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**Distributed multiscale computing**

Borgdorff, J.

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# Bibliography

- [1] Car-Parinello Molecular Dynamics: <http://www.cpmc.org>, 2013.
- [2] Large-scale atomic/molecular massively parallel simulator: <http://lammps.sandia.gov>, 2013.
- [3] A. Abdulle and M. E. Huber. Discontinuous Galerkin finite element heterogeneous multiscale method for advection-diffusion problems with multiple scales. *Numerische Mathematik*, 2013. doi: 10.1007/s00211-013-0578-9.
- [4] A. Abdulle, W. E. B. Engquist, and E. Vanden-Eijnden. The heterogeneous multiscale method. *Acta Numerica*, 21:1–87, 2012. doi: 10.1017/S0962492912000025.
- [5] A. Adel and S. Adel. A Meta-ontology for Architecture Description Languages and MDA Platforms. In *2008 International Conference on Computational Intelligence for Modelling, Control and Automation*. IEEE, Dec. 2008. doi: 10.1109/CIMCA.2008.62.
- [6] E. Agullo, C. Coti, T. Herault, J. Langou, S. Peyronnet, A. Rezmerita, F. Cappello, and J. J. Dongarra. QCG-OMPI: MPI applications on grids. *Future Generation Computer Systems*, Nov. 2010. doi: 10.1016/j.future.2010.11.015.
- [7] B. A. Allan and R. Armstrong. Ccaffeine Framework: Composing and Debugging Applications Iteratively and Running them Statically. . In *Compframe 2005 workshop*, Atlanta, GA, Feb. 2005. Sandia National Laboratories.
- [8] B. A. Allan, R. Armstrong, D. E. Bernholdt, F. Bertrand, K. Chiu, T. L. Dahlgren, K. B. Damevski, W. R. Elwasif, M. Govindaraju, D. S. Katz, J. A. Kohl, M. Krishnan, J. W. Larson, S. Lefantzi, M. J. Lewis, A. D. Malony, L. C.

- McInnes, J. Nieplocha, B. Norris, J. Ray, T. L. Windus, and S. Zhou. A Component Architecture for High-Performance Scientific Computing. *International Journal of High-Performance Computing Applications*, 20(2):163–202, July 2006. doi: 10.1177/1094342006064488.
- [9] R. Allen and D. Garlan. A formal basis for architectural connection. *ACM Transactions on Software Engineering and Methodology*, 6(3):213–249, July 1997. doi: 10.1145/258077.258078.
- [10] A. Arbona, A. Artigues, C. Bona-Casas, J. Massó, B. Miñano, A. Rigo, M. Trias, and C. Bona. Simflowny: A general-purpose platform for the management of physical models and simulation problems. *Computer Physics Communications*, 184(10):2321–2331, Oct. 2013. doi: 10.1016/j.cpc.2013.04.012.
- [11] C. W. Armstrong, R. W. Ford, and G. D. Riley. Coupling integrated Earth System Model components with BFG2. *Concurrency and Computation: Practice and Experience*, 21(6):767–791, Apr. 2009. doi: 10.1002/cpe.1348.
- [12] F. Baccelli, A. Jean-Marie, and Z. Liu. A survey on solution methods for task graph models. In N. Götz, U. Herzog, and M. Rettelbach, editors, *QMIPS-Workshop on Formalism, Principles and State-of-the-art*, pages 163–183, Erlangen, Germany, Sept. 1993.
- [13] Y. Bar-Yam. Multiscale Complexity / Entropy. *Advances in Complex Systems*, (7):47–63, 2004.
- [14] Y. Bar-Yam, D. Harmon, and Y. Bar-Yam. Computationally tractable pairwise complexity profile. *Complexity*, 18(5):20–27, Feb. 2013. doi: 10.1002/cplx.21437.
- [15] A. Barker and J. Van Hemert. Scientific workflow: a survey and research directions. In *7th International Conference on Parallel processing and Applied Mathematics (PPAM 2007), Proceedings of the*, pages 746–753. University of Edinburgh, Springer-Verlag Berlin/Heidelberg, Sept. 2007. ISBN 3-540-68105-1, 978-3-540-68105-2. doi: 10.1007/978-3-540-68111-3\_78.
- [16] M. Ben Belgacem, B. Chopard, and A. Parmigiani. Coupling Method for Building a Network of Irrigation Canals on a Distributed Computing Envi-

- ronment. In G. C. Sirakoulis and S. Bandini, editors, *ACRI 2012*, pages 309–318. Springer-Verlag Berlin Heidelberg, 2012. ISBN 978-3-642-33350-7. doi: 10.1007/978-3-642-33350-7\_32.
- [17] M. Ben Belgacem, B. Chopard, J. Borgdorff, M. Mamonski, K. Rycerz, and D. Harezlak. Distributed Multiscale Computations Using the MAPPER Framework. *Procedia Computer Science*, 18:1106–1115, 2013. doi: 10.1016/j.procs.2013.05.276.
- [18] M. O. Bernabeu, R. W. Nash, D. Groen, H. B. Carver, J. Hetherington, T. Krüger, and P. V. Coveney. Impact of blood rheology on wall shear stress in a model of the middle cerebral artery. *Interface Focus*, 3:20120094, Feb. 2013. doi: 10.1098/rsfs.2012.0094.
- [19] J. Borgdorff, J.-L. Falcone, E. Lorenz, B. Chopard, and A. G. Hoekstra. A principled approach to distributed multiscale computing, from formalization to execution. In *Proceedings of the IEEE 7th International Conference on e-Science Workshops*, pages 97–104, 5-8 Dec. 2011, Stockholm, Sweden, 2011. IEEE Computer Society Press. doi: 10.1109/eScienceW.2011.9.
- [20] J. Borgdorff, C. Bona-Casas, M. Mamonski, K. Kurowski, T. Piontek, B. Bosak, K. Rycerz, E. Ciepiela, T. Gubała, D. Harezlak, M. Bubak, E. Lorenz, and A. G. Hoekstra. A Distributed Multiscale Computation of a Tightly Coupled Model Using the Multiscale Modeling Language. *Procedia Computer Science*, 9:596–605, 2012. doi: 10.1016/j.procs.2012.04.064.
- [21] J. Borgdorff, D. Groen, S. Ferlin, I. Saverchenko, J. L. Suter, A. G. Hoekstra, and P. V. Coveney. Multiscale Simulations on distributed European e-Infrastructures. *inSiDE*, 10(1), Apr. 2012. URL: [http://inside.hlr.rs.de/html/Edition\\_01\\_12/article\\_24.html](http://inside.hlr.rs.de/html/Edition_01_12/article_24.html).
- [22] J. Borgdorff, J.-L. Falcone, E. Lorenz, C. Bona-Casas, B. Chopard, and A. G. Hoekstra. Foundations of distributed multiscale computing: Formalization, specification, and analysis. *Journal of Parallel and Distributed Computing*, 73: 465–483, 2013. doi: 10.1016/j.jpdc.2012.12.011.
- [23] J. Borgdorff, M. Mamonski, B. Bosak, D. Groen, M. Ben Belgacem, K. Kurowski, and A. G. Hoekstra. Multiscale Computing with the Multiscale

- Modeling Library and Runtime Environment. *Procedia Computer Science*, 18: 1097–1105, Jan. 2013. doi: 10.1016/j.procs.2013.05.275.
- [24] J. Borgdorff, D. Groen, and M. Mamonski. Adding MUSCLE to Multiscale Simulations. *HPCWire*, 2013. URL: <http://www.hpcwire.com/2013/12/11/adding-muscle-multiscale-simulations/>.
- [25] J. Borgdorff, M. Ben Belgacem, C. Bona-Casas, L. Fazendeiro, D. Groen, O. Hoenen, A. Mizeranschi, J. L. Suter, D. P. Coster, P. V. Coveney, W. Dubitzky, A. G. Hoekstra, P. Strand, and B. Chopard. Performance of Distributed Multiscale Simulations. *Phil. Trans. R. Soc. A*, *accepted*, 2014.
- [26] J. Borgdorff, M. Mamonski, B. Bosak, K. Kurowski, M. Ben Belgacem, B. Chopard, D. Groen, P. V. Coveney, and A. G. Hoekstra. Distributed Multiscale Computing with MUSCLE 2, the Multiscale Coupling Library and Environment. *Journal of Computational Science*, *in press*, 2014. doi: 10.1016/j.jocs.2014.04.004.
- [27] B. Bosak, J. Komasa, P. Kopta, K. Kurowski, M. Mamonski, and T. Piontek. New Capabilities in QosCosGrid Middleware for Advanced Job Management, Advance Reservation and Co-allocation of Computing Resources – Quantum Chemistry Application Use Case. In M. Bubak, T. Szepieniec, and K. Wiatr, editors, *Lecture Notes in Computer Science*, pages 40–55–55. Springer Berlin Heidelberg, Berlin, Heidelberg, 2012. ISBN 978-3-642-28267-6. doi: 10.1007/978-3-642-28267-6\_4.
- [28] A. Brandt. *Principles of Systematic Upscaling*. wisdom.weizmann.ac.il, 2010.
- [29] J. Q. Broughton, F. F. Abraham, N. Bernstein, and E. Kaxiras. Concurrent coupling of length scales: Methodology and application. *Physical Review B*, 60(4):2391–2403, July 1999. doi: 10.1103/PhysRevB.60.2391.
- [30] M. Bubak, K. Górka, T. Gubała, M. Malawski, and K. Zając. Component-Based System for Grid Application Workflow Composition. In G. Goos, J. Hartmanis, J. Leeuwen, J. J. Dongarra, D. Laforenza, and S. Orlando, editors, *LNCS 2840*, pages 611–618. Springer Berlin Heidelberg, 2003. ISBN 978-3-540-20149-6. doi: 10.1007/978-3-540-39924-7\_82.

- [31] A. Caiazzo, J.-L. Falcone, B. Chopard, and A. G. Hoekstra. Asymptotic analysis of Complex Automata models for reaction–diffusion systems. *Applied Numerical Mathematics*, 59(8):2023–2034, Aug. 2009. doi: 10.1016/j.apnum.2009.04.001.
- [32] A. Caiazzo, D. J. W. Evans, J.-L. Falcone, J. Hegewald, E. Lorenz, B. Stahl, D. Wang, J. Bernsdorf, B. Chopard, J. Gunn, D. R. Hose, M. Krafczyk, P. V. Lawford, R. H. Smallwood, D. Walker, and A. G. Hoekstra. A Complex Automata approach for In-stent Restenosis: two-dimensional multiscale modeling and simulations. *Journal of Computational Science*, 2(1):9–17, Mar. 2011. doi: 10.1016/j.jocs.2010.09.002.
- [33] H. Casanova, F. Desprez, and F. Suter. On cluster resource allocation for multiple parallel task graphs. *Journal of Parallel and Distributed Computing*, 70: 1193–1203, 2010. doi: 10.1016/j.jpdc.2010.08.017.
- [34] Center for Advanced Computing Research, Caltech. Pyre: A Python Framework. <http://www.cacr.caltech.edu/projects/pyre/>, 2005.
- [35] CERFACS. OpenPALM 4.1.4. [http://www.cerfacs.fr/globc/PALM\\_WEB/](http://www.cerfacs.fr/globc/PALM_WEB/), 2013.
- [36] B. Chopard, J.-L. Falcone, A. G. Hoekstra, and J. Borgdorff. A Framework for Multiscale and Multiscience Modeling and Numerical Simulations. In C. Calude, J. Kari, I. Petre, and G. Rozenberg, editors, *LNCS 6714*, pages 2–8. Springer-Verlag Berlin Heidelberg, 2011. ISBN 978-3-642-21340-3. doi: 10.1007/978-3-642-21341-0\_2.
- [37] B. Chopard, J. Borgdorff, and A. G. Hoekstra. A Framework for multiscale modelling. *Phil. Trans. R. Soc. A*, *accepted*, 2014.
- [38] W. W. Chu, L. Holloway, M.-T. Lan, and K. Efe. Task Allocation in Distributed Data Processing. *Computer*, 13(11):57–69, Nov. 1980. doi: 10.1109/MC.1980.1653419.
- [39] E. Ciepiela, D. Harezlak, J. Kocot, T. Bartynski, M. Kasztelnik, P. Nowakowski, T. Gubała, M. Malawski, and M. Bubak. Exploratory Programming in the Virtual Laboratory. In *Proceedings of the 2010 International*

*Multiconference on Computer Science and Information Technology*, pages 621–628. Institute of Computer Science, AGH, Krakow, Poland, Oct. 2010.

- [40] D. P. Coster, V. Basiuk, G. Pereverzev, D. Kalupin, R. Zagorksi, R. Stankiewicz, P. Huynh, and F. Imbeaux. The European Transport Solver. *IEEE Transactions on Plasma Science*, 38(9):2085–2092, 2010. doi: 10.1109/TPS.2010.2056707.
- [41] J. Dada and P. Mendes. Multi-scale modelling and simulation in systems biology. *Integrative Biology*, (3):86–96, 2011. doi: 10.1039/coib00075b.
- [42] W. E and B. Engquist. The Heterogeneous Multiscale Methods. *Communications of Mathematical Sciences*, 1(1):87–132, 2003.
- [43] W. E, B. Engquist, and Z. Huang. Heterogeneous multiscale method: A general methodology for multiscale modeling. *Physical Review B*, 67(9):092101, Mar. 2003. doi: 10.1103/PhysRevB.67.092101.
- [44] W. E, B. Engquist, X. Li, W. Ren, and E. Vanden-Eijnden. Heterogeneous multiscale methods: A review. *Communications in Computational Physics*, 2(3):367–450, 2007.
- [45] H. El-Rewini, H. H. Ali, and T. Lewis. Task scheduling in multiprocessing systems. *Computer*, 28(12):27–37, Dec. 1995. doi: 10.1109/2.476197.
- [46] D. J. W. Evans, P. V. Lawford, J. Gunn, D. Walker, D. R. Hose, R. H. Smallwood, B. Chopard, M. Krafczyk, J. Bernsdorf, and A. G. Hoekstra. The application of multiscale modelling to the process of development and prevention of stenosis in a stented coronary artery. *Philosophical Transactions of the Royal Society A*, 366:3343–3360, 2008. doi: 10.1098/rsta.2008.0081.
- [47] J.-L. Falcone, B. Chopard, and A. G. Hoekstra. MML: towards a Multiscale Modeling Language. *Procedia Computer Science*, 1(1):819–826, 2010. doi: 10.1016/j.procs.2010.04.089.
- [48] D. A. Fedosov and G. E. Karniadakis. Triple-decker: Interfacing atomistic–mesoscopic–continuum flow regimes. *Journal of Computational Physics*, 228(4):1157–1171, 2009. doi: 10.1016/j.jcp.2008.10.024.

- [49] A. Finkelstein, J. Hetherington, L. Li, O. Margoninski, P. Saffrey, R. Seymour, and A. Warner. Computational challenges of systems biology. *Computer*, 37(5): 26– 33, May 2004. doi: 10.1109/MC.2004.1297236.
- [50] J. Fish. Bridging the scales in nano engineering and science. *Journal of Nanoparticle Research*, 8(5):577–594, Sept. 2006. doi: 10.1007/s11051-006-9090-9.
- [51] I. Foster. Globus Toolkit Version 4: Software for Service-Oriented Systems. *Journal of computer science and technology*, 21(4):513–520–520, 2006. doi: 10.1007/s11390-006-0513-y.
- [52] I. Foster, C. Kesselman, J. M. Nick, and S. Tuecke. The Physiology of the Grid. Globus Project, 2002.
- [53] Y. Frauel, D. P. Coster, B. Guillerminet, F. Imbeaux, A. Jackson, C. Konz, M. Owsiak, M. Plociennik, B. D. Scott, and P. Strand. Easy use of high performance computers for fusion simulations. *Fusion Engineering and Design*, 87(12): 2057–2062, Dec. 2012. doi: 10.1016/j.fusengdes.2012.04.015.
- [54] R. M. Fujimoto. Parallel discrete event simulation. *Communications of the ACM*, 33(10):30–53, Oct. 1990. doi: 10.1145/84537.84545.
- [55] D. Garlan. Formal Modeling and Analysis of Software Architecture: Components, Connectors, and Events. In G. Goos, J. Hartmanis, J. Leeuwen, M. Bernardo, and P. Inverardi, editors, *Lecture Notes in Computer Science*, pages 1–24. Springer-Verlag Berlin, Heidelberg, 2003. ISBN 978-3-540-20083-3. doi: 10.1007/978-3-540-39800-4\_1.
- [56] D. Givon, R. Kupferman, and A. Stuart. Extracting macroscopic dynamics: model problems and algorithms. *Nonlinearity*, (17):R55–R127, 2004. doi: 10.1088/0951-7715/17/6/R01.
- [57] Globus. GridFTP 5.2. <http://www.globus.org/toolkit/data/gridftp/>, 2012.
- [58] T. Goodale, G. Allen, G. Lanfermann, J. Massó, T. Radke, E. Seidel, and J. Shalf. The Cactus Framework and Toolkit: Design and Applications. In J. M. L. M. Palma, A. A. Sousa, J. J. Dongarra, and V. Hernández, editors,



- LNCS 2565*, pages 197–227. Springer-Verlag Berlin Heidelberg, Apr. 2003. ISBN 978-3-540-00852-1. doi: 10.1007/3-540-36569-9\_13.
- [59] D. Groen, S. Rieder, P. Grosso, C. de Laat, and S. F. Portegies Zwart. A lightweight communication library for distributed computing. *Computational Science & Discovery*, 3(1):015002, Jan. 2010. doi: 10.1088/1749-4699/3/1/015002.
- [60] D. Groen, J. Borgdorff, C. Bona-Casas, J. Hetherington, R. W. Nash, S. J. Zasada, I. Saverchenko, M. Mamonski, K. Kurowski, M. O. Bernabeu, A. G. Hoekstra, and P. V. Coveney. Flexible composition and execution of high performance, high fidelity multiscale biomedical simulations. *Interface Focus*, 3(2): 20120087, Apr. 2013. doi: 10.1098/rsfs.2012.0087.
- [61] D. Groen, J. Hetherington, H. B. Carver, R. W. Nash, M. O. Bernabeu, and P. V. Coveney. Analysing and modelling the performance of the HemeLB lattice-Boltzmann simulation environment. *Journal of Computational Science*, 4(5):412–422, 2013. doi: 10.1016/j.jocs.2013.03.002.
- [62] D. Groen, S. J. Zasada, and P. V. Coveney. Survey of Multiscale and Multiphysics Applications and Communities. *IEEE Computing in Science and Engineering, preprint*, pages doi:10.1109-MCSE.2013.47, 2013. doi: 10.1109/MCSE.2013.47.
- [63] T. Gubała, M. Bubak, and P. M. A. Sloot. Semantic Integration for Research Environments. In *Handbook of Research on Computational Grid Technologies for Life Sciences, Biomedicine, and Healthcare*, pages 514–530. IGI Global, Hershey, PA, USA, 2009. ISBN 9781605663753. doi: 10.4018/978-1-60566-374-6.ch026.
- [64] J. Hegewald. The Multiscale Coupling Library and Environment (MUSCLE). <http://muscle.berlios.de/>, jan 2010.
- [65] J. Hegewald, M. Krafczyk, J. Tölke, and A. G. Hoekstra. An agent-based coupling platform for complex automata. In *ICCS 2008, LNCS 5102*, pages 227–233. Springer-Verlag Berlin Heidelberg, 2008. doi: 10.1007/978-3-540-69387-1\_25.
- [66] C. A. R. Hoare. Communicating sequential processes. *Communications of the ACM*, 21(8):666–677, Aug. 1978. doi: 10.1145/359576.359585.

- [67] A. G. Hoekstra, E. Lorenz, J.-L. Falcone, and B. Chopard. Toward a Complex Automata Formalism for MultiScale Modeling. *International Journal for Multiscale Computational Engineering*, 5(6):491–502, 2007. doi: 10.1615/IntJMultCompEng.v5.i6.60.
- [68] A. G. Hoekstra, E. Lorenz, J.-L. Falcone, and B. Chopard. Towards a complex automata framework for multi-scale modeling: formalism and the scale separation map. In *ICCS 2007, Part I, LNCS 4487*, pages 922–930, 2007.
- [69] A. G. Hoekstra, J.-L. Falcone, and A. Caiazzo. Multi-scale Modeling with Cellular Automata: The Complex Automata Approach. In *LNCS*, pages 192–199. Springer-Verlag Berlin Heidelberg, 2008. doi: 10.1007/978-3-540-79992-4\_25.
- [70] A. G. Hoekstra, A. Caiazzo, E. Lorenz, and J.-L. Falcone. Complex automata: multi-scale modeling with coupled cellular automata. In A. G. Hoekstra, J. Kroc, and P. M. A. Sloot, editors, *Simulating Complex Systems by Cellular Automata*, pages 29–57. Springer-Verlag Berlin, Heidelberg, 2010. doi: 10.1007/978-3-642-12203-3\_3.
- [71] A. G. Hoekstra, B. Chopard, and P. V. Coveney. Multiscale Modelling and Simulation: a position paper. *Philosophical Transactions of the Royal Society A*, submitted, 2014.
- [72] O. Hoenen, L. Fazendairo, B. D. Scott, J. Borgdorff, A. G. Hoekstra, P. Strand, and D. P. Coster. Designing and running turbulence transport simulations using a distributed multiscale computing approach. In *EPS 2013, Europhysics Conference Abstracts*, 37D, page P4.155, 2013. ISBN 2-914771-84-3.
- [73] O. Hoenen, L. Fazendairo, B. D. Scott, J. Borgdorff, A. G. Hoekstra, P. Strand, and D. P. Coster. Designing and running turbulence transport simulations using a distributed multiscale computing approach. In *EPS 2013, Europhysics Conference Abstracts*, 37D, page P4.155, 2013. ISBN 2-914771-84-3.
- [74] iMatix Corporation. ZeroMQ: The Intelligent Transport Layer. <http://www.zeromq.org/>, 2013.
- [75] G. D. Ingram and I. T. Cameron. Challenges in Multiscale Modelling and its Application to Granulation Systems. *Developments in Chemical Engineering and Mineral Processing*, 12(3-4):293–308, 2004. doi: 10.1002/apj.5500120406.

- [76] G. D. Ingram, I. T. Cameron, and K. M. Hantos. Classification and analysis of integrating frameworks in multiscale modelling. *Chemical engineering science*, 59:2171–2187, 2004. doi: 10.1016/j.ces.2004.02.010.
- [77] D. Jefferson. Virtual time. *ACM Transactions on Programming Languages and ...*, 1985.
- [78] W. Joppich, M. Kürschner, and the MpCCI team. MpCCI—a tool for the simulation of coupled applications. *Concurrency and Computation: Practice and Experience*, 18(2):183–192, 2005. doi: 10.1002/cpe.913.
- [79] J. W. Jukema, J. J. W. Verschuren, T. A. N. Ahmed, and P. H. A. Quax. Restenosis after PCI. Part 1: pathophysiology and risk factors. *Nature Reviews Cardiology*, 9(1):53–62, Sept. 2011. doi: 10.1038/nrcardio.2011.132.
- [80] A. Kastrati, D. Hall, and A. Schömig. Long-term outcome after coronary stenting. *Current Controlled Trials in Cardiovascular Medicine*, 1(1):48–54, 2000.
- [81] J. Kennedy and R. Eberhart. Particle swarm optimization. In *Neural Networks, 1995. Proceedings., IEEE International Conference on*, pages 1942–1948, Perth, WA, 1995. doi: 10.1109/ICNN.1995.488968.
- [82] I. G. Kevrekidis and G. Samaey. Equation-free multiscale computation: Algorithms and applications. *Annual review of physical chemistry*, 2009.
- [83] D. Kim, J. W. Larson, and K. Chiu. Toward Malleable Model Coupling. *Procedia Computer Science*, 4:312–321, 2011. doi: doi:10.1016/j.procs.2011.04.033.
- [84] V. Kravtsov, A. Schuster, D. Carmeli, K. Kurowski, and W. Dubitzky. Grid-enabling complex system applications with QoSCosGrid: An architectural perspective. In *Proceedings of the 2008 International Conference on Grid Computing & Applications*, pages 168–174, Las Vegas, Nevada, USA, 2008.
- [85] T. Krüger. *Computer Simulation Study of Collective Phenomena in Dense Suspensions of Red Blood Cells under Shear*. Vieweg+Teubner Verlag, Wiesbaden, 2012. ISBN 978-3-8348-2376-2. doi: 10.1007/978-3-8348-2376-2.
- [86] K. Kurowski, W. Back, W. Dubitzky, L. Gulyás, G. Kampis, M. Mamonski, G. Szemes, and M. T. Swain. Complex System Simulations with QoSCosGrid.

- In G. Allen, J. Nabrzyski, E. Seidel, G. Albada, J. J. Dongarra, and P. M. A. Sloot, editors, *Lecture Notes in Computer Science*, pages 387–396–396. Springer Berlin Heidelberg, Berlin, Heidelberg, 2009. ISBN 978-3-642-01970-8. doi: 10.1007/978-3-642-01970-8\_38.
- [87] Y.-K. Kwok and I. Ahmad. Benchmarking and Comparison of the Task Graph Scheduling Algorithms. *Journal of Parallel and Distributed Computing*, 59(3): 381–422, Dec. 1999. doi: 10.1006/jpdc.1999.1578.
- [88] L. Lamport. Time, clocks, and the ordering of events in a distributed system. *Communications of the ACM*, 21(7):558–565, 1978.
- [89] J. W. Larson, R. L. Jacob, I. Foster, and J. Guo. The model coupling toolkit. In V. N. Alexandrov, J. J. Dongarra, B. A. Juliano, R. S. Renner, and C. J. K. Tan, editors, *ICCS 2001, LNCS 2073*, pages 185–194. Springer-Verlag Berlin Heidelberg, 2001. doi: 10.1007/3-540-45545-0\_27.
- [90] J. Li, W. Ge, J. Zhang, and M. Kwauk. Multi-scale compromise and multi-level correlation in complex systems. *Chemical Engineering Research and Design*, 83 (A6):574–582, 2005. doi: 10.1205/cherd.05093.
- [91] M. J. Litzkow. Remote Unix: Turning idle workstations into cycle servers. In *Proceedings of the Summer USENIX Conference*, 1987.
- [92] F. Liu, M. Sosonkina, and R. Bramley. A New Approach: Component-Based Multi-physics Coupling through CCA-LISI. In D. Taniar et al., editors, *ICCSA 2010, Part II, LNCS 6017*, pages 503–518. Springer-Verlag Berlin / Heidelberg, 2010.
- [93] C. M. Lloyd, M. D. B. Halstead, and P. F. Nielsen. CellML: its future, present and past. *Progress in Biophysics and Molecular Biology*, 85(2-3):433–450, June 2004. doi: 10.1016/j.pbiomolbio.2004.01.004.
- [94] E. Lorenz and A. G. Hoekstra. Heterogeneous Multiscale Simulations of Suspension Flow. *Multiscale Modeling & Simulation*, 9(4):1301–1326, Oct. 2011. doi: 10.1137/100818522.
- [95] B. Ludäscher, I. Altintas, C. Berkley, D. Higgins, E. Jaeger, M. Jones, E. A. Lee, J. Tao, and Y. Zhao. Scientific workflow management and the Kepler system.

- Concurrency and Computation: Practice and Experience*, 18(10):1039–1065, 2006. doi: 10.1002/cpe.994.
- [96] J. Maassen and H. E. Bal. SmartSockets: Solving the Connectivity Problems in Grid Computing. In *High performance distributed computing (HPDC'07), 16th International Symposium*, pages 1–10, Monterey, California, USA, June 2007. ACM. doi: 10.1145/1272366.1272368.
- [97] P.-O. Malaterre and J.-P. Baume. Modeling and regulation of irrigation canals: existing applications and ongoing researches. In *Systems, Man, and Cybernetics, 1998. 1998 IEEE International Conference on*, pages 3850–3855. IEEE, 1998. ISBN 0-7803-4778-1. doi: 10.1109/ICSMC.1998.726688.
- [98] M. Mamoński. GFD.179 – Smoa Computing HPC Basic Profile Adoption – Experience Report. Technical report, Open Grid Forum, 2011.
- [99] A. Mandal, K. Kennedy, C. Koelbel, G. Marin, J. Mellor-Crummey, B. Liu, and L. Johnsson. Scheduling strategies for mapping application workflows onto the grid. In *Proceedings of the 14th IEEE International Symposium on High Performance Distributed Computing*, pages 125–134. IEEE Computer Society, July 2005. doi: 10.1109/HPDC.2005.1520947.
- [100] S. Manini, K. Passera, W. Huberts, L. Botti, L. Antiga, and A. Remuzzi. Computational model for simulation of vascular adaptation following vascular access surgery in haemodialysis patients. *Computer Methods in Biomechanics and Biomedical Engineering*, pages 1–10, Jan. 2013. doi: 10.1080/10255842.2012.745857.
- [101] D. Marbach, J. C. Costello, R. Küffner, N. M. Vega, R. J. Prill, D. M. Camacho, K. R. Allison, The DREAM5 Consortium, M. Kellis, J. J. Collins, and G. Stolovitzky. Wisdom of crowds for robust gene network inference. *Nature Methods*, 9(8):796–804, July 2012. doi: 10.1038/nmeth.2016.
- [102] O. Marcou, B. Chopard, and S. El Yacoubi. Modeling of Irrigation Channels — a Comparative Study. *International Journal of Modern Physics C*, 18(04):739, 2007. doi: 10.1142/S0129183107011005.

- [103] D. A. Menasce and R. R. Muntz. Locking and Deadlock Detection in Distributed Data Bases. *IEEE Transactions on Software Engineering*, SE-5(3):195–202, May 1979. doi: 10.1109/TSE.1979.234181.
- [104] MessagePack. Messagepack 0.6.6. <http://msgpack.org>, 2012.
- [105] F. Migliavacca and G. Dubini. Computational modeling of vascular anastomoses. *Biomechanics and Modeling in Mechanobiology*, 3(4):235–250, Mar. 2005. doi: 10.1007/s10237-005-0070-2.
- [106] R. Milner. A calculus of communicating systems. Springer-Verlag Berlin/New York, 1980. ISBN 0-387-10235-3.
- [107] L. Mountrakis, E. Lorenz, and A. G. Hoekstra. Where do the platelets go? A simulation study of fully resolved blood flow through aneurysmal vessels. *Interface Focus*, 3(2):20120089–20120089, Feb. 2013. doi: 10.1098/rsfs.2012.0089.
- [108] L. Mountrakis, E. Lorenz, and A. G. Hoekstra. Validation of an efficient two-dimensional model for dense suspensions of red blood cells. *International Journal of Modern Physics C*, 2014.
- [109] A. Moustapha, A. R. Assali, S. Sdringola, W. K. Vaughn, R. D. Fish, O. Rosales, G. Schroth, Z. Krajcer, R. W. Smalling, and H. V. Anderson. Percutaneous and surgical interventions for in-stent restenosis: long-term outcomes and effect of diabetes mellitus. *Journal of the American College of Cardiology*, 37(7):1877–1882, June 2001. doi: 10.1016/S0735-1097(01)01231-1.
- [110] D. Noble. Modeling the Heart—from Genes to Cells to the Whole Organ. *Science*, 295(5560):1678–1682, Mar. 2002. doi: 10.1126/science.1069881.
- [111] C. Obiol-Pardo, J. Gomis-Tena, F. Sanz, J. Saiz, and M. Pastor. A Multiscale Simulation System for the Prediction of Drug-Induced Cardiotoxicity. *Journal of Chemical Information and Modeling*, 51(2):483–492, Feb. 2011. doi: 10.1021/ci100423z.
- [112] W. W. H. F. W. S. Organization, editor. *Global atlas on cardiovascular disease prevention and control*. Policies, strategies and interventions. World Health Organization, Geneva, Switzerland, 2012. ISBN 978 92 4 156437 3.

- [113] C. C. Pantelides. New challenges and opportunities for process modelling. In *Computer Aided Chemical Engineering*, pages 15–26. Elsevier, 2001. ISBN 9780444507099. doi: 10.1016/S1570-7946(01)80003-1.
- [114] A. Parmigiani, J. Latt, M. Ben Belgacem, and B. Chopard. A Lattice Boltzmann simulation of the Rhone river. *Int. J. Mod. Phys. C*, 24(11):1340008, 2013. doi: 10.1142/S0129183113400081.
- [115] P. Pathmanathan, M. O. Bernabeu, and R. Bordas. Chaste: a test-driven approach to software development for biological modelling. *Computer Physics Communications*, 2009.
- [116] C. S. Peskin. The immersed boundary method. *Acta Numerica*, 11:479–517, July 2003. doi: 10.1017/S0962492902000077.
- [117] C. A. Petri. *Kommunikation mit Automaten*. PhD thesis, Institut für instrumentelle Mathematik, Bonn, 1962.
- [118] S. F. Portegies Zwart, S. L. W. McMillan, A. van Elteren, F. I. Pelupessy, and N. de Vries. Multi-physics simulations using a hierarchical interchangeable software interface. *Computer Physics Communications*, 184(3):456–468, Mar. 2013. doi: 10.1016/j.cpc.2012.09.024.
- [119] R. Prodan and T. Fahringer. Dynamic scheduling of scientific workflow applications on the grid: a case study. *Proceedings of the 2005 ACM symposium on Applied computing*, pages 687–694, 2005. doi: 10.1145/1066677.1066835.
- [120] R. Quax, A. Apolloni, and P. M. A. Sloot. Towards understanding the behavior of physical systems using information theory. *The European Physical Journal Special Topics*, 222(6):1389–1401, Sept. 2013. doi: 10.1140/epjst/e2013-01933-9.
- [121] P. Reiher and D. Jefferson. Virtual time based dynamic load management in the time warp operating system. *Transactions of the Society for Computer ...*, 1990.
- [122] A. J. Ryan. Emergence is coupled to scope, not level. *Complexity*, 13(2):67–77, 2007. doi: 10.1002/cplx.20203.
- [123] K. Rycerz, M. Bubak, E. Ciepiela, D. Harezlak, T. Gubała, J. Meizner, and M. Pawlik. Composing, Execution and Sharing of Multiscale Applications. *Future Generation Computer Systems*, submitted, 2014.

- [124] B. D. Scott. Free-energy conservation in local gyrofluid models. *Physics of Plasmas (1994-present)*, 12(102307):-, 2005. doi: 10.1063/1.2064968.
- [125] P. M. A. Sloot and A. G. Hoekstra. Multi-scale modelling in computational biomedicine. *Briefings in bioinformatics*, 11(1):142–152, Jan. 2010. doi: 10.1093/bib/bbp038.
- [126] P. M. A. Sloot, A. Tirado-Ramos, I. Altintas, M. Bubak, and C. Boucher. From Molecule to Man: Decision Support in Individualized E-Health. *Computer*, 39(11):40–46, Nov. 2006. doi: 10.1109/MC.2006.380.
- [127] J. Southern, J. Pitt-Francis, J. Whiteley, D. Stokeley, H. Kobashi, R. Nobes, K. Yoshimasa, and D. Gavaghan. Multi-scale computational modelling in biology and physiology. *Progress in Biophysics and Molecular Biology*, (96):60–89, 2008. doi: 10.1016/j.pbiomolbio.2007.07.019.
- [128] E. Steinhart. The Physics of Information. In L. Floridi, editor, *The Philosophy of Computing and Information*, pages 178–185. Blackwell Publishing, 2004. ISBN 0-631-22918-3.
- [129] W. P. Stevens, G. J. Myers, and L. L. Constantine. Structured design. *IBM Systems Journal*, 13(2):115–139, 1974. doi: 10.1147/sj.132.0115.
- [130] S. Succi. *The Lattice Boltzmann Equation: For Fluid Dynamics and Beyond*. Numerical Mathematics and Scientific Computation. Oxford University Press, 2001. ISBN 9780198503989.
- [131] Sun Microsystems. XDR: External Data Representation standard. RFC 1014, June 1987.
- [132] J. L. Suter and P. V. Coveney. Computer simulation study of the materials properties of intercalated and exfoliated poly(ethylene)glycol clay nanocomposites. *Soft Matter*, 5(11):2239–2251, Apr. 2009. doi: 10.1039/b822666k.
- [133] J. L. Suter, D. Groen, L. Kabalan, and P. V. Coveney. Distributed Multiscale Simulations of Clay-Polymer Nanocomposites. *MRS Proceedings*, 1470:mrss12-1470-xx02-07, Jan. 2012. doi: 10.1557/opl.2012.1009.



- [134] M. T. Swain, T. Hunniford, W. Dubitzky, J. Mandel, and N. Palfreyman. Reverse-Engineering Gene-Regulatory Networks using Evolutionary Algorithms and Grid Computing. *Journal of Clinical Monitoring and Computing*, 19(4-5):329–337, Oct. 2005. doi: 10.1007/s10877-005-0678-x.
- [135] M. T. Swain, J. J. Mandel, and W. Dubitzky. Comparative study of three commonly used continuous deterministic methods for modeling gene regulation networks. *BMC Bioinformatics*, 11(1):459, 2010. doi: 10.1186/1471-2105-11-459.
- [136] H. Tahir. *Modelling and simulating the dynamics of in-stent restenosis in porcine coronary arteries*. PhD thesis, Universiteit van Amsterdam, Amsterdam, The Netherlands, 2013.
- [137] H. Tahir, A. G. Hoekstra, E. Lorenz, P. V. Lawford, D. R. Hose, J. Gunn, and D. J. W. Evans. Multiscale simulations of the dynamics of in-stent restenosis: impact of stent deployment and design. *Interface Focus*, 1(3):365–373, Apr. 2011. doi: 10.1098/rsfs.2010.0024.
- [138] H. Tahir, C. Bona-Casas, and A. G. Hoekstra. Modelling the influence of re-endothelialization on in-stent restenosis. In *VPH 2012*, London, UK, Sept. 2012.
- [139] H. Tahir, C. Bona-Casas, and A. G. Hoekstra. Modelling the Effect of a Functional Endothelium on the Development of In-Stent Restenosis. *PLOS ONE*, 8(6):e66138, June 2013. doi: 10.1371/journal.pone.0066138.
- [140] H. Tahir, C. Bona-Casas, A. J. Narracott, J. Iqbal, J. Gunn, P. V. Lawford, and A. G. Hoekstra. Endothelial repair process and its relevance to longitudinal neointimal tissue patterns: comparing histology with in silico modelling. *Journal of The Royal Society Interface*, 11(94):20140022–20140022, Feb. 2014. doi: 10.1161/CIRCULATIONAHA.107.720730.
- [141] H. Talebi, M. Silani, S. P. A. Bordas, P. Kerfriden, and T. Rabczuk. A computational library for multiscale modeling of material failure. *Computational Mechanics*, pages 1–25, Dec. 2013. doi: 10.1007/s00466-013-0948-2.
- [142] D. Thain, T. Tannenbaum, and M. Livny. Distributed computing in practice: the Condor experience. *Concurrency and Computation: Practice and Experience*, 17(2-4):323–356, 2005. doi: 10.1002/cpe.938.

- [143] The COAST project. Complex automata. <http://www.complex-automata.org/>, 2007.
- [144] The MAPPER project. <http://www.mapper-project.eu/>, 2010.
- [145] S. Valcke, E. Guilyardi, and C. Larsson. PRISM and ENES: a European approach to Earth system modelling. *Concurrency and Computation: Practice and Experience*, 18(2):247–262, 2005. doi: 10.1002/cpe.915.
- [146] L. G. Valiant. A bridging model for parallel computation. *Communications of the ACM*, 33(8):103–111, Aug. 1990. doi: 10.1145/79173.79181.
- [147] W. M. P. van der Aalst. The application of Petri nets to workflow management. *Journal of Circuits Systems and Computers*, 8(1):21–66, 1998.
- [148] D. G. Vlachos. A Review of Multiscale Analysis: Examples from Systems Biology, Materials Engineering, and Other Fluid–Surface Interacting Systems. *Advances in Chemical Engineering*, 30:1–61, 2005. doi: 10.1016/S0065-2377(05)30001-9.
- [149] G. Weikum and G. Vossen. *Transactional Information Systems: Theory, Algorithms, and the Practice of Concurrency Control and Recovery*. The Morgan Kaufmann Series in Data Management Systems. Elsevier, 2001. ISBN 9780080519562.
- [150] K. Wolstencroft, R. Haines, D. Fellows, A. Williams, D. Withers, S. Owen, S. Soiland-Reyes, I. Dunlop, A. Nenadic, P. Fisher, J. Bhagat, K. Belhajjame, F. Bacall, A. Hardisty, A. Nieva de la Hidalga, M. P. Balcazar Vargas, S. Sufi, and C. Goble. The Taverna workflow suite: designing and executing workflows of Web Services on the desktop, web or in the cloud. *Nucleic Acids Research*, 41(W1):W557–W561, June 2013. doi: 10.1093/nar/gkt328.
- [151] A. Yang and W. Marquardt. An ontological conceptualization of multiscale models. *Computers & Chemical Engineering*, (33):822–837, 2009. doi: 10.1016/j.compchemeng.2008.11.015.
- [152] T. Yang and A. Gerasoulis. DSC: scheduling parallel tasks on an unbounded number of processors. *Parallel and Distributed Systems, IEEE Transactions on*, 5(9):951–967, Sept. 1994. doi: 10.1109/71.308533.

- [153] J. Yu, R. Buyya, and K. Ramamohanarao. Workflow Scheduling Algorithms for Grid Computing. In F. Xhafa and A. Abraham, editors, *Studies in Computational Intelligence*, pages 173–214. Springer Berlin Heidelberg, Berlin, Heidelberg, 2008. ISBN 978-3-540-69260-7. doi: 10.1007/978-3-540-69277-5\_7.
- [154] S. J. Zasada and P. V. Coveney. Virtualizing access to scientific applications with the Application Hosting Environment. *Computer Physics Communications*, 180(12):2513–2525, Dec. 2009. doi: 10.1016/j.cpc.2009.06.008.
- [155] S. J. Zasada, M. Mamonski, D. Groen, J. Borgdorff, I. Saverchenko, T. Piontek, K. Kurowski, and P. V. Coveney. Distributed Infrastructure for Multiscale Computing. In *2012 IEEE/ACM 16th International Symposium on Distributed Simulation and Real Time Applications (DS-RT)*, pages 65–74. IEEE, 2012. ISBN 978-1-4673-2954-5. doi: 10.1109/DS-RT.2012.17.
- [156] K. Zuse. Rechnender Raum. *Elektronische Datenverarbeitung*, 8:336–344, 1967.