Siwar Badreddine

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Research interest

High dimensional problems arising in molecular simulations, Tensor algorithms, Algorithmic complexity, Low-rank approximation methods, Numerical linear algebra, Numerical analysis, Quantum chemistry.

Education

- **Sorbonne university/INRIA Paris** — Paris, France
  Studying towards Ph.D — *Oct. 2020 - Present*
  - **Thesis title**: Tensor techniques for high dimensional problems arising in quantum chemistry
  - **Thesis topics**: We focus on high-dimensional problems arising in molecular simulations. These problems have extreme dimensions and when represented by tensors, they can also have large ranks. We will thus examine efficient algorithms for solving eigenvalue problems from molecular simulations in which the operator is represented as a tensor. In particular, we are interested in approaches such as DRMG that address high dimensional problems. This Ph.D is part of the EMC2 project.
  - **Advisor**: Laura Grigori
- **ENSTA ParisTech** — Paris, France
  Master of Science in Applied Mathematics and Engineering — *Sep. 2017 - Sep. 2020*
  - **Courses taken**
    Fast algorithms for the solution of scattering problems by boundary element methods.
    Modeling and simulation of complex systems at different scales.
    Parallel programming with MPI.
    Derivative-free optimization.
    Finite volume and finite elements methods.
    Scientific visualization.
  - **Double degree with National Engineering School of Tunis.**

Experience

- **INRIA (National Institute for Research in Digital Science and Technology)** — Paris, France
  Final year project — *Mar. 2020 - Aug. 2020*
  - **Low-rank approximation of the high dimensional two-electron integral tensor and its application in quantum chemistry.)**:
    * Evaluation of the high-dimensional two-electron integrals with long-range interaction (fourth-order tensors) that are vital in large-scale applications of accurate electronic-structure methods in quantum chemistry.
    * Development of a novel numerical approximation method based on Chebyshev interpolation method and Gaussian quadrature rule for numerical integration to get a faster and more accurate solution of the two-electron integrals (six-dimensional integrals).
    * Compression of the fourth-order tensor by using low-rank decomposition methods such as truncated singular value decomposition, truncated randomized singular value decomposition, QR decomposition, and interpolative decomposition.

    Programming Languages: *Matlab, Python.*
- **CEA (The Alternative Energies and Atomic Energy Commission)** — Paris, France
  Research internship — *May 2019 -Aug. 2019*
  - **Data analysis**:

* Data analysis (Felix data) taken in 2018 from the Atlas experiment at Cern's Large Hadron Collider (LHC) for proton collisions to test the working performances of Liquid Argon Trigger Digitizer Board in the electromagnetic calorimeter.
* The use of statistical techniques to identify types of problems found in the data and to spot anomalous structures while analyzing the electronic noise signal.
* Implementation of sorting methods and simulation codes in order to select the interesting data by sorting between real and anomalous events.

Programming Languages: *C++, Python.*

Software and academic Projects

- **SCATensor**: *(ongoing)* A package in Julia that aims to implement ALS and MALS algorithms (known in quantum Chemistry as DMRG) with improved version.

  Important features:

  - Efficient construction of ab initio Hamiltonian operators and eigenfunctions using a block sparse tensor train representation.
  - Optimized algorithms for performing fast block sparse tensor contractions.
  - Efficient compression of block sparse tensors.

  Programming Languages: Julia.
- **Academic projects**:

  - Simulation of dynamic crowd behaviors using the finite element method.
  - Recommendation engine.
  - Parallel computing to solve structured and unstructured problems from the heat equation using the MPI library.
  - Solving scattering problems using low rank approximations and hierarchical matrices.
  - Time series analysis and prediction.

  Programming Languages: C++, Matlab, R.

Skills

- **Programming Languages**: Julia, Python, Matlab
- **Sporadically Used:**: C++, R
- **Technologies**: Git
- **Languages**: Native; Arabic. Advanced; English, French.

Conferences, Awards and Miscellaneous Information

- **IPAM workshop** — University of California, Los Angeles, USA
  New Mathematics for the Exascale: Applications to Materials Science. — *Mar. 2023*
- **Visiting scholar** — University of California, Berkeley, USA
  Jan. 2023
- **EMC2 Seminar** — LJLL, Sorbonne university
  Dec. 2022
- **7th IMA conference.** — Birmingham,Uk
  Conference on Numerical Linear Algebra and Optimization. — *Jul. 2022*
- **Householder symposium 2020.** — Selva di Fassano, Italy
  Symposium on Numerical Linear Algebra. — *Jun. 2022*
- **Participation to the CEMRACS 2021 summer school.** — Marseille, France
  Project on DMRG. — *Jul. 2021 - Aug. 2021*
- **SIAM CSE 2021 Conference**
  SIAM Student Travel Award 2021 — *Mar. 2021*

Part-time teaching

- **EFREI PARIS engineering school of digital technologies** — Paris, France
  Bachelor's degree of Science classes: Linear algebra courses — *Jan. 2022 - May. 2022*
- **Sorbonne university** — Paris, France
  Master 1 classes: Introduction to Python programming and PDE's approximation with Python — *Mar. 2021 - May. 2021*

References

- **Laura Grigori**
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  Alpines group, INRIA Paris, France
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