Computing Patterns for High Performance Multiscale Computing

Results

Project Information

ComPat

Grant agreement ID: 671564

Project website

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10.3030/671564

Project closed

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24 June 2015

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1 October 2015

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30 September 2018

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€ 4 122 864,36

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€ 3 942 885,00

Coordinated by
UNIVERSITEIT VAN AMSTERDAM
Netherlands

CORDIS provides links to public deliverables and publications of HORIZON projects.

Links to deliverables and publications from FP7 projects, as well as links to some specific result types such as dataset and software, are dynamically retrieved from OpenAIRE.

Deliverables

Documents, reports (21)

Interim Report on Instantiating Computing Patterns for HPMC Applications

Interim report about our progress in employing multiscale computing patterns in actual scientific applications. It will contain an assessment of the efficacy of the patterns as well as recommendations and best practices for their instantiation.

Report on Application Software Readiness

Report the specific requirements of the applications as identified during Task 3.1.

Quality Assurance Plan

To manage and support the project Quality Control, a documented Quality Assurance Plan will be set up and maintained to monitor all deliverables before finalising them. The deliverable also contains a detailed risk analysis and contingency planning.

First Dissemination Report

Review events and dissemination results of past year and proposes actions for the coming one, including update of dissemination action plan.

First progress report on the Experimental Execution Environment

This deliverable will present the progress in the installation, configuration, and usage of the Experimental Execution Environment. This deliverable will also include the first version of the ComPat Experimental Execution Environment user guide.

Report on integration of ComPat services with multiscale coupling libraries and patterns

A document describing the final integration of ComPat services with multiscale coupling libraries and patterns including references to ComPat applications executed on the ComPat Pan-European Experimental Execution Environment.

Report and software on design of tools and required actions to support performance tools for multiscale

Report on an analyses of the requirements for the tools (debug, profile and analyse performance) and design and architecture of a solution appropriate to support the multiscale patterns.

Architecture of the ComPat system

A document describing the overall architecture of the ComPat system including relationships between developed in the project toolkits and services.

Report on Existing Software Suitability and Adaptation

Report on what software will be used in the project, how it compares to other software packages, and outline a detailed plan for their adaptation and

integration, as well as report on MML implementation and status report on implementation of the multiscale computing patterns.

Final report on the Experimental Execution Environment
An update of deliverable D6.3.

Final report on high level tools, including performance profiling and modelling
Report on the status of the tools, and on the validation of the impact of measurement and analysis on the applications – and on the accuracy of the modelling tools as applied to simulations at the scales of machines available during the latter months of the project.

Report on the assessment of operational procedures and definition of the ComPat operational model

Report on Instantiating Computing Patterns and performance measurements and prediction of HPMC Application
Report on the performance of all selected multiscale applications as measured on the Experimental Execution Environment and other available resources. It will give a detailed account of various metrics of resource usage, including wall clock time, data throughput, scalability and energy consumption. It will furnish detailed performance predictions for all selected multiscale applications on future exascale systems. This report will, as a major outcome of this project, present a forecast of the actual impact that exascale resources may have on future science applications by leveraging extreme parallelism.

Final Report on Multiscale Computing Patterns, including their Performance
Final report on the performance of all selected multiscale applications as measured on the Experimental Execution Environment and selected production environments. It will give a detailed account of various metrics of resource usage, including wall clock time, data throughput, scalability and energy consumption. It will also provide a detailed account on the performance prediction models.

First Report on Multiscale Computing Patterns and Algorithms
First report on the algorithms and components used to construct the Multiscale Computing Patterns, details of the actual implementation, and preliminary results on performance measurements.

First Report on status of performance profiling of multiscale simulations
First report on an analysis of the changes and impact on the initial simulations using the initial tools, including any architectural changes required since D4.1.

First Report on ComPat middleware services

A document summarizing the status of development of services offering a set of key capabilities for toolkits and patterns from WP2, including QoS on computational Tier-0/1 resources, dynamic multi-cluster co-allocation of resources, energy optimization and multi-cluster deployment and execution of ComPat multiscale simulations consisting of cooperating sub-models.

Third Dissemination Report
Review events and dissemination results of second project period.

Second Dissemination Report
Review events and dissemination results and propose actions for the coming one, including update of dissemination action plan.

Detailed Dissemination Action plan

Project Handbook
To ensure a consistent implementation of the management of the project, UvA will produce a project procedure handbook that will be easily accessible to all Partners.

Publications

Other (12)

High-throughput Binding Affinity Calculations at Extreme Scales
Author(s): Dakka, Jumana; Turilli, Matteo; Wright, David W; Zasada, Stefan J; Balasubramanian, Vivek; Wan, Shunzhou; Coveney, Peter V; Jha, Shantenu
Published in: BioMed Central, Issue 1, 2018
Publisher: Springer Nature

Multiscale Computing for Science and Engineering in the Era of Exascale Performance
Author(s): A. G. Hoekstra, B. Chopard, D. Coster, S. Portegies Zwar, P. V. Coveney
Published in: 2018
Publisher: The Royal Society Publishing
DOI: 10.1098/rsta.2018.0144

The heterogeneous multiscale method applied to inelastic polymer mechanics
Author(s): M. Vassaux, R. Richardson, P. V. Coveney
Published in: 2018

Publisher: The Royal Society Publishing
DOI: 10.1098/rsta.2018.0150

Application of the Extreme Scaling Computing Pattern on Multiscale Fusion Plasma Modelling
Author(s): O. O. Luk, O. Hoenen, O. Perks, K. Brabazon, T. Piontek, P. Kopta, B. Bosak, A. Bottino, B. D. Scott, D. P. Coster
Published in: 2018
Publisher: The Royal Society
DOI: 10.1098/rsta.2018.0152

ComPat Framework for Multiscale Simulations Applied to Fusion Plasmas
Author(s): O. Luk, O. Hoenen, A. Bottino, B. Scott, D. Coster
Published in: Computer Physics Communications, 2018
Publisher: Elsevier

Load Balancing Massively Parallel Cell-based Blood Flow Simulations
Author(s): S. Alowayyed, V. Azizi, G. Zavodszky and A. G. Hoekstra
Published in: Computer Physics Communications, 2018
Publisher: Elsevier

Predicting Queue Wait Time Probabilities for Multi-Scale Computing
Author(s): V. Jancauskas, T. Piontek, P. Kopta, B. Bosak
Published in: Philosophical Transactions of the Royal Society, 2018
Publisher: The Royal Society

Development of a multiscale simulation approach for forced migration
Author(s): D. Groen
Published in: ICCS 2018, Springer Lecture Notes in Computer Science (LNCS), 2018
Publisher: Springer

Modelling Refugees Escaping Violent Events: A Feasibility Study From An Input Data Perspective
Author(s): N. T. Chan, D. Suleimenova, D. Bell, D. Groen
Published in: Proceedings of the Operational Research Society Simulation Workshop 2018, 2018
Publisher: The Operational Research Society

Big Data: the End of the Scientific Method?
Author(s): Sauro Succi, Peter V. Coveney
Published in: Phil Trans R Soc (Series A), 2018
Publisher: The Royal Society
DOI: 10.1098/rsta.2018.0145

A Distributed Multi-agent Market Place for HPC Compute Cycle Resource Trading”

Author(s): S. J. Zasada and P. V. Coveney
Published in: CoRR, 2015
Publisher: Cornell University Library

Mastering the scales: A survey on the benefits of multiscale computing software
Author(s): D. Groen, J. Knap, P. Neumann, D. Suleimenova, L. Veen, K. Leiter
Published in: Philosophical Transactions A: Mathematical, Physical and Engineering Sciences, 2018
Publisher: The Royal Society
DOI: 10.1098/rsta.2018.0147

Peer reviewed articles (33)

SiMon: Simulation Monitor for Computational Astrophysics
Author(s): Penny Xuran Qian, Maxwell Xu Cai, Simon Portegies Zwart, Ming Zhu
Published in: Publications of the Astronomical Society of the Pacific, Issue 129/979, 2017, Page(s) 094503, ISSN 0004-6280
Publisher: University of Chicago Press
DOI: 10.1088/1538-3873/aa7c49

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

The Role of Multiscale Protein Dynamics in Antigen Presentation and T Lymphocyte Recognition
Author(s): R. Charlotte Eccleston, Shunzhou Wan, Neil Dalchau, Peter V. Coveney
Published in: Frontiers in Immunology, Issue 8, 2017, ISSN 1664-3224
Publisher: Frontiers
DOI: 10.3389/fimmu.2017.00797

Cellular Level In-silico Modeling of Blood Rheology with An Improved Material Model for Red Blood Cells
Author(s): Gábor Závodszky, Britt van Rooij, Victor Azizi, Alfons Hoekstra
Published in: Frontiers in Physiology, Issue 8, 2017, Page(s) 563, ISSN 1664-042X

Publisher: Frontiers Research Foundation
DOI: 10.3389/fphys.2017.00563

Validation of Patient-Specific Cerebral Blood Flow Simulation Using Transcranial Doppler Measurements

Author(s): Derek Groen, Robin A. Richardson, Rachel Coy, Ulf D. Schiller, Hoskote Chandrashekar, Fergus Robertson, Peter V. Coveney
Published in: Frontiers in Physiology, Issue 9, 2018, ISSN 1664-042X
Publisher: Frontiers Research Foundation
DOI: 10.3389/fphys.2018.00721

Load balancing of parallel cell-based blood flow simulations

Author(s): S. Alowayyed, G. Závodszky, V. Azizi, A.G. Hoekstra
Published in: Journal of Computational Science, Issue 24, 2018, Page(s) 1-7, ISSN 1877-7503
Publisher: Elsevier BV
DOI: 10.1016/j.jocs.2017.11.008

Stability of exomoons around the Kepler transiting circumbinary planets

Author(s): Adrian S Hamers, Maxwell X Cai, Javier Roa, Nathan Leigh
Published in: Monthly Notices of the Royal Astronomical Society, Issue 480/3, 2018, Page(s) 3800-3811, ISSN 0035-8711
Publisher: Blackwell Publishing Inc.
DOI: 10.1093/mnras/sty2117

Multiscale computing in the exascale era

Author(s): Saad Alowayyed, Derek Groen, Peter V. Coveney, Alfons G. Hoekstra
Published in: Journal of Computational Science, Issue 22, 2017, Page(s) 15-25, ISSN 1877-7503
Publisher: Elsevier BV
DOI: 10.1016/j.jocs.2017.07.004

Graphene-Graphene Interactions: Friction, Superlubricity, and Exfoliation

Author(s): Robert C. Sinclair, James L. Suter, Peter V. Coveney
Published in: Advanced Materials, Issue 30/13, 2018, Page(s) 1705791, ISSN 0935-9648
Publisher: United Nations Industrial Developement Organization
DOI: 10.1002/adma.201705791

The Oceanographic Multipurpose Software Environment (OMUSE v1.0)

Author(s): Inti Pelupessy, Ben van Werkhoven, Arjen van Elteren, Jan Viebahn, Adam Candy, Simon Portegies Zwart, Henk Dijkstra
Published in: Geoscientific Model Development, Issue 10/8, 2017, Page(s)

3167-3187, ISSN 1991-9603
Publisher: Copernicus Publications
DOI: 10.5194/gmd-10-3167-2017

Numerical verification of the microscopic time reversibility of Newton's equations of motion: Fighting exponential divergence
Author(s): Simon F. Portegies Zwart, Tjarda C.N. Boekholt
Published in: Communications in Nonlinear Science and Numerical Simulation, Issue 61, 2018, Page(s) 160-166, ISSN 1007-5704
Publisher: Elsevier BV
DOI: 10.1016/j.cnsns.2018.02.002

Chemically Specific Multiscale Modeling of the Shear-Induced Exfoliation of Clay–Polymer Nanocomposites
Author(s): James L. Suter, Peter V. Coveney
Published in: ACS Omega, Issue 3/6, 2018, Page(s) 6439-6445, ISSN 2470-1343
Publisher: ACS
DOI: 10.1021/acsomega.8b00542

A Comparison of Fully-Coupled 3D In-Stent Restenosis Simulations to In-vivo Data
Author(s): Pavel S. Zun, Tatiana Anikina, Andrew Svitenkov, Alfons G. Hoekstra
Published in: Frontiers in Physiology, Issue 8, 2017, ISSN 1664-042X
Publisher: Frontiers Research Foundation
DOI: 10.3389/fphys.2017.00284

The signatures of the parental cluster on field planetary systems
Author(s): Maxwell Xu Cai, Simon Portegies Zwart, Arjen van Elteren
Published in: Monthly Notices of the Royal Astronomical Society, Issue 474/4, 2017, Page(s) 5114-5121, ISSN 0035-8711
Publisher: Blackwell Publishing Inc.
DOI: 10.1093/mnras/stx3064

The dynamics of stellar discs in live dark-matter haloes
Author(s): M S Fujii, J Bédorf, J Baba, S Portegies Zwart
Published in: Monthly Notices of the Royal Astronomical Society, Issue 477/2, 2018, Page(s) 1451-1471, ISSN 0035-8711
Publisher: Blackwell Publishing Inc.
DOI: 10.1093/mnras/sty711

PolNet: A Tool to Quantify Network-Level Cell Polarity and Blood Flow in Vascular Remodeling
Author(s): Miguel O. Bernabeu, Martin L. Jones, Rupert W. Nash, Anna Pezzarossa, Peter V. Coveney, Holger Gerhardt, Claudio A. Franco
Published in: Biophysical Journal, Issue 114/9, 2018, Page(s) 2052-2058,

ISSN 0006-3495
Publisher: Biophysical Society
DOI: 10.1016/j.bpj.2018.03.032

The Oceanographic Multipurpose Software Environment
Author(s): Inti Pelupessy, Ben van Werkhoven, Arjen van Elteren, Jan Viebahn, Adam Candy, Simon Portegies Zwart, Henk Dijkstra
Published in: Geoscientific Model Development Discussions, 2016, Page(s) 1-36, ISSN 1991-962X
Publisher: EGU
DOI: 10.5194/gmd-2016-178

Stability of multiplanetary systems in star clusters
Author(s): Maxwell Xu Cai (□□), M. B. N. Kouwenhoven, Simon F. Portegies Zwart, Rainer Spurzem
Published in: Monthly Notices of the Royal Astronomical Society, Issue 470/4, 2017, Page(s) 4337-4353, ISSN 0035-8711
Publisher: Blackwell Publishing Inc.
DOI: 10.1093/mnras/stx1464

Simulations of stripped core-collapse supernovae in close binaries
Author(s): Alex Rimoldi, Simon Portegies Zwart, Elena Maria Rossi
Published in: Computational Astrophysics and Cosmology, Issue 3/1, 2016, ISSN 2197-7909
Publisher: Springer
DOI: 10.1186/s40668-016-0015-4

Hemocell: a high-performance microscopic cellular library
Author(s): Gábor Zavodszky, Britt van Rooij, Victor Azizi, Saad Alowayyed, Alfons Hoekstra
Published in: Procedia Computer Science, Issue 108, 2017, Page(s) 159-165, ISSN 1877-0509
Publisher: Elsevier
DOI: 10.1016/j.procs.2017.05.084

The evolution of hierarchical triple star-systems
Author(s): Silvia Toonen, Adrian Hamers, Simon Portegies Zwart
Published in: Computational Astrophysics and Cosmology, Issue 3/1, 2016, ISSN 2197-7909
Publisher: Springer
DOI: 10.1186/s40668-016-0019-0

On the calculation of equilibrium thermodynamic properties from molecular dynamics

Author(s): Peter V. Coveney, Shunzhou Wan
Published in: Physical Chemistry Chemical Physics, Issue 18/44, 2016, Page(s) 30236-30240, ISSN 1463-9076
Publisher: Royal Society of Chemistry
DOI: 10.1039/c6cp02349e

Uncertainty Quantification of a Multiscale Model for In-Stent Restenosis
Author(s): Anna Nikishova, Lourens Veen, Pavel Zun, Alfons G. Hoekstra
Published in: Cardiovascular Engineering and Technology, 2018, ISSN 1869-408X
Publisher: Springer Pub. Co.,
DOI: 10.1007/s13239-018-00372-4

The origin of interstellar asteroidal objects like 1I/2017 U1 'Oumuamua
Author(s): Simon Portegies Zwart, Santiago Torres, Inti Pelupessy, Jeroen Bédorf, Maxwell X Cai
Published in: Monthly Notices of the Royal Astronomical Society: Letters, Issue 479/1, 2018, Page(s) L17-L22, ISSN 1745-3933
Publisher: Blackwell Publishing
DOI: 10.1093/mnrasl/sly088

Multiscale modeling: recent progress and open questions
Author(s): Bastien Chopard, Jean-Luc Falcone, Pierre Kunzli, Lourens Veen, Alfons Hoekstra
Published in: Multiscale and Multidisciplinary Modeling, Experiments and Design, Issue 1/1, 2018, Page(s) 57-68, ISSN 2520-8160
Publisher: Springer
DOI: 10.1007/s41939-017-0006-4

Patterns for High Performance Multiscale Computing
Author(s): 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
Published in: Future Generation Computer Systems, Issue 91, 2019, Page(s) 335-346, ISSN 0167-739X
Publisher: Elsevier BV
DOI: 10.1016/j.future.2018.08.045

Towards the virtual artery: a multiscale model for vascular physiology at the physics–chemistry–biology interface
Author(s): Alfons G. Hoekstra, Saad Alowayyed, Eric Lorenz, Natalia Melnikova, Lampros Mountrakis, Britt van Rooij, Andrew Svitenkov, Gábor Závodszky, Pavel Zun
Published in: Philosophical Transactions of the Royal Society A: Mathematical,

Physical and Engineering Sciences, Issue 374/2080, 2016, Page(s) 20160146, ISSN 1364-503X
Publisher: Royal Society of London
DOI: 10.1098/rsta.2016.0146

Rapid and Reliable Binding Affinity Prediction of Bromodomain Inhibitors: A Computational Study
Author(s): Shunzhou Wan, Agastya P. Bhati, Stefan J. Zasada, Ian Wall, Darren Green, Paul Bamborough, Peter V. Coveney
Published in: Journal of Chemical Theory and Computation, Issue 13/2, 2017, Page(s) 784-795, ISSN 1549-9618
Publisher: American Chemical Society
DOI: 10.1021/acs.jctc.6b00794

FabSim: Facilitating computational research through automation on large-scale and distributed e-infrastructures
Author(s): Derek Groen, Agastya P. Bhati, James Suter, James Hetherington, Stefan J. Zasada, Peter V. Coveney
Published in: Computer Physics Communications, Issue 207, 2016, Page(s) 375-385, ISSN 0010-4655
Publisher: Elsevier BV
DOI: 10.1016/j.cpc.2016.05.020

Mechanism of Exfoliation and Prediction of Materials Properties of Clay–Polymer Nanocomposites from Multiscale Modeling
Author(s): James L. Suter, Derek Groen, Peter V. Coveney
Published in: Nano Letters, Issue 15/12, 2015, Page(s) 8108-8113, ISSN 1530-6984
Publisher: American Chemical Society
DOI: 10.1021/acs.nanolett.5b03547

LB3D: A parallel implementation of the Lattice-Boltzmann method for simulation of interacting amphiphilic fluids
Author(s): S. Schmieschek, L. Shamardin, S. Frijters, T. Krüger, U.D. Schiller, J. Harting, P.V. Coveney
Published in: Computer Physics Communications, 2017, ISSN 0010-4655
Publisher: Elsevier BV
DOI: 10.1016/j.cpc.2017.03.013

Evaluation and Characterization of Trk Kinase Inhibitors for the Treatment of Pain: Reliable Binding Affinity Predictions from Theory and Computation
Author(s): Shunzhou Wan, Agastya P. Bhati, Sarah Skerratt, Kiyoyuki Omoto, Veerabahu Shanmugasundaram, Sharan K. Bagal, Peter V. Coveney
Published in: Journal of Chemical Information and Modeling, Issue 57/4, 2017, Page(s) 897-909, ISSN 1549-9596

Publisher: American Chemical Society
DOI: 10.1021/acs.jcim.6b00780

Rapid, Accurate, Precise, and Reliable Relative Free Energy Prediction Using Ensemble Based Thermodynamic Integration
Author(s): Agastya P. Bhati, Shunzhou Wan, David W. Wright, Peter V. Coveney
Published in: Journal of Chemical Theory and Computation, Issue 13/1, 2016, Page(s) 210-222, ISSN 1549-9618
Publisher: American Chemical Society
DOI: 10.1021/acs.jctc.6b00979

Conference proceedings (3)

Concurrent and Adaptive Extreme Scale Binding Free Energy Calculations
Author(s): Dakka, Jumana; Farkas-Pall, Kristof; Turilli, Matteo; Wright, David W; Coveney, Peter V; Jha, Shantenu
Published in: arXiv, Issue 1, 2018
Publisher: arXiv

From Thread to Transcontinental Computer: Disturbing Lessons in Distributed Supercomputing
Author(s): Derek Groen, Simon Portegies Zwart
Published in: 2015 IEEE 11th International Conference on e-Science, 2015, Page(s) 565-571, ISBN 978-1-4673-9325-6
Publisher: IEEE
DOI: 10.1109/eScience.2015.81

Optimization of Multiscale fusion Plasma Simulations within the ComPat Framework
Author(s): O. Luk, O. Hoenen, A. Bottino, B. Scott, D. Coster
Published in: EPS Proceedings, Issue P1, 2018, Page(s) 1102, ISBN 979-10-96389-08-7
Publisher: European Physical Society

Monographic books (1)

Astrophysical Recipes: the Art of AMUSE
Author(s): S. Portegies Zwart and S. McMillan
Published in: AAS IOP Astronomy, 2018
Publisher: IOP

Datasets

Datasets via OpenAIRE (2)

LB3D: A parallel implementation of the Lattice-Boltzmann method for mesoscale simulation of interacting amphiphilic fluids
Author(s): Schmieschek, S.
Published in: Mendeley

FabSim: Facilitating computational research through automation on large-scale and distributed e-infrastructures
Author(s): Groen, Derek
Published in: Mendeley

Software

Software via OpenAIRE (1)

PolNet
Author(s): Bernabeu, Miguel O.
Publisher: bio.tools

Other Research Products

Other Research Products via OpenAire (1)

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

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