A Centre of Excellence in Computational Biomedicine

Résultats

Informations projet

CompBioMed

N° de convention de subvention: 675451

DOI
10.3030/675451

Projet clôturé

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3 Juin 2016

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Coordonné par
UNIVERSITY COLLEGE LONDON
Royaume-Uni

CORDIS fournit des liens vers les livrables publics et les publications des projets HORIZON.

Les liens vers les livrables et les publications des projets du 7e PC, ainsi que les liens vers certains types de résultats spécifiques tels que les jeux de données et les logiciels, sont récupérés dynamiquement sur OpenAIRE.

Livrables

Documents, rapports (26)

Report on Efficient HPC usage by the Biomedicine community

Report which describes the uptake of biomedicine applications on various European e-infrastructures, and the use of community applications on HPC systems facilitated by this project.

Report on Deployment of Deep Track Tools and Services to Improve Efficiency of Research and Facilitating Access to CoE Capabilities
Report on progress in and impact of deployment of these tools in support of complex workflows (including multiscale models) on available HPC environments.

Project Handbook
WP1 will produce a project handbook outlining the project's procedures, legal obligations and reporting processes, to assist each partner.

Report on dissemination and training material
Report on dissemination and training material as produced by the project.

Training Plan
A report with a detailed training plan, including both training events, ways of delivery, and partners responsible for the training.

Quality Assurance Plan
To manage the project's quality control process, a Quality Assurance Plan will be created to assist internal reviewers in monitoring all deliverables before they are finalised and submitted to the commission. The deliverable will also contain a detailed risk analysis and contingency planning.

Report on existing solutions in support of biomedical applications
This is a public document, which describes the existing solutions (tools, services, datasets) that can be of benefit to a range of new biomedical research applications.

Dissemination Action Plan
A detailed and comprehensive report on the dissemination actions that will be carried out by the project.

Report on the Impact of Modelling and Simulation within Biomedical Research as enabled by CompBioMed
This report will be a major outcome of the project and will present an overview of the impact to date of computational approaches in biomedical research, together with a forecast of the anticipated impact that these methods and associated technologies will have within academia, industry and healthcare.

Report on best practices for e-infrastructure application usage

Report which will cover usage of the e-infrastructure from an applications point of view.

First report on training and dissemination
Report on delivered training and dissemination actions as well as update to the training plan and dissemination action plan

Report on Extreme Scaling of and Porting of Exemplar Applications to Novel Architectures
Report on the implementation of high fidelity CompBioMed applications on emerging HPC architectures on the path to the exascale and on porting to new and maturing architectures.

Report on selected emerging use cases for existing solutions
As part of T6.2, an updated version of D6.1.1 will be produced at M24, to address emerging use cases.

Final report on the end-user solutions
A final update of the public document, describing all the end-user solutions.

Final Report on Industrial and cPPP Collaboration
A detailed report on our engagement with industrial stakeholders and ETH4HPC, and our Innovation Exchange Programme, throughout the course of the CompBioMed project

Innovation Plan
We will deliver an innovation plan, to be adhered to by all members of the consortium, to promote the innovation and commercialisation aspects of this project.

Report on computing and data needs of the biomedical community
Report which identifies the needs for infrastructure usage and access models for the biomedicine community

Final training and dissemination report
A report on the training and dissemination actions, as well as delivery of a reusable set of training materials, as developed and used during the project.

Sustainability Plan
A plan to ensure the sustainability of our CompBioMed Centre of Excellence

Preparing data infrastructures for large-scale resources: report on the optimization activities
Report which describes the selected optimization tasks, and the outcome of these tasks.

Final Public Report
A non-confidential summary of the final status of the project.

Interim Report on Industrial and cPPP Collaboration
A report on our initial engagement with industrial stakeholders and ETH4HPC, and our Innovation Exchange Programme.

Report on Application Software Readiness and Fast Track Exploitation
Report on the applications and research being undertaken within the CompBioMed environment based on the initial, Fast Track deployment.

Report on Workflow system provision
This report will describe the initial workflow system deployment conducted in T6.5

Report on the optimization activities
A report that describes the progress achieved in the optimisation activities (T6.3).

Report on access mechanisms to HPC systems
Report on the various access models to HPC systems for scientific usage, in particular for the biomedicine community

Open Research Data Pilot (1)

Data Management Plan
WP1 will produce a Data Management Plan in M6.

Sites Web, dépôts de brevet, vidéos, etc. (3)

Release of Community Software Repository
We will make available our community software repository to members of the computational biomedicine research community

Website Release
The project website will provide a focal point for the dissemination activities of the project.

Deployment of project informatics platform

We will make a release of our project informatics platform for community members to use.

Publications

Articles approuvés par les pairs (75)

Computational techniques for ECG analysis and interpretation in light of their contribution to medical advances

Auteurs: Aurore Lyon, Ana Mincholé, Juan Pablo Martínez, Pablo Laguna, Blanca Rodriguez
Publié dans: Journal of The Royal Society Interface, Numéro 15/138, 2018, Page(s) 20170821, ISSN 1742-5689
Éditeur: The Royal Society
DOI: 10.1098/rsif.2017.0821

Unlocking data sets by calibrating populations of models to data density: A study in atrial electrophysiology

Auteurs: Brodie A. J. Lawson, Christopher C. Drovandi, Nicole Cusimano, Pamela Burrage, Blanca Rodriguez, Kevin Burrage
Publié dans: Science Advances, Numéro 4/1, 2018, Page(s) e1701676, ISSN 2375-2548
Éditeur: American Association for the Advancement of Science
DOI: 10.1126/sciadv.1701676

Model for pressure drop and flow deflection in the numerical simulation of stents in aneurysms

Auteurs: Sha Li, Jonas Latt, Bastien Chopard
Publié dans: International Journal for Numerical Methods in Biomedical Engineering, Numéro 34/3, 2018, Page(s) e2949, ISSN 2040-7939
Éditeur: John Wiley & Sons Ltd.
DOI: 10.1002/cnm.2949

Atrial Fibrillation Dynamics and Ionic Block Effects in Six Heterogeneous Human 3D Virtual Atria with Distinct Repolarization Dynamics

Auteurs: Carlos Sánchez, Alfonso Bueno-Orovio, Esther Pueyo, Blanca Rodríguez
Publié dans: Frontiers in Bioengineering and Biotechnology, Numéro 5, 2017, ISSN 2296-4185
Éditeur: Frontiers Research Foundation
DOI: 10.3389/fbioe.2017.00029

In silico evaluation of arrhythmia

Auteurs: Xin Zhou, Alfonso Bueno-Orovio, Blanca Rodriguez
Publié dans: Current Opinion in Physiology, Numéro 1, 2018, Page(s) 95-103, ISSN 2468-8673
Éditeur: Elsevier
DOI: 10.1016/j.cophys.2017.11.003

Rapid and accurate assessment of GPCR-ligand interactions Using the fragment molecular orbital-based density-functional tight-binding method

Auteurs: Inaki Morao, Dmitri G. Fedorov, Roger Robinson, Michelle Southey, Andrea Townsend-Nicholson, Mike J. Bodkin, Alexander Heifetz
Publié dans: Journal of Computational Chemistry, Numéro 38/23, 2017, Page(s) 1987-1990, ISSN 0192-8651
Éditeur: John Wiley & Sons Inc.
DOI: 10.1002/jcc.24850

Modeling Patient-Specific Magnetic Drug Targeting Within the Intracranial Vasculature

Auteurs: Alexander Patronis, Robin A. Richardson, Sebastian Schmieschek, Brian J. N. Wylie, Rupert W. Nash, Peter V. Coveney
Publié dans: Frontiers in Physiology, Numéro 9, 2018, ISSN 1664-042X
Éditeur: Frontiers Research Foundation
DOI: 10.3389/fphys.2018.00331

Rapid, Accurate, Precise, and Reliable Relative Free Energy Prediction Using Ensemble Based Thermodynamic Integration

Auteurs: Agastya P. Bhati, Shunzhou Wan, David W. Wright, Peter V. Coveney
Publié dans: Journal of Chemical Theory and Computation, Numéro 13/1, 2016, Page(s) 210-222, ISSN 1549-9618
Éditeur: American Chemical Society
DOI: 10.1021/acs.jctc.6b00979

Rapid and Reliable Binding Affinity Prediction of Bromodomain Inhibitors: A Computational Study

Auteurs: Shunzhou Wan, Agastya P. Bhati, Stefan J. Zasada, Ian Wall, Darren Green, Paul Bamborough, Peter V. Coveney
Publié dans: Journal of Chemical Theory and Computation, Numéro 13/2, 2017, Page(s) 784-795, ISSN 1549-9618
Éditeur: American Chemical Society
DOI: 10.1021/acs.jctc.6b00794

Multiscale computing in the exascale era

Auteurs: Saad Alowayyed, Derek Groen, Peter V. Coveney, Alfons G. Hoekstra
Publié dans: Journal of Computational Science, Numéro 22, 2017, Page(s) 15-25, ISSN 1877-7503

Éditeur: Elsevier BV
DOI: 10.1016/j.jocs.2017.07.004

Evaluation and Characterization of Trk Kinase Inhibitors for the Treatment of Pain: Reliable Binding Affinity Predictions from Theory and Computation
Auteurs: Shunzhou Wan, Agastya P. Bhati, Sarah Skerratt, Kiyoyuki Omoto, Veerabahu Shanmugasundaram, Sharan K. Bagal, Peter V. Coveney
Publié dans: Journal of Chemical Information and Modeling, Numéro 57/4, 2017, Page(s) 897-909, ISSN 1549-9596
Éditeur: American Chemical Society
DOI: 10.1021/acs.jcim.6b00780

A Comparison of Fully-Coupled 3D In-Stent Restenosis Simulations to In-vivo Data
Auteurs: Pavel S. Zun, Tatiana Anikina, Andrew Svitenkov, Alfons G. Hoekstra
Publié dans: Frontiers in Physiology, Numéro 8, 2017, ISSN 1664-042X
Éditeur: Frontiers Research Foundation
DOI: 10.3389/fphys.2017.00284

Phenotypic variability in LQT3 human induced pluripotent stem cell-derived cardiomyocytes and their response to antiarrhythmic pharmacologic therapy: An in silico approach
Auteurs: Michelangelo Paci, Elisa Passini, Stefano Severi, Jari Hyttinen, Blanca Rodriguez
Publié dans: Heart Rhythm, Numéro 14/11, 2017, Page(s) 1704-1712, ISSN 1547-5271
Éditeur: Elsevier BV
DOI: 10.1016/j.hrthm.2017.07.026

Parameter Estimation of Platelets Deposition: Approximate Bayesian Computation With High Performance Computing
Auteurs: Ritabrata Dutta, Bastien Chopard, Jonas Lätt, Frank Dubois, Karim Zouaoui Boudjeltia, Antonietta Mira
Publié dans: Frontiers in Physiology, Numéro 9, 2018, ISSN 1664-042X
Éditeur: Frontiers Research Foundation
DOI: 10.3389/fphys.2018.01128

Cellular Level In-silico Modeling of Blood Rheology with An Improved Material Model for Red Blood Cells
Auteurs: Gábor Závodszky, Britt van Rooij, Victor Azizi, Alfons Hoekstra
Publié dans: Frontiers in Physiology, Numéro 8, 2017, ISSN 1664-042X
Éditeur: Frontiers Research Foundation
DOI: 10.3389/fphys.2017.00563

β-Adrenergic receptor stimulation inhibits proarrhythmic alternans in postinfarction border zone cardiomyocytes: a computational analysis

Auteurs: Jakub Tomek, Blanca Rodriguez, Gil Bub, Jordi Heijman
Publié dans: American Journal of Physiology-Heart and Circulatory Physiology, Numéro 313/2, 2017, Page(s) H338-H353, ISSN 0363-6135
Éditeur: American Physiological Society
DOI: 10.1152/ajpheart.00094.2017

The Role of Multiscale Protein Dynamics in Antigen Presentation and T Lymphocyte Recognition
Auteurs: R. Charlotte Eccleston, Shunzhou Wan, Neil Dalchau, Peter V. Coveney
Publié dans: Frontiers in Immunology, Numéro 8, 2017, ISSN 1664-3224
Éditeur: Frontiers Research Foundation
DOI: 10.3389/fimmu.2017.00797

Dynamic and Kinetic Elements of μ-Opioid Receptor Functional Selectivity
Auteurs: Abhijeet Kapoor, Gerard Martinez-Rosell, Davide Provasi, Gianni de Fabritiis, Marta Filizola
Publié dans: Scientific Reports, Numéro 7/1, 2017, ISSN 2045-2322
Éditeur: Nature Publishing Group
DOI: 10.1038/s41598-017-11483-8

An Ensemble-Based Protocol for the Computational Prediction of Helix–Helix Interactions in G Protein-Coupled Receptors using Coarse-Grained Molecular Dynamics
Auteurs: Nojood A. Altwaijry, Michael Baron, David W. Wright, Peter V. Coveney, Andrea Townsend-Nicholson
Publié dans: Journal of Chemical Theory and Computation, Numéro 13/5, 2017, Page(s) 2254-2270, ISSN 1549-9618
Éditeur: American Chemical Society
DOI: 10.1021/acs.jctc.6b01246

Host genotype and time dependent antigen presentation of viral peptides: predictions from theory
Auteurs: R. Charlotte Eccleston, Peter V. Coveney, Neil Dalchau
Publié dans: Scientific Reports, Numéro 7/1, 2017, Page(s) 14367, ISSN 2045-2322
Éditeur: Nature Publishing Group
DOI: 10.1038/s41598-017-14415-8

Functional identification of islet cell types by electrophysiological fingerprinting
Auteurs: Linford J. B. Briant, Quan Zhang, Elisa Vergari, Joely A. Kellard, Blanca Rodriguez, Frances M. Ashcroft, Patrik Rorsman
Publié dans: Journal of The Royal Society Interface, Numéro 14/128, 2017, Page(s) 20160999, ISSN 1742-5689
Éditeur: The Royal Society
DOI: 10.1098/rsif.2016.0999

The application of the screen-model based approach for stents in cerebral aneurysms
Auteurs: Sha Li, Jonas Latt, Bastien Chopard
Publié dans: Computers & Fluids, 2018, ISSN 0045-7930
Éditeur: Pergamon Press Ltd.
DOI: 10.1016/j.compfluid.2018.02.007

Predicting Binding Free Energies of PDE2 Inhibitors. The Difficulties of Protein Conformation
Auteurs: Laura Pérez-Benito, Henrik Keränen, Herman van Vlijmen, Gary Tresadern
Publié dans: Scientific Reports, Numéro 8/1, 2018, ISSN 2045-2322
Éditeur: Nature Publishing Group
DOI: 10.1038/s41598-018-23039-5

Load balancing of parallel cell-based blood flow simulations
Auteurs: S. Alowayyed, G. Závodszky, V. Azizi, A.G. Hoekstra
Publié dans: Journal of Computational Science, Numéro 24, 2018, Page(s) 1-7, ISSN 1877-7503
Éditeur: Elsevier BV
DOI: 10.1016/J.JOCS.2017.11.008

Distinct ECG Phenotypes Identified in Hypertrophic Cardiomyopathy Using Machine Learning Associate With Arrhythmic Risk Markers
Auteurs: Aurore Lyon, Rina Ariga, Ana Mincholé, Masliza Mahmod, Elizabeth Ormondroyd, Pablo Laguna, Nando de Freitas, Stefan Neubauer, Hugh Watkins, Blanca Rodriguez
Publié dans: Frontiers in Physiology, Numéro 9, 2018, ISSN 1664-042X
Éditeur: Frontiers Research Foundation
DOI: 10.3389/fphys.2018.00213

Investigating the mechanical response of paediatric bone under bending and torsion using finite element analysis
Auteurs: Zainab Altai, Marco Viceconti, Amaka C. Offiah, Xinshan Li
Publié dans: Biomechanics and Modeling in Mechanobiology, 2018, ISSN 1617-7959
Éditeur: Springer Verlag
DOI: 10.1007/s10237-018-1008-9

Three-dimensional cardiac fibre disorganization as a novel parameter for ventricular arrhythmia stratification after myocardial infarction
Auteurs: Daniel G León, Mariña López-Yunta, José Manuel Alfonso-Almazán, Manuel Marina-Breysse, Jorge G Quintanilla, Javier Sánchez-González, Carlos Galán-Arriola, Francisco Castro-Núñez, Juan José González-Ferrer, Borja Ibáñez, Julián Pérez-Villacastín, Nicasio Pérez-Castellano, Valentín Fuster, José Jalife, Mariano Vázquez, Jazmín Aguado-Sierra, David Filgueiras-Rama

Publié dans: EP Europace, Numéro 21/5, 2019, Page(s) 822-832, ISSN 1099-5129
Éditeur: Oxford University Press
DOI: 10.1093/europace/euy306

Implications of bipolar voltage mapping and magnetic resonance imaging resolution in biventricular scar characterization after myocardial infarction

Auteurs: Mariña López-Yunta, Daniel G León, José Manuel Alfonso-Almazán, Manuel Marina-Breysse, Jorge G Quintanilla, Javier Sánchez-González, Carlos Galán-Arriola, Victoria Cañadas-Godoy, Daniel Enríquez-Vázquez, Carlos Torres, Borja Ibáñez, Julián Pérez-Villacastín, Nicasio Pérez-Castellano, José Jalife, Mariano Vázquez, Jazmín Aguado-Sierra, David Filgueiras-Rama
Publié dans: EP Europace, Numéro 21/1, 2018, Page(s) 163-174, ISSN 1099-5129
Éditeur: Oxford University Press
DOI: 10.1093/europace/euy192

LigVoxel: inpainting binding pockets using 3D-convolutional neural networks

Auteurs: Miha Skalic, Alejandro Varela-Rial, José Jiménez, Gerard Martínez-Rosell, Gianni De Fabritiis
Publié dans: Bioinformatics, Numéro 35/2, 2018, Page(s) 243-250, ISSN 1367-4803
Éditeur: Oxford University Press
DOI: 10.1093/bioinformatics/bty583

Bridging the computational gap between mesoscopic and continuum modeling of red blood cells for fully resolved blood flow

Auteurs: Christos Kotsalos, Jonas Latt, Bastien Chopard
Publié dans: Journal of Computational Physics, Numéro 398, 2019, Page(s) 108905, ISSN 0021-9991
Éditeur: Academic Press
DOI: 10.1016/j.jcp.2019.108905

Strategies of data layout and cache writing for input-output optimization in high performance scientific computing: Applications to the forward electrocardiographic problem

Auteurs: Louie Cardone-Noott, Blanca Rodriguez, Alfonso Bueno-Orovio
Publié dans: PLOS ONE, Numéro 13/8, 2018, Page(s) e0202410, ISSN 1932-6203
Éditeur: Public Library of Science
DOI: 10.1371/journal.pone.0202410

K DEEP : Protein–Ligand Absolute Binding Affinity Prediction via 3D-Convolutional Neural Networks

Auteurs: José Jiménez, Miha Škalič, Gerard Martínez-Rosell, Gianni De Fabritiis
Publié dans: Journal of Chemical Information and Modeling, Numéro 58/2, 2018, Page(s) 287-296, ISSN 1549-9596
Éditeur: American Chemical Society
DOI: 10.1021/acs.jcim.7b00650

Nasal sprayed particle deposition in a human nasal cavity under different inhalation conditions
Auteurs: Hadrien Calmet, Kiao Inthavong, Beatriz Eguzkitza, Oriol Lehmkuhl, Guillaume Houzeaux, Mariano Vázquez
Publié dans: PLOS ONE, Numéro 14/9, 2019, Page(s) e0221330, ISSN 1932-6203
Éditeur: Public Library of Science
DOI: 10.1371/journal.pone.0221330

Application of ESMACS binding free energy protocols to diverse datasets: Bromodomain-containing protein 4
Auteurs: David W. Wright, Shunzhou Wan, Christophe Meyer, Herman van Vlijmen, Gary Tresadern, Peter V. Coveney
Publié dans: Scientific Reports, Numéro 9/1, 2019, ISSN 2045-2322
Éditeur: Nature Publishing Group
DOI: 10.1038/s41598-019-41758-1

Simulations meet machine learning in structural biology
Auteurs: Adrià Pérez, Gerard Martínez-Rosell, Gianni De Fabritiis
Publié dans: Current Opinion in Structural Biology, Numéro 49, 2018, Page(s) 139-144, ISSN 0959-440X
Éditeur: Elsevier BV
DOI: 10.1016/j.sbi.2018.02.004

Complex Congenital Heart Disease Associated With Disordered Myocardial Architecture in a Midtrimester Human Fetus
Auteurs: Patricia Garcia-Canadilla, Hector Dejea, Anne Bonnin, Vedrana Balicevic, Sven Loncaric, Chong Zhang, Constantine Butakoff, Jazmin Aguado-Sierra, Mariano Vázquez, Laurence H. Jackson, Daniel J. Stuckey, Cristoph Rau, Marco Stampanoni, Bart Bijnens, Andrew C. Cook
Publié dans: Circulation: Cardiovascular Imaging, Numéro 11/10, 2018, ISSN 1941-9651
Éditeur: Lippincott Williams & Wilkins Ltd.
DOI: 10.1161/circimaging.118.007753

Big data: the end of the scientific method?
Auteurs: Sauro Succi, Peter V. Coveney
Publié dans: Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, Numéro 377/2142, 2019, Page(s)

20180145, ISSN 1364-503X
Éditeur: Royal Society of London
DOI: 10.1098/rsta.2018.0145

A Mechanistic Model for Predicting Cell Surface Presentation of Competing Peptides by MHC Class I Molecules
Auteurs: Denise S. M. Boulanger, Ruth C. Eccleston, Andrew Phillips, Peter V. Coveney, Tim Elliott, Neil Dalchau
Publié dans: Frontiers in Immunology, Numéro 9, 2018, ISSN 1664-3224
Éditeur: Frontiers Research Foundation
DOI: 10.3389/fimmu.2018.01538

Patterns for High Performance Multiscale Computing
Auteurs: S. Alowayyed, T. Piontek, J.L. Suter, O. Hoenen, D. Groen, O. Luk, B. Bosak, P. Kopta, K. Kurowski, O. Perks, K. Brabazon, V. Jancauskas, D. Coster, P.V. Coveney, A.G. Hoekstra
Publié dans: Future Generation Computer Systems, Numéro 91, 2019, Page(s) 335-346, ISSN 0167-739X
Éditeur: Elsevier BV
DOI: 10.1016/j.future.2018.08.045

A modeling and machine learning approach to ECG feature engineering for the detection of ischemia using pseudo-ECG
Auteurs: Carlos A. Ledezma, Xin Zhou, Blanca Rodríguez, P. J. Tan, Vanessa Díaz-Zuccarini
Publié dans: PLOS ONE, Numéro 14/8, 2019, Page(s) e0220294, ISSN 1932-6203
Éditeur: Public Library of Science
DOI: 10.1371/journal.pone.0220294

Are CT-Based Finite Element Model Predictions of Femoral Bone Strengthening Clinically Useful?
Auteurs: Marco Viceconti, Muhammad Qasim, Pinaki Bhattacharya, Xinshan Li
Publié dans: Current Osteoporosis Reports, Numéro 16/3, 2018, Page(s) 216-223, ISSN 1544-1873
Éditeur: Current Science Inc.
DOI: 10.1007/s11914-018-0438-8

Left Ventricular Trabeculations Decrease the Wall Shear Stress and Increase the Intra-Ventricular Pressure Drop in CFD Simulations
Auteurs: Federica Sacco, Bruno Paun, Oriol Lehmkuhl, Tinen L. Iles, Paul A. Iaizzo, Guillaume Houzeaux, Mariano Vázquez, Constantine Butakoff, Jazmin Aguado-Sierra
Publié dans: Frontiers in Physiology, Numéro 9, 2018, ISSN 1664-042X

Éditeur: Frontiers Research Foundation
DOI: 10.3389/fphys.2018.00458

Modelling variability in cardiac electrophysiology: a moment-matching approach
Auteurs: Eliott Tixier, Damiano Lombardi, Blanca Rodriguez, Jean-Frédéric Gerbeau
Publié dans: Journal of The Royal Society Interface, Numéro 14/133, 2017, Page(s) 20170238, ISSN 1742-5689
Éditeur: The Royal Society
DOI: 10.1098/rsif.2017.0238

Validation of Patient-Specific Cerebral Blood Flow Simulation Using Transcranial Doppler Measurements
Auteurs: Derek Groen, Robin A. Richardson, Rachel Coy, Ulf D. Schiller, Hoskote Chandrashekar, Fergus Robertson, Peter V. Coveney
Publié dans: Frontiers in Physiology, Numéro 9, 2018, ISSN 1664-042X
Éditeur: Frontiers Research Foundation
DOI: 10.3389/fphys.2018.00721

High-throughput binding affinity calculations at extreme scales
Auteurs: Jumana Dakka, Matteo Turilli, David W. Wright, Stefan J. Zasada, Vivek Balasubramanian, Shunzhou Wan, Peter V. Coveney, Shantenu Jha
Publié dans: BMC Bioinformatics, Numéro 19/S18, 2018, ISSN 1471-2105
Éditeur: BioMed Central
DOI: 10.1186/s12859-018-2506-6

Uncertainty Quantification in Alchemical Free Energy Methods
Auteurs: Agastya P. Bhati, Shunzhou Wan, Yuan Hu, Brad Sherborne, Peter V. Coveney
Publié dans: Journal of Chemical Theory and Computation, Numéro 14/6, 2018, Page(s) 2867-2880, ISSN 1549-9618
Éditeur: American Chemical Society
DOI: 10.1021/acs.jctc.7b01143

Machine Learning of Coarse-Grained Molecular Dynamics Force Fields
Auteurs: Jiang Wang, Simon Olsson, Christoph Wehmeyer, Adrià Pérez, Nicholas E. Charron, Gianni de Fabritiis, Frank Noé, Cecilia Clementi
Publié dans: ACS Central Science, 2019, ISSN 2374-7943
Éditeur: American Chemical Society
DOI: 10.1021/acscentsci.8b00913

δ-cells and β-cells are electrically coupled and regulate α-cell activity via somatostatin
Auteurs: L. J. B. Briant, T. M. Reinbothe, I. Spiliotis, C. Miranda, B. Rodriguez, P. Rorsman

Publié dans: The Journal of Physiology, Numéro 596/2, 2018, Page(s) 197-215, ISSN 0022-3751
Éditeur: Blackwell Publishing Inc.
DOI: 10.1113/JP274581

Human In Silico Drug Trials Demonstrate Higher Accuracy than Animal Models in Predicting Clinical Pro-Arrhythmic Cardiotoxicity

Auteurs: Elisa Passini, Oliver J. Britton, Hua Rong Lu, Jutta Rohrbacher, An N. Hermans, David J. Gallacher, Robert J. H. Greig, Alfonso Bueno-Orovio, Blanca Rodriguez
Publié dans: Frontiers in Physiology, Numéro 8, 2017, ISSN 1664-042X
Éditeur: Frontiers Research Foundation
DOI: 10.3389/fphys.2017.00668

PolNet: A Tool to Quantify Network-Level Cell Polarity and Blood Flow in Vascular Remodeling

Auteurs: Miguel O. Bernabeu, Martin L. Jones, Rupert W. Nash, Anna Pezzarossa, Peter V. Coveney, Holger Gerhardt, Claudio A. Franco
Publié dans: Biophysical Journal, Numéro 114/9, 2018, Page(s) 2052-2058, ISSN 0006-3495
Éditeur: Biophysical Society
DOI: 10.1016/j.bpj.2018.03.032

Influence of fiber connectivity in simulations of cardiac biomechanics

Auteurs: D Gil, R Aris, A Borras, E Ramirez, R Sebastian, M Vazquez
Publié dans: International Journal of Computer Assisted Radiology and Surgery, Numéro 14/1, 2019, Page(s) 63-72, ISSN 1861-6410
Éditeur: Springer Verlag
DOI: 10.1007/s11548-018-1849-9

Ensemble-Based Replica Exchange Alchemical Free Energy Methods: The Effect of Protein Mutations on Inhibitor Binding

Auteurs: Agastya P. Bhati, Shunzhou Wan, Peter V. Coveney
Publié dans: Journal of Chemical Theory and Computation, Numéro 15/2, 2018, Page(s) 1265-1277, ISSN 1549-9618
Éditeur: American Chemical Society
DOI: 10.1021/acs.jctc.8b01118

Fully coupled fluid-electro-mechanical model of the human heart for supercomputers

Auteurs: Alfonso Santiago, Jazmín Aguado-Sierra, Miguel Zavala-Aké, Ruben Doste-Beltran, Samuel Gómez, Ruth Arís, Juan C. Cajas, Eva Casoni, Mariano Vázquez
Publié dans: International Journal for Numerical Methods in Biomedical Engineering, Numéro 34/12, 2018, Page(s) e3140, ISSN 2040-7939

Éditeur: John Wiley & Sons Ltd.
DOI: 10.1002/cnm.3140

PlayMolecule BindScope: large scale CNN-based virtual screening on the web
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Auteurs: B. Czaja, G. Závodszky, V. Azizi Tarksalooyeh, A. G. Hoekstra
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Inflow and outflow boundary conditions for 2D suspension simulations with the immersed boundary lattice Boltzmann method
Auteurs: Victor W. Azizi Tarksalooyeh, Gábor Závodszky, Britt J. M. van Rooij, Alfons G. Hoekstra
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Auteurs: Anna Nikishova, Lourens Veen, Pavel Zun, Alfons G. Hoekstra
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Auteurs: Federica Sacco, Bruno Paun, Oriol Lehmkuhl, Tinen L. Iles, Paul A. Iaizzo, Guillaume Houzeaux, Mariano Vázquez, Constantine Butakoff, Jazmin Aguado-Sierra
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Mechanisms Underlying Allosteric Molecular Switches of Metabotropic Glutamate Receptor 5
Auteurs: Claudia Llinas del Torrent, Nil Casajuana-Martin, Leonardo Pardo, Gary Tresadern, Laura Pérez-Benito
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Auteurs: Jakub Tomek, Guoliang Hao, Markéta Tomková, Andrew Lewis, Carolyn Carr, David J. Paterson, Blanca Rodriguez, Gil Bub, Neil Herring
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Auteurs: Philipp Berg, Samuel Voß, Gábor Janiga, Sylvia Saalfeld, Aslak W. Bergersen, Kristian Valen-Sendstad, Jan Bruening, Leonid Goubergrits, Andreas Spuler, Tin Lok Chiu, Anderson Chun On Tsang, Gabriele Copelli, Benjamin Csippa, György Paál, Gábor Závodszky, Felicitas J. Detmer, Bong J. Chung, Juan R. Cebral, Soichiro Fujimura, Hiroyuki Takao, Christof Karmonik, Saba Elias, Nicole M. Cancelliere
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Éditeur: American Institute of Physics
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Autres (5)

Rapid, concurrent and adaptive extreme scale binding free energy calculation

Auteurs: Dakka, Jumana; Farkas-Pall, Kristof; Balasubramanian, Vivek; Turilli, Matteo; Wright, David W; Wan, Shunzhou; Zasada, Stefan; Coveney, Peter V; Jha, Shantenu
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High-throughput Binding Affinity Calculations at Extreme Scales

Auteurs: Dakka, Jumana; Turilli, Matteo; Wright, David W; Zasada, Stefan J; Balasubramanian, Vivek; Wan, Shunzhou; Coveney, Peter V; Jha, Shantenu
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Auteurs: Galvelis, Raimondas; Doerr, Stefan; Damas, Joao M.; Harvey, Matt J.; De Fabritiis, Gianni
Publié dans: Numéro 2, 2019
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Auteurs: P.V. Coveney and R. Highfield
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Éditeur: Institute and Faculty of Actuaries

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Auteurs: Alexander Heifetz, Michelle Southey, Inaki Morao, Andrea Townsend-Nicholson, Mike J. Bodkin
Publié dans: Methods in Molecular Biology, 2017, Page(s) 375-394
Éditeur: Springer New York
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Auteurs: Andrew Potterton, Alexander Heifetz, Andrea Townsend-Nicholson
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Understanding Malaria Induced Red Blood Cell Deformation Using Data-Driven Lattice Boltzmann Simulations

Auteurs: Joey Sing Yee Tan, Gábor Závodszky, Peter M. A. Sloot
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DOI: 10.1007/978-3-319-93698-7_30

Optimizing Parallel Performance of the Cell Based Blood Flow Simulation Software HemoCell

Auteurs: Victor Azizi Tarksalooyeh, Gábor Závodszky, Alfons G. Hoekstra
Publié dans: Computational Science – ICCS 2019 - 19th International Conference, Faro, Portugal, June 12–14, 2019, Proceedings, Part III, Numéro 11538, 2019, Page(s) 537-547, ISBN 978-3-030-22743-2
Éditeur: Springer International Publishing
DOI: 10.1007/978-3-030-22744-9_42

Actes de conférence (1)

Concurrent and Adaptive Extreme Scale Binding Free Energy Calculations

Auteurs: Jumana Dakka, Kristof Farkas-Pall, Matteo Turilli, David W. Wright, Peter V. Coveney, Shantenu Jha
Publié dans: 2018 IEEE 14th International Conference on e-Science (e-Science), 2018, Page(s) 189-200, ISBN 978-1-5386-9156-4

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Ensemble de données

Ensemble de données via OpenAIRE (16)

Scalasca summary analysis of HemeLB application execution with 13824 MPI processes on SuperMUC-NG
Auteurs: Brian J. N. Wylie
Publié dans: Zenodo

Scalasca summary analysis of HemeLB application execution with 300000 MPI processes on SuperMUC-NG
Auteurs: Brian J. N. Wylie
Publié dans: Zenodo

Scalasca trace analysis of HemeLB application execution with 13824 MPI processes on SuperMUC-NG
Auteurs: Brian J. N. Wylie
Publié dans: Zenodo

Data for the paper "Humeral Fractures in Non-Ambulant Infants: CT-Based Finite Element Investigation Indicates an Unlikely Mechanism "
Auteurs: Tai, Zainab Al; Viceconti, Marco; Xinshan Li; Amaka Offiah
Publié dans: The University of Sheffield

Scalasca summary analysis of HemeLB_GPU application execution with 129 MPI processes on JUWELS/V100
Auteurs: Wylie, Brian J. N.
Publié dans: Zenodo

The effect of stiffened diabetic red blood cells on wall shear stress in a reconstructed 3D microaneurysm
Auteurs: Czaja, Benjamin; de Bouter, Jonathan; Heisler, Morgan; Závodszky, Gábor; Karst, Sonja; Sarunic, Marinko; Maberley, David; Hoekstra, Alfons; Sarunic, Marinko
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Data for the paper "The effect of boundary constraints on patient classification using finite element predicted risk of fracture "
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Publié dans: The University of Sheffield

Data for the paper "Investigating the mechanical response of paediatric bone under bending and torsion using finite element analysis"
Auteurs: Tai, Zainab Al; Viceconti, Marco; Amaka Offiah; Xinshan Li
Publié dans: The University of Sheffield

Supplementary Information for "Parametric Analysis of an Efficient Boundary Condition to Control Outlet Flow Rates in Large Arterial Networks"
Auteurs: Lo, Sharp C. Y.; McCullough, Jon; Coveney, Peter
Publié dans: University College London

Development and performance of a HemeLB GPU code for human-scale blood flow simulation
Auteurs: John Ballantyne
Publié dans: Mendeley

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Voir les 16 résultats

Logiciel

Logiciel via OpenAIRE (2)

UCL-CCS/brd4-diverse-esmacs: submission-version
Auteurs: Wright, David W
Éditeur: Zenodo
DOI: 10.5281/zenodo.1484050; 10.5281/zenodo.1484049

PolNet
Auteurs: Bernabeu, Miguel O.
Éditeur: bio.tools

Autres produits de recherche

Autres produits de recherche via OpenAire (5)

Exascale Potholes for HPC: Execution Performance and Variability Analysis of the Flagship Application Code HemeLB
Auteurs: Brian J. N. Wylie
Publié dans: Zenodo

Movie microcontraction simulation from Identifying the start of a platelet aggregate by the shear rate and the cell-depleted layer
Auteurs: B.J.M. Van Rooij; G. Závodszky; V.W. Azizi Tarksalooyeh; A.G. Hoekstra
Publié dans: The Royal Society

Analysis report examination with Cube
Auteurs: Brian J. N. Wylie
Publié dans: Zenodo

Supplementary Figures
Auteurs: Lo, Sharp C. Y.; McCullough, Jon; Coveney, Peter
Publié dans: University College London

Concurrent and Adaptive Extreme Scale Binding Free Energy Calculations
Auteurs: Dakka, J; Farkas-Pall, K; Turilli, M; Wright, DW; Coveney, PV; Jha, S

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