals . . . . . 324
    - 10.2.7 Row Projection Methods and Banded Systems . . . . . 325
  - 10.3 Multiplicative Schwarz Preconditioner with GMRES. . . . . 326
    - 10.3.1 Algebraic Domain Decomposition of a Sparse Matrix . . . . . 327
    - 10.3.2 Block Multiplicative Schwarz. . . . . 329
    - 10.3.3 Block Multiplicative Schwarz as a Preconditioner for Krylov Methods. . . . . 336
  - References. . . . . 340

<b>11</b>	<b>Large Symmetric Eigenvalue Problems</b> . . . . .	<b>343</b>
11.1	Computing Dominant Eigenpairs and Spectral Transformations . . . . .	343
11.1.1	Spectral Transformations . . . . .	345
11.1.2	Use of Sturm Sequences . . . . .	349
11.2	The Lanczos Method . . . . .	350
11.2.1	The Lanczos Tridiagonalization . . . . .	350
11.2.2	The Lanczos Eigensolver . . . . .	352
11.3	A Block Lanczos Approach for Solving Symmetric Perturbed Standard Eigenvalue Problems . . . . .	356
11.3.1	Starting Vectors for $A(S_i)x = \lambda X$ . . . . .	356
11.3.2	Starting Vectors for $A(S_i)^{-1}x = \mu x$ . . . . .	358
11.3.3	Extension to the Perturbed Symmetric Generalized Eigenvalue Problems . . . . .	359
11.3.4	Remarks . . . . .	360
11.4	The Davidson Methods . . . . .	363
11.4.1	General Framework . . . . .	363
11.4.2	Convergence . . . . .	364
11.4.3	Types of Correction Steps . . . . .	366
11.5	The Trace Minimization Method for the Symmetric Generalized Eigenvalue Problem . . . . .	368
11.5.1	Derivation of the Trace Minimization Algorithm . . . . .	370
11.5.2	Practical Considerations . . . . .	373
11.5.3	Acceleration Techniques . . . . .	378
11.5.4	A Davidson-Type Extension . . . . .	381
11.5.5	Implementations of TRACEMIN . . . . .	384
11.6	The Sparse Singular-Value Problem . . . . .	386
11.6.1	Basics . . . . .	386
11.6.2	Subspace Iteration for Computing the Largest Singular Triplets . . . . .	390
11.6.3	The Lanczos Method for Computing a Few of the Largest Singular Triplets . . . . .	392
11.6.4	The Trace Minimization Method for Computing the Smallest Singular Triplets . . . . .	395
11.6.5	Davidson Methods for the Computation of the Smallest Singular Values . . . . .	398
11.6.6	Refinement of Left Singular Vectors . . . . .	399
	References . . . . .	402

**Part IV Matrix Functions and Characteristics**

**12 Matrix Functions and the Determinant** . . . . . 409

12.1 Matrix Functions. . . . . 410

12.1.1 Methods Based on the Product Form  
of the Denominator . . . . . 412

12.1.2 Methods Based on Partial Fractions. . . . . 414

12.1.3 Partial Fractions in Finite Precision . . . . . 418

12.1.4 Iterative Methods and the Matrix Exponential. . . . . 424

12.2 Determinants . . . . . 428

12.2.1 Determinant of a Block-Tridiagonal Matrix . . . . . 429

12.2.2 Counting Eigenvalues with Determinants . . . . . 431

References. . . . . 434

**13 Computing the Matrix Pseudospectrum** . . . . . 439

13.1 Grid Based Methods . . . . . 440

13.1.1 Limitations of the Basic Approach . . . . . 440

13.1.2 Dense Matrix Reduction . . . . . 442

13.1.3 Thinning the Grid: The Modified GRID Method. . . . . 443

13.2 Dimensionality Reduction on the Domain: Methods  
Based on Path Following . . . . . 446

13.2.1 Path Following by Tangents. . . . . 446

13.2.2 Path Following by Triangles. . . . . 450

13.2.3 Descending the Pseudospectrum . . . . . 454

13.3 Dimensionality Reduction on the Matrix: Methods  
Based on Projection . . . . . 458

13.3.1 An EIGTOOL Approach for Large Matrices . . . . . 459

13.3.2 Transfer Function Approach. . . . . 460

13.4 Notes . . . . . 463

References. . . . . 464

**Index** . . . . . 467



<http://www.springer.com/978-94-017-7187-0>

Parallelism in Matrix Computations

Gallopoulos, E.; Philippe, B.; Sameh, A.H.

2016, XXX, 473 p. 58 illus., Hardcover

ISBN: 978-94-017-7187-0