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| Nota di contenuto | Invited Papers -- Cells as Computation -- Formal Modeling of C. elegans Development: A Scenario-Based Approach -- Regular Papers -- Causal ?-Calculus for Biochemical Modelling -- Graphs for Core Molecular Biology -- Contribution of Computational Tree Logic to Biological Regulatory Networks: Example from Pseudomonas Aeruginosa -- Modeling Cellular Behavior with Hybrid Automata: Bisimulation and Collapsing -- Multiscale Modeling of Alternative Splicing Regulation -- A Method for Estimating Metabolic Fluxes from Incomplete Isotopomer Information -- Dynamic Bayesian Network and Nonparametric Regression for Nonlinear Modeling of Gene Networks |

from Time Series Gene Expression Data -- Discrete Event Simulation for a Better Understanding of Metabolite Channeling - A System Theoretic Approach -- Mathematical Modeling of the Influence of RKIP on the ERK Signaling Pathway -- A Method to Identify Essential Enzymes in the Metabolism: Application to Escherichia Coli -- Symbolic Model Checking of Biochemical Networks -- Presentation Abstracts -- Coupled Oscillator Models for a Set of Communicating Cells -- Representing and Simulating Protein Functional Domains in Signal Transduction Using Maude -- A Core Modeling Language for the Working Molecular Biologist (Abstract) -- Integrating Simulation Packages via Systems Biology Mark-Up Language -- Recreating Biopathway Databases towards Simulation -- How to Synthesize an Optimized Genetic ?-Switching System? A System-Theoretic Approach Based on SQP -- Simulation Sudy of the TNF? Mediated NF-?B Signaling Pathway -- Detection and Analysis of Unexpected State Components in Biological Systems -- Model Validation of Biological Pathways Using Petri Nets - Demonstrated for Apoptosis -- An Overview of Data Models for the Analysis of Biochemical Pathways -- Discrete Event Systems and Client-Server Model for Signaling Mechanisms -- Position Papers -- Enhanced Operational Semantics in Systems Biology -- Issues in Computational Methods for Functional Genomics and Systems Biology -- Integrating Biological Process Modelling with Gene Expression Data and Ontologies for Functional Genomics (Position Paper) -- Computer Simulation of Protocells -- How to Solve Semantic Puzzles of Systems Biology -- Evolution as Design Engineer -- Inference, Modeling and Simulation of Gene Networks.

Sommario/riassunto

Molecularbiologyhasuntilnowmainlyfocussedonindividualmolecules,on theirpropertiesasisolatedentitiesorascomplexesinverysimplemodelsyste ms. However,
biologicalmoleculesinlivingsystemsparticipateinverycomplexn- works, includingregulatorynetworksforgeneexpression,intracellularmetabolic networksandbothintra-andintercellularcommunicationnetworks. Suchn- worksareinvolvedinthemaintenance(homeostasis)
aswellasthedi'erentiation
ofcellularsystemsofwhichwehaveaveryincompleteunderstanding. Nevertheless,
theprogressinmolecularbiologyhasmadepossiblethedetailed descriptionofthecomponentsthatconstitutelivingsystems,
notablygenesand proteins. Large-
scalegenomesequencingmeansthatwecan(atleastinpr- ciple) delineateallmacromolecularcomponentsofagivencellularsystem,and microarrayexperimentsaswellaslarge-
scaleproteomicswillsoongiveuslarge
amountsofexperimentaldataongeneregulation,molecularinteractionsand cellularnetworks. Thechallengeofthe21stcenturywillbetounderstandhow theseindividualcomponentsintegrateintocomplexsystemsandthefunctio n andevolutionofthesesystems,thusscalingupfrommolecularbiologytos- temsbiology.
Bycombiningexperimentaldatawithadvancedformaltheories fromcomputerscience,"theformallanguageforbiologicalsystems" tospecify
dynamicmodelsofinteractingmolecularentitieswouldbeessentialfor:(i)- derstandingthenormalbehaviourofcellularprocesses,
andhowchangesmay a'ectthe processesandcausedisease-
itmaybepossibletocorrelategenetic
propertiesandsymptomsinnewandmoree'cientways,basedonanactual- derstandingofhowvariousprocessesinteract;(ii)
providingpredictabilityand ?exibilitytoacademic,pharmaceutical,

biotechnologyandmedicalresearchers studyinggeneorproteinfunctions. Inparticular,itmaysavetimebyreducing thenumberofexperimentsneeded, ifinadequatehypothesescanbeexcludedby computersimulation. InresponsetothecallforpapersWeresubmittedtoCMSB2003. Allthe submittedpaperswerereviewedandtheprogrammecommittee (listedbelow) selected11high-qualitypapersforpublicationinthisvolume. Thecareofthe reviewersandoftheprogrammecommitteemembersinreviewingthepapers wassurelyvaluable. Afurther11paperswereselectedonlyforpresentationat theworkshopinordertostimulatediscussions(anabstractisincluded). AttheworkshopEhudShapiroandMichaelSterngavetwoinvited talks whosetopicsaredescribedinpapersincludedinthisvolume. Theprogramme committeedecidedtoacceptforpublicationinthisvolumealsosomeposition papers that highlight the research trends in this new ?eld of computational methodsinsystemsbiology. Thereasonisthatbecausethisisthe'rstedition ofaworkshopinthisfast-growing'eldalargeviewofpotentialtopicsofresearch wasconsideredextremelyimportant. Rovereto,December2002 CorradoPriami ProgrammeCommitteeofCMSB 2003 CorradoPriami (Chair),UniversityofTrento(Italy), CharlesAu'ray,CNRS,Villejuif(France), CosimaBaldari,Universit`adiSiena(Italy), AlexanderBockmayr, Universit´eHenriPoincar´e(France), LucaCardelli, MicrosoftResearchCambridge(UK), VincentDanos,Universit´eParisVII (France), PierpaoloDegano,Universitad ` iPisa(Italy), Francois ¸ Fages, INRIA,Rocquencourt(France), DrabløsFinn, NorwegianUniversityofScienceandTechnology,Trondheim(N- way), MonikaHeiner,BrandenburgUniversityofTechnologyatCottbus(Germany), InaKoch,UniversityofAppliedSciencesBerlin,(Germany), JohnE. Ladbury, UniversityCollegeLondon(UK), PatrickLincoln,SRI(USA), SatoruMiyano, UniversityofTokyo(Japan), GordonPlotkin,UniversityofEdinburgh(UK), SimonPlyte,PharmaciaCorporation(Italy), AvivRegev, WeizmannInstituteofScience(Israel), MagaliRoux-Rouqui´e, BSMIPasteurInstitute(France), VincentSchachter,HybrigenicsParis (France), MasaruTomita,KeioUniversity(Japan), AdelindeUhrmacher, UniversityofRostock(Germany), AlfonsoValencia,CNB-CSIC, CentroNacionaldeBiotecnologia(Spain), OlafWolkenhauer,UMIST, Manchester(UK) Local Organizing Committee Corrado Priami, Linda Brodo, Michela de Concini, Debora Schuch da Rosa Machado, andtheUniversityofTrentoEventsandMeetingsO'ce. List ofReferees F. Abascal,N. Chabrier,A. Cimatti,M. Curti,M. D. Devignes,S. Gnesi, J. Guijarro,K. Hafez,E. Klipp,C. Laneve,P. LopezRomero,F. Luccio, R. Marangoni,M. Padron,M. C. Pinotti,R. Rizzi,S. Tini. Acknowledgement TheworkshopwassponsoredandpartiallysupportedbytheuniversityofTren to, ComunediRovereto,APT,andtheEUprojectIST-32072-DEGAS. Table of Contents IInvitedPapers CellsasComputation. . . . . 1 AmitaiRegevandEhudShapiro FormalModelingofC. elegansDevelopment: AScenario-BasedApproach . . . 4 Na"aman Kam,David Harel,Hillel Kugler, RamiMarelly, AmirPnueli, E. JaneAlbertHubbard, andMichael J. Stern IIRegularPapers Causal?-CalculusforBiochemicalModelling . . . . . 21 Michele Curti,Pierpaolo Degano, andCosima Tatiana Baldari GraphsforCoreMolecularBiology . . . . . 34 Vincent Danos and Cosimo Laneve ContributionofComputationalTreeLogic toBiologicalRegulatoryNetworks: ExamplefromPseudomonasAeruginosa. . . . . 47 SabinePeresandJean-PaulComet ModelingCellularBehaviorwithHybridAutomata: BisimulationandCollapsing. . . . . .

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