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and Exercises; Chapter 8. The Gibbs Ensemble; 8.1 The Gibbs Ensemble Technique; 8.2 The Partition Function; 8.3 Monte Carlo Simulations; 8.4 Applications; 8.5 Questions and Exercises; Chapter 9. Other Methods to Study Coexistence; 9.1 Semigrand Ensemble; 9.2 Tracing Coexistence Curves; Chapter 10. Free Energies of Solids; 10.1 Thermodynamic Integration; 10.2 Free Energies of Solids
10.3 Free Energies of Molecular Solids10.4 Vacancies and Interstitials; Chapter 11. Free Energy of Chain Molecules; 11.1 Chemical Potential as Reversible Work; 11.2 Rosenbluth Sampling; Part IV: Advanced Techniques; Chapter 12. Long-Range Interactions; 12.1 Ewald Sums; 12.2 Fast Multipole Method; 12.3 Particle Mesh Approaches; 12.4 Ewald Summation in a Slab Geometry; Chapter 13. Biased Monte Carlo Schemes; 13.1 Biased Sampling Techniques; 13.2 Chain Molecules; 13.3 Generation of Trial Orientations; 13.4 Fixed Endpoints; 13.5 Beyond Polymers; 13.6 Other Ensembles; 13.7 Recoil Growth
13.8 Questions and ExercisesChapter 14. Accelerating Monte Carlo Sampling; 14.1 Parallel Tempering; 14.2 Hybrid Monte Carlo; 14.3 Cluster Moves; Chapter 15. Tackling Time-Scale Problems; 15.1 Constraints; 15.2 On-the-Fly Optimization: Car-Parrinello Approach; 15.3 Multiple Time Steps; Chapter 16. Rare Events; 16.1 Theoretical Background; 16.2 Bennett-Chandler Approach; 16.3 Diffusive Barrier Crossing; 16.4 Transition Path Ensemble; 16.5 Searching for the Saddle Point; Chapter 17. Dissipative Particle Dynamics; 17.1 Description of the Technique; 17.2 Other Coarse-Grained Techniques
Part V: Appendices

Sommario/riassunto

Understanding Molecular Simulation: From Algorithms to Applications explains the physics behind the ""recipes"" of molecular simulation for materials science. Computer simulators are continuously confronted with questions concerning the choice of a particular technique for a given application. A wide variety of tools exist, so the choice of technique requires a good understanding of the basic principles. More importantly, such understanding may greatly improve the efficiency of a simulation program. The implementation of simulation methods is illustrated in pseudocodes and their practic

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Nota di contenuto	Contents; Preface; Acknowledgements; Metamorphoses of a Discipline: Rethinking Canadian Literature within Institutional Contexts; Against Institution: Established Law, Custom, or Purpose; From Canadian Trance to TransCanada: White Civility to Wry Civility in the CanLit Project; Subtitling CanLit: Keywords; Oratory on Oratory; TransCanada, Literature: No Direction Home; World Famous across Canada, or TransNational Localities; Diasporic Citizenship: Contradictions and Possibilities for Canadian Literature; Acts of Citizenship: Erin Moure's O Cidadan and the Limits of Worldliness

	Trans-Scan: Globalization, Literary Hemispheric Studies, Citizenship as ProjectTransubracination: How Writers of Colour Became CanLit; Institutional Genealogies in the Global Net of Fundamentalisms, Families, and Fantasies; TransCanada Collectives: Social Imagination, the Cunning of Production, and the Multilateral Sublime; Notes; Works Cited; Contributors; Index
Sommario/riassunto	The study of Canadian literature-CanLit-has undergone dramatic changes since it became an area of specialization in the 1960s and '70s. As new global forces in the 1990s undermined its nation-based critical assumptions, its theoretical focus and research methods lost their immediacy. The contributors to Trans.Can.Lit address cultural policy, citizenship, white civility, and the celebrated status of diasporic writers, unabashedly recognizing the imperative to transfigure the disciplinary and institutional frameworks within which Canadian literature is produced, disseminated, studied,