Research Software Engineering for Multiscale Simulators

IPES (Innovative Parallel numErical Solvers) Research Group

Antônio Tadeu Azevedo Gomes (LNCC)

Laboratório Nacional de Computação Científica - LNCC

December 19, 2023

Laboratório
Nacional de
Computação
Científica

The IPES Research Group

MHM

Most of our developments on numerical simulators are based on the family of Multiscale Hybrid-Mixed (MHM) methods, which provides a multi-level strategy to approximate the solution of boundary value problems with heterogeneous coefficients.

HPC

We devise numerical simulators to run at scale, exploring massively parallel architectures and developing code with bleeding-edge technologies.

Machine learning

We explore machine-learning techniques to predict resource consumption and to act as surrogates of numerical simulations.

The IPES Team

A multidisciplinary group with mathematicians, computer scientists and engineers.

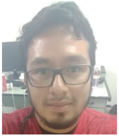
Antônio Tadeu Gomes

- Ph.D. in Computer Science from PUC-Rio, Brazil (2005).
- Coordinator of the Steering Committee of the SDumont supercomputing facility.
- Main interests in the broad area of systems modeling, encompassing networked systems, distributed systems, numerical simulation systems, high-performance computing systems, and machine learning systems.

Frédéric Valentin

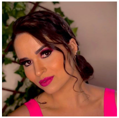
- PhD in applied mathematics from the Sorbonne Universités - Paris VI, France (1999).
- INRIA International Chair from 2018 to 2023.
- Research lies in devising and analyzing innovative numerical methods and mathematical models for multiscale phenomena appearing in engineering and life science problems.

Roberto Souto (LNCC)

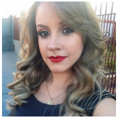


Juan Fabian (Postdoc)

Julio da Fonseca (Postdoc)



Larissa Martins (PhD Student)

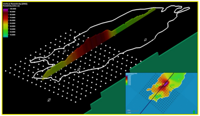


Larissa Miguez (PhD Student)

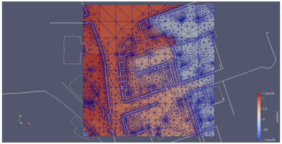
Weslley Pereira (NREL, US)

Diego Paredes (UdeC, CL)

Projects in Energy



INVMULTIFIS: Development of multi-physics data inversion software with optimization via artificial intelligence (2022-2025)

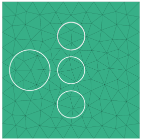


EOLIS: Efficient Off-LIne numerical Strategies for multi-query problems (2021-2023)

PADEF: Parallelism and Analysis of Accuracy, Performance and Applicability in Simulators based on Finite Element Methods (2018-2020)

PHOTOM: Photovoltaic Solar Devices in Multiscale Computational Simulations (2018-2020)

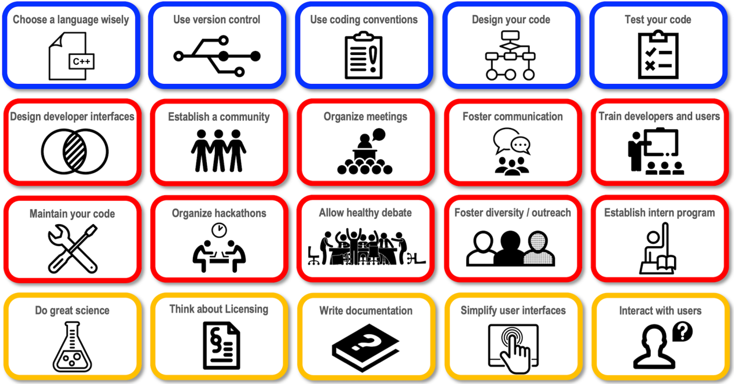
HPC4e: High-Performance Computing for Energy (2016-2019)



HOMAR: High-performance Multiscale Algorithms for wave pRopagation problems (2015-2018)

HOSCAR: High performance cOmputing and SCientific dAta management dRiven by highly demanding applications (2013-2015)

Research Software Issues



Source: Better together: Elements of successful scientific software development in a distributed collaborative community (https://doi.org/10.1371/journal.pcbi.1007507)

Selected Publications

Journals

1. Fernando, H.; Martins, L.; Pereira, W.; Valentin, F. A petrov–galerkin multiscale hybrid-mixed method for the darcy equation on polytopes. Computational and Applied Mathematics, 42(4):173, 2023.
2. Gomes, A. T. A.; Pereira W.; Valentin, F. The MHM Method for Linear Elasticity on Polytopal Meshes. IMA Journal of Numerical Analysis, 2022.
3. Chaumont-Frelet, T.; Valentin, F. A multiscale hybrid-mixed method for the helmholtz equation in heterogeneous domains. SIAM J. Numer. Anal., 58(2):1029–1067, 2020.
4. Lanteri, S.; Paredes, D.; Scheid, C.; Valentin, F. The multiscale hybrid-mixed method for the Maxwell equations in heterogeneous media. SIAM Multiscale Model. Simul., 16(4):1648–1683, 2018.
5. Harder, C.; Paredes, D.; Valentin, F. On a multiscale hybrid-mixed method for advective-reactive dominated problems with heterogenous coefficients. SIAM Multiscale Model. and Simul., 13(2):491–518, 2015.
6. Harder, C.; Paredes, D.; Valentin, F. A family of multiscale hybrid-mixed finite element methods for the Darcy equation with rough coefficients. J. Comput. Phys., 245:107–130, 2013.

Conference papers

1. Boito, F.; Gomes, A.T.A.; Peyrondet, L. Teylo, L. I/O Performance of Multiscale Finite Element Simulations on HPC environments. In: 34th SBAC-PAD Workshops, Bordeaux, FR, 2022. p. 9-16.
2. Gomes, A. T. A. ; da Silva, L. M. ; Valentin, F. Improving Boundary Layer Predictions Using Parametric Physics-Aware Neural Networks. In: 9th CARLA, Porto Alegre, BR, 2022.
3. Fabian, J. H. L. ; Gomes, A. T. A. ; Ogasawara, E. Estimating the execution time of the coupled stage in multiscale numerical simulations. In: 7th CARLA, Cuenca, EQ, 2020.
4. Fabian, J. H. L. ; Gomes, A. T. A. ; Ogasawara, E. Estimating the execution time of fully-online multiscale numerical simulations. In: XXI WSCAD. Santo André, BR, 2020.
5. Gomes, A.T.A.; Paredes, D.; Pereira, W.S.; Souto, R.P.; Valentin, F. A Multiscale Hybrid-Mixed Method for the Elastodynamic Model with Rough Coefficients. In: XXXVIII CILAMCE, Florianopolis, BR, 2017.

Courses, Software...

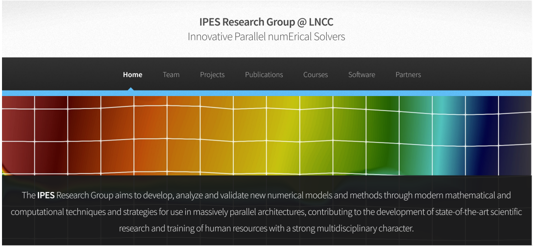
Courses

1. Valentin, F.; Gomes, A.T.A. The Multiscale Hybrid-Mixed Finite Element Method: Origin, Theory and Practice (L'École Doctorale en Sciences Fondamentales et Appliquées – Université Côte d'Azur, January/2023).
2. Valentin, F.; Gomes, A.T.A.; Pereira W.S. MC-A03: The MHM Method: Theory and Practice (LNCC Summer School - February/2022).
3. Valentin, F.; Gomes, A.T.A.; Pereira W.S. MC-A06: The MHM Method: Theory and Practice (LNCC Summer School - February/2021).
4. Valentin, F.; Gomes, A.T.A.; Pereira W.S. MC-A: Multiscale Methods: Theory and Practice (LNCC Summer School - March/2020).

Softwares

1. MSL Core: C++ library for implementing key concepts present in most FEM-based simulators.
2. MSL CG: C++ library for implementing key concepts present in Continuous Galerkin-based simulators.
3. MSL MHM: C++ library for implementing simulators based on the family of MHM methods.
4. MSL Python: Simple Python wrapper over the FEniCS platform for implementing simulators based on the family of MHM methods.
5. MSL FreeFEM++: Simple implementation of the MHM method on the FreeFEM++ platform.

http://ipes.lncc.br



Thank You!

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