

Scientific Report on SNSF project 172710
Numerical methods for stationary and time-dependent
multiscale problems

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1 Summary of the research work and its results

- 1.1 Multiscale inverse problems
- 1.2 Statistical inference of multiscale SDEs
- 1.3 Probabilistic numerical methods for forward and inverse problems
- 1.4 Discontinuous Galerkin discretization of elliptic PDEs
- 1.5 Stabilized explicit multirate methods for stiff equations
- 1.6 Novel cell problems for reduced resonance errors in the FE-HMM

2 Research Output

TO DO

References

- [1] A. ABDULLE, I. ALMUSLIMANI, AND G. VILMART, *Optimal explicit stabilized integrator of weak order 1 for stiff and ergodic stochastic differential equations*, SIAM/ASA J. Uncertain. Quantif., 6 (2018), pp. 937–964, <https://doi.org/10.1137/17M1145859>.
- [2] A. ABDULLE, D. ARJMAND, AND E. PAGANONI, *Exponential decay of the resonance error in numerical homogenization via parabolic and elliptic cell problems*, C. R. Math. Acad. Sci. Paris, 357 (2019), pp. 545–551, <https://doi.org/10.1016/j.crma.2019.05.011>.
- [3] A. ABDULLE, D. ARJMAND, AND E. PAGANONI, *Analytical and numerical study of a modified cell problem for the numerical homogenization of multiscale random fields*. arXiv preprint arXiv:2007.10828, 2020.
- [4] A. ABDULLE, D. ARJMAND, AND E. PAGANONI, *An elliptic local problem with exponential decay of the resonance error for numerical homogenization*. arXiv preprint arXiv:2001.06315, 2020.
- [5] A. ABDULLE, D. ARJMAND, AND E. PAGANONI, *A parabolic local problem with exponential decay of the resonance error for numerical homogenization*, Math. Models Methods Appl. Sci., (2021), pp. 1–40, <https://doi.org/10.1142/S0218202521500603>.
- [6] A. ABDULLE AND A. DI BLASIO, *Numerical homogenization and model order reduction for multiscale inverse problems*, Multiscale Model. Simul., 17 (2019), pp. 399–433, <https://doi.org/10.1137/16M1091320>.

- [7] A. ABDULLE AND A. DI BLASIO, *A Bayesian Numerical Homogenization Method for Elliptic Multiscale Inverse Problems*, SIAM/ASA J. Uncertain. Quantif., 8 (2020), pp. 414–450, <https://doi.org/10.1137/18M1187891>.
- [8] A. ABDULLE, L. GANDER, AND G. ROSILHO DE SOUZA, *Optimal stabilized explicit integrators for stiff discrete noise stochastic differential equations*. arXiv preprint arXiv:2106.09339, 2021.
- [9] A. ABDULLE AND G. GAREGNANI, *Random time step probabilistic methods for uncertainty quantification in chaotic and geometric numerical integration*, Stat. Comput., 30 (2020), pp. 907–932, <https://doi.org/10.1007/s11222-020-09926-w>.
- [10] A. ABDULLE AND G. GAREGNANI, *A probabilistic finite element method based on random meshes: A posteriori error estimators and Bayesian inverse problems*, Comput. Methods Appl. Mech. Engrg., 384 (2021), p. 113961, <https://doi.org/10.1016/j.cma.2021.113961>.
- [11] A. ABDULLE, G. GAREGNANI, G. A. PAVLIOTIS, A. M. STUART, AND A. ZANONI, *Drift estimation of multiscale diffusions based on filtered data*, Found. Comput. Math., (2021), <https://doi.org/https://doi.org/10.1007/s10208-021-09541-9>.
- [12] A. ABDULLE, G. GAREGNANI, AND A. ZANONI, *Ensemble Kalman Filter for Multiscale Inverse Problems*, Multiscale Model. Simul., 18 (2020), pp. 1565–1594, <https://doi.org/10.1137/20M1348431>.
- [13] A. ABDULLE, M. J. GROTE, AND G. ROSILHO DE SOUZA, *Stabilized explicit multirate methods for stiff differential equations*. arXiv preprint arXiv:2006.00744, 2020.
- [14] A. ABDULLE, G. A. PAVLIOTIS, AND G. VILMART, *Accelerated convergence to equilibrium and reduced asymptotic variance for Langevin dynamics using Stratonovich perturbations*, C. R. Math. Acad. Sci. Paris, 357 (2019), pp. 349–354, <https://doi.org/10.1016/j.crma.2019.04.008>.
- [15] A. ABDULLE, G. A. PAVLIOTIS, AND A. ZANONI, *Eigenfunction martingale estimating functions and filtered data for drift estimation of discretely observed multiscale diffusions*. arXiv preprint arXiv:2104.10587, 2021.
- [16] A. ABDULLE AND G. ROSILHO DE SOUZA, *A local discontinuous Galerkin gradient discretization method for linear and quasilinear elliptic equations*, ESAIM Math. Model. Numer. Anal., 53 (2019), pp. 1269–1303, <https://doi.org/10.1051/m2an/2019022>.
- [17] A. ABDULLE AND G. ROSILHO DE SOUZA, *A posteriori error analysis of a local adaptive discontinuous Galerkin method for convection-diffusion-reaction equations*. arXiv preprint arXiv:2004.07148, 2020.
- [18] A. ABDULLE AND G. ROSILHO DE SOUZA, *Explicit stabilized multirate methods for stiff stochastic differential equations*. arXiv preprint arXiv:2010.15193, 2020.
- [19] A. ABDULLE AND G. ROSILHO DE SOUZA, *Instabilities and order reduction phenomenon of an interpolation based multirate Runge–Kutta–Chebyshev method*. arXiv preprint arXiv:2003.03154, 2020.
- [20] M. CROCI AND G. ROSILHO DE SOUZA, *Mixed-precision explicit stabilized Runge–Kutta methods for single- and multi-scale differential equations*. arXiv preprint arXiv:2109.12153, 2021.
- [21] G. GAREGNANI, *Sampling methods for Bayesian inference involving convergent noisy approximations of forward maps*. arXiv preprint arXiv:2111.03491, 2021.
- [22] G. GAREGNANI AND A. ZANONI, *Robust estimation of effective diffusions from multiscale data*. arXiv preprint arXiv:2109.03132, 2021.
- [23] G. A. PAVLIOTIS AND A. ZANONI, *Eigenfunction martingale estimators for interacting particle systems and their mean field limit*. arXiv preprint arXiv:2112.04870, 2021.
- [24] A. ZANONI, *Homogenization results for the generator of multiscale Langevin dynamics in weighted Sobolev spaces*. arXiv preprint arXiv:2112.04921, 2021.

3 Output Data

3.1 Scientific publications

Journal articles

- [1] A. ABDULLE, I. ALMUSLIMANI, AND G. VILMART, *Optimal explicit stabilized integrator of weak order 1 for stiff and ergodic stochastic differential equations*, SIAM/ASA J. Uncertain. Quantif., 6 (2018), pp. 937–964, <https://doi.org/10.1137/17M1145859>
- [2] A. ABDULLE, D. ARJMAND, AND E. PAGANONI, *Exponential decay of the resonance error in numerical homogenization via parabolic and elliptic cell problems*, C. R. Math. Acad. Sci. Paris, 357 (2019), pp. 545–551, <https://doi.org/10.1016/j.crma.2019.05.011>
- [3] A. ABDULLE, D. ARJMAND, AND E. PAGANONI, *A parabolic local problem with exponential decay of the resonance error for numerical homogenization*, Math. Models Methods Appl. Sci., (2021), pp. 1–40, <https://doi.org/10.1142/S0218202521500603>
- [4] A. ABDULLE AND A. DI BLASIO, *Numerical homogenization and model order reduction for multiscale inverse problems*, Multiscale Model. Simul., 17 (2019), pp. 399–433, <https://doi.org/10.1137/16M1091320>
- [5] A. ABDULLE AND A. DI BLASIO, *A Bayesian Numerical Homogenization Method for Elliptic Multiscale Inverse Problems*, SIAM/ASA J. Uncertain. Quantif., 8 (2020), pp. 414–450, <https://doi.org/10.1137/18M1187891>
- [6] A. ABDULLE AND G. GAREGNANI, *Random time step probabilistic methods for uncertainty quantification in chaotic and geometric numerical integration*, Stat. Comput., 30 (2020), pp. 907–932, <https://doi.org/10.1007/s11222-020-09926-w>
- [7] A. ABDULLE AND G. GAREGNANI, *A probabilistic finite element method based on random meshes: A posteriori error estimators and Bayesian inverse problems*, Comput. Methods Appl. Mech. Engrg., 384 (2021), p. 113961, <https://doi.org/10.1016/j.cma.2021.113961>
- [8] A. ABDULLE, G. GAREGNANI, G. A. PAVLIOTIS, A. M. STUART, AND A. ZANONI, *Drift estimation of multiscale diffusions based on filtered data*, Found. Comput. Math., (2021), <https://doi.org/https://doi.org/10.1007/s10208-021-09541-9>
- [9] A. ABDULLE, G. GAREGNANI, AND A. ZANONI, *Ensemble Kalman Filter for Multiscale Inverse Problems*, Multiscale Model. Simul., 18 (2020), pp. 1565–1594, <https://doi.org/10.1137/20M1348431>
- [10] A. ABDULLE, G. A. PAVLIOTIS, AND G. VILMART, *Accelerated convergence to equilibrium and reduced asymptotic variance for Langevin dynamics using Stratonovich perturbations*, C. R. Math. Acad. Sci. Paris, 357 (2019), pp. 349–354, <https://doi.org/10.1016/j.crma.2019.04.008>
- [11] A. ABDULLE AND G. ROSILHO DE SOUZA, *A local discontinuous Galerkin gradient discretization method for linear and quasilinear elliptic equations*, ESAIM Math. Model. Numer. Anal., 53 (2019), pp. 1269–1303, <https://doi.org/10.1051/m2an/2019022>

Preprints submitted for publication

- [1] A. ABDULLE, D. ARJMAND, AND E. PAGANONI, *An elliptic local problem with exponential decay of the resonance error for numerical homogenization*. arXiv preprint arXiv:2001.06315, 2020
- [2] A. ABDULLE, D. ARJMAND, AND E. PAGANONI, *Analytical and numerical study of a modified cell problem for the numerical homogenization of multiscale random fields*. arXiv preprint arXiv:2007.10828, 2020

- [3] A. ABDULLE, L. GANDER, AND G. ROSILHO DE SOUZA, *Optimal stabilized explicit integrators for stiff discrete noise stochastic differential equations*. arXiv preprint arXiv:2106.09339, 2021
- [4] A. ABDULLE, M. J. GROTE, AND G. ROSILHO DE SOUZA, *Stabilized explicit multirate methods for stiff differential equations*. arXiv preprint arXiv:2006.00744, 2020
- [5] A. ABDULLE, G. A. PAVLIOTIS, AND A. ZANONI, *Eigenfunction martingale estimating functions and filtered data for drift estimation of discretely observed multiscale diffusions*. arXiv preprint arXiv:2104.10587, 2021
- [6] A. ABDULLE AND G. ROSILHO DE SOUZA, *A posteriori error analysis of a local adaptive discontinuous Galerkin method for convection-diffusion-reaction equations*. arXiv preprint arXiv:2004.07148, 2020
- [7] A. ABDULLE AND G. ROSILHO DE SOUZA, *Explicit stabilized multirate methods for stiff stochastic differential equations*. arXiv preprint arXiv:2010.15193, 2020
- [8] M. CROCI AND G. ROSILHO DE SOUZA, *Mixed-precision explicit stabilized Runge–Kutta methods for single- and multi-scale differential equations*. arXiv preprint arXiv:2109.12153, 2021
- [9] G. GAREGNANI, *Sampling methods for Bayesian inference involving convergent noisy approximations of forward maps*. arXiv preprint arXiv:2111.03491, 2021
- [10] G. GAREGNANI AND A. ZANONI, *Robust estimation of effective diffusions from multiscale data*. arXiv preprint arXiv:2109.03132, 2021
- [11] G. A. PAVLIOTIS AND A. ZANONI, *Eigenfunction martingale estimators for interacting particle systems and their mean field limit*. arXiv preprint arXiv:2112.04870, 2021
- [12] A. ZANONI, *Homogenization results for the generator of multiscale Langevin dynamics in weighted Sobolev spaces*. arXiv preprint arXiv:2112.04921, 2021

Technical Reports

- [1] A. ABDULLE AND G. ROSILHO DE SOUZA, *Instabilities and order reduction phenomenon of an interpolation based multirate Runge–Kutta–Chebyshev method*. arXiv preprint arXiv:2003.03154, 2020

3.2 Academic events

Giacomo Garegnani has given the following presentations on the topics of the project:

- **Workshop presentation:** *Calibration of probabilistic numerical methods*, Dagstuhl Seminar “Probabilistic Numerical Methods – From Theory to Implementation”, October 2021, Dagstuhl, Germany
- **Conference presentation:** *Random mesh FEM: A probabilistic approach to the FEM*, European Finite Element Fair, September 2021, Paris, France
- **Seminar presentation:** *Filtering the data: An alternative to subsampling for drift estimation of multiscale diffusions*, RWTH Aachen University, January 2021, Aachen, Germany
- **Conference presentation (cancelled due to Covid19):** *Model misspecification and uncertainty quantification for drift estimation in multiscale diffusion processes*, SIAM conference on uncertainty quantification, March 2020, Garching, Germany
- **Seminar presentation:** *A pre-processing technique for asymptotically correct drift estimation in multiscale diffusion processes*, Imperial College London, February 2020, London, UK

- **Seminar presentation:** *Bayesian inference of multiscale differential equations*, Caltech, August 2019, Pasadena, US
- **Seminar presentation:** *Bayesian inference of multiscale diffusion processes*, MATHICSE retreat, June 2019, Champéry, Switzerland
- **Summer school presentation:** *Probabilistic Runge–Kutta methods for uncertainty quantification of numerical errors in geometric integration*, FoMICS-DADSi Summer School on Data Assimilation, September 2018, Lugano, Switzerland
- **Conference presentation:** *Uncertainty quantification of numerical errors in geometric integration via random time steps*, AIMS Conference on Dynamical Systems, Differential Equations and Applications, July 2018, Taipei, Taiwan
- **Seminar presentation:** *Probabilistic geometric integration of ordinary differential equations*, MATHICSE retreat, June 2018, Sainte-Croix, Switzerland
- **Conference presentation:** *Random time steps geometric integrators of ordinary differential equations for uncertainty quantification of numerical errors*, Swiss Numerics Day, April 2018, ETH Zürich, Switzerland
- **Seminar presentation:** *Uncertainty quantification of numerical errors in geometric integration via random time steps*, Max Planck Institute for Intelligent Systems, March 2018, Tübingen, Germany
- **Seminar presentation:** *Probabilistic Runge–Kutta methods for ODEs: Chaotic problems and geometric properties*, MATHICSE retreat, June 2017, Leysin, Switzerland

Andrea Zanoni has given the following presentations on the topics of the project:

- **Conference presentation (upcoming):** *Data-driven homogenization of multiscale Langevin dynamics*, SIAM Conference on uncertainty quantification, April 2022, Atlanta, US
- **Conference presentation:** *Inference of effective diffusions from multiscale data*, Swiss Numerics Day, September 2021, Lausanne, Switzerland
- **Conference presentation:** *Solution of multiscale inverse problems through filtering techniques and numerical homogenization*, 14th WCCM & ECCOMAS Congress 2020, January 2021, virtual event

Andrea Di Blasio has given the following presentations on the topics of the project:

- **Conference presentation:** *Model order reduction and numerical homogenization for solving Bayesian multiscale inverse problems*, EUROMECH colloquium, August 2018, Bad-Herrenalb, Germany
- **Seminar presentation:** *Numerical methods for solving Bayesian multiscale inverse problems*, MATHICSE retreat, June 2018, Sainte-Croix, Switzerland
- **Conference presentation:** *Numerical homogenization and model order reduction for solving linear elasticity problems in perforated domains*, ECCM – ECFD 2018, June 2018, Glasgow, UK
- **Conference presentation:** *Model order reduction and Bayesian techniques for multiscale inverse problems*, COMPLAS 2017, September 2017, Barcelona, Spain
- **Conference presentation:** *Numerical homogenization and Bayesian techniques for multiscale inverse problems*, EQUADIFF 2017, July 2017, Bratislava, Slovakia
- **Seminar presentation:** *Using numerical homogenization for solving elliptic multiscale inverse problems*, MATHICSE retreat, June 2017, Leysin, Switzerland

- **Conference presentation:** *Solving elliptic multiscale inverse problems using Bayesian techniques and numerical homogenization*, Swiss Numerics Day, April 2017, Basel, Switzerland
- **Seminar presentation:** *A reduced basis method for multiscale inverse problems*, MATH-ICSE retreat, June 2016, Leysin, Switzerland
- **Conference poster:** *A reduced basis method for multiscale inverse problems*, Swiss Numerics Day, April 2016, Fribourg, Switzerland

Giacomo Rosilho de Souza has given the following presentations on the topics of the project:

- **Conference presentation:** *Multirate stabilized explicit methods based on a modified equation for problems with multiple scales*, SIAM conference on computational science and engineering (CSE21), March 2021, virtual event
- **Workshop presentation:** *Multirate stabilized explicit methods for deterministic and stochastic differential equations without clear-cut scale separation*, CECAM workshop “Multiscale simulations of soft matter: New method developments and mathematical foundations”, September 2020, Mainz, Germany, virtual event
- **Seminar presentation:** *Multirate explicit stabilized integrators for stiff differential equations*, Universität Basel, November 2019, Basel, Switzerland
- **Conference presentation:** *Stabilized explicit multirate methods for ordinary and stochastic differential equations with multiple scales*, SciCADE International Conference on Scientific Computation and Differential Equations, July 2019, Innsbruck, Austria
- **Seminar presentation:** *Multirate explicit stabilized integrators for stiff differential equations*, MATHICSE seminar, June 2019, Champéry, Switzerland
- **Seminar presentation:** *A local discontinuous Galerkin FEM for linear and quasilinear elliptic equations*, MATHICSE seminar, June 2018, Sainte-Croix, Switzerland
- **Conference presentation:** *A priori and a posteriori analysis of a local scheme for elliptic equations*, Swiss Numerics Day, April 2018, Zürich, Switzerland
- **Seminar presentation:** *Predictor corrector local time stepping scheme for parabolic equations*, MATHICSE seminar, June 2017, Leysin, Switzerland
- **Seminar presentation:** *Two local time stepping techniques for parabolic equations*, MATHICSE seminar, June 2016, Leysin, Switzerland

Assyr Abdulle has given the following presentations on the topics of the project:

- **Workshop presentation:** *Learning effective models from multiscale data: filtering and Bayesian inference*, Oberwolfach workshop “Geometric Numerical Integration”, March 2021, Oberwolfach, Germany
- **Workshop presentation:** *Stabilized explicit multirate methods for ordinary and stochastic differential equations with multiple scales*, Workshop on multiscale methods for deterministic and stochastic dynamics, January 2020, Geneva, Switzerland
- **Plenary conference presentation:** *Numerical methods for wave propagation in heterogeneous media*, 14th International Conference on Mathematical and Numerical Aspects of Wave Propagation (WAVES 2019), August 2019, Vienna, Austria
- **Workshop presentation:** *A Bayesian approach for multiscale inverse problems*, Banff International Research Station workshop “Integrating the integrators for nonlinear evolution equations: from analysis to numerical methods, high-performance computing and applications”, December 2018, Banff, Canada

- **Workshop presentation:** *Bayesian numerical homogenization methods for multiscale inverse problems*, Workshop on Numerical methods for multiscale PDEs, September 2018, Cargèse, France
- **Workshop presentation:** *Bayesian multiscale inverse problems and probabilistic numerical methods*, Workshop on Interplay of multiscale data assimilation and data science with advanced PDE discretizations, Erwin Schrödinger International Institute for Mathematics and Physics (ESI), June 2018, Vienna, Austria
- **Workshop presentation:** *Probabilistic numerical methods and Bayesian multiscale inverse problems*, Workshop on Data driven modelling of complex systems, Alan Turing Institute, May 2018, London, UK

3.3 Knowledge transfer events

Giacomo Garegnani participated in the following knowledge transfer events:

- **Summer school:** Dobbiaco summer school on Probabilistic Numerics, June 2017, Dobbiaco, Italy
- **Workshop:** Workshop on probabilistic numerical methods, Alan Turing Institute, April 2018, London, UK
- **Co-Supervision of Master Projects:**
 - Andrea Zaroni, *Ensemble Kalman filter for multiscale inverse problems*, EPFL, 2019 – co-supervised with Assyr Abdulle and Sandro Salsa (Politecnico di Milano)
 - Aleksa Stanković, *Probabilistic methods for differential equations: adaptivity and Bayesian inverse problems*, EPFL, 2018 – co-supervised with Assyr Abdulle
- **Co-Supervision of Semester Projects:**
 - Daniele Hamm, *Numerical study of an iterative filtering method for drift estimation of multiscale diffusions*, EPFL, 2021 – co-supervised with Assyr Abdulle
 - Anne-Sophie Van De Velde, *Parameter estimation in multiscale Langevin dynamics with particle filters and Monte Carlo methods*, EPFL, 2020 – co-supervised with Assyr Abdulle
 - Wojciech Reise, *Probabilistic solvers for ordinary differential equations*, EPFL, 2019 – co-supervised with Assyr Abdulle

Giacomo Rosilho de Souza participated in the following knowledge transfer events:

- **Co-Supervision of Master Projects:**
 - Lia Gander, *Optimized Chebyshev methods for discrete stochastic simulations*, EPFL, 2019 – co-supervised with Assyr Abdulle
 - Tristan Chanay, *Optimal explicit stabilized method for jump-diffusion processes*, EPFL, 2021 – co-supervised with Assyr Abdulle

3.4 Collaboration

The following national and international collaborations took place:

- Prof. Grigorios A. Pavliotis, Department of Mathematics, Imperial College London, London, UK; including:
 - scientific visit of Prof. Grigorios A. Pavliotis at EPFL (March 2019)
 - scientific visit of Giacomo Garegnani at Imperial College London (3.2.2020-7.2.2020)

– planned scientific visit of Andrea Zanoni at Imperial College London (14.02.2022-18.03.2022)

- Prof. Andrew M. Stuart, Department of Computing and Mathematical Sciences, Caltech, Pasadena, US; including a scientific visit of Giacomo Garegnani at Caltech (19.08.2019-20-09-2019)
- Prof. Marcus J. Grote, Departement Mathematik und Informatik, Universität Basel, Basel, Switzerland
- MER Gilles Vilmart, Section de Mathématiques, Université de Geneve, Geneva, Switzerland

3.5 Awards

- Giacomo Rosilho de Souza won the John Butcher prize in numerical analysis for the talk *Multirate explicit stabilized integrators for stiff differential equations* that he gave at the SciCADE conference, held in July 2019, Innsbruck, Austria
- Giacomo Garegnani won a SIAM travel award to join the SIAM conference on uncertainty quantification, held in March 2020, Garching, Germany (cancelled due to Covid19)