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[Inici](#) > BSC hosts its 3rd Doctoral Symposium

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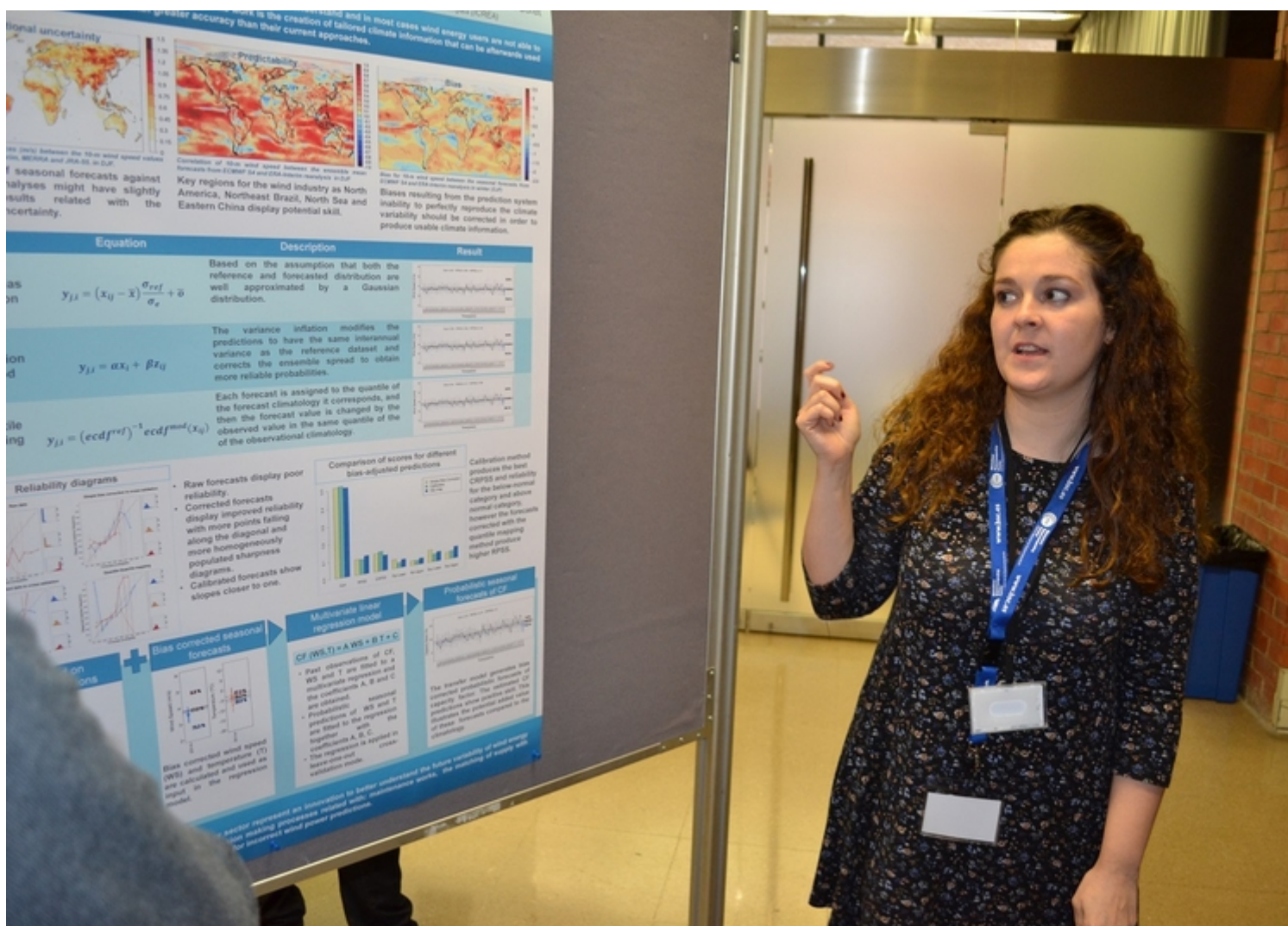
In this third edition of the BSC Doctoral Symposium we had six different sessions of talks tackling the topics of: Postdoc research at BSC; Algorithms, Physics & Data Science Algorithms, Numerical Methods and Data Science; Life Sciences; Simulations and Modelling; and Performance. The posters were exhibited and presented during four poster sessions that created lively discussion and gave the authors the opportunity to explain their research and results. The directors of BSC strongly supported the creation of the symposium and its organisation and Mateo Valero, Director of BSC, gave the opening speech.

The keynote speaker, Prof. Francisco Doblas Reyes, gave the lecture: Big Data for the Study of Climate Change and Air Quality. He is Director of the Department of Earth Sciences at BSC and ICREA research professor at the Catalan Institute of Climate (IC3). At BSC he coordinates the largest FP7 project on climate prediction. The Department hosts more than 50 engineers, physicists, mathematicians and other air quality and climate researchers who try to bring the latest developments in supercomputing and Big Data to provide the best information and services. He is author of more than 100 peer-reviewed papers.

The training courses given by researchers from Computer Science Department, reviewed the fundamental Algorithms and Techniques for Data and Computationally Intensive Problems (Prof. Vassil Alexandrov, ICREA-BSC) and introduced Scientific Visualisation of Data (Dr. Javier Espinosa) as well as provided some practice regarding these concepts.

For further details, please visit the Symposium webpage: <http://www.bsc.es/doctoral-symposium-2016>

More photos available [here](#).



- Dynamic Library transparent to the user
 - No need to analyze nor modify the application
- Tries to maximize the utilization of computational resources
 - Manages the number of threads in the shared memory level
 - Compatible with MPI, OpenMP and/or OmpSs
- Has two modules independent and compatible:

LeWI

Lend When Idle

- Motivation: Avoid expensive process of optimizing applications
- Can solve imbalance from:
 - Input Data
 - Computational Heterogeneity
 - Noise



- Lend CPU when not using it
- Intranode resource sharing

Success story:
• App 1: 1000 nodes, 1000 MPI processes, 1 thread per node, 1 thread per process

• With DLB & LeWI: 2000 MPI processes, 1 thread per node, 1 thread per process

DROM

Dynamic Resource Ownership Management

- Motivation: Allow dynamic reassignment of resources depending on demand
- Enables different scheduling policies in HPC systems
 - Prioritize applications
 - Maximize utilization
 - Fair sharing
- Can work in cooperation with the job scheduler



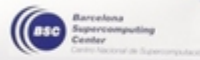
- CPUs can be removed from a running application and given to another one
 - To a new application to allow interactive simulation (maximize utilization)
 - To an existing application to prioritize its execution

Interactive simulation:
- Red: Running simulation in 16 CPUs
- Pink: Co-allocate analysis in 4 CPUs



Enhanced Monte Carlo methods for Sparse Approximate Matrix Inversion

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Introduction

An enhanced version of a parallel stochastic Sparse Approximate Inverse (SAI) preconditioner for general matrices is presented. This method is used in contrast to the well known stochastic preconditioner Modified Sparse approximate Inverse Preconditioner (MSPAI). The new proposal features 2 main advantages:
 - Lower computational complexity with respect to the matrix size.
 - Better parallelism.

The behavior of the proposed algorithm is studied, its performance measured, evaluated and compared with MSPAI.

Our Approach

The preconditioner can be transformed a complex $A^{-1}A$ into a simpler equivalent form. MSPAI preconditioner use an approximation of the inverse matrix to reduce the complexity as follows:

$$A^{-1}x = k$$

$$A^{-1}Ax = A^{-1}k$$

$$E^{-1}x = A^{-1}k$$

Conclusions

- A Monte Carlo based preconditioner for general matrices has been proposed as an alternative to MSPAI algorithm.
- Monte Carlo approach has shown to produce preconditioners of comparable quality to the stochastic MSPAI ones.
- Proposed approach generates preconditioners more efficiently, outperforming or matching the deterministic approach, especially for the problem sizes.
- Further improvements are needed by Monte Carlo for the preconditioner compared to MSPAI.

References:
 - O. Esquivel, D. Davila, V. Alexandrov, "A New Sparse Monte Carlo Preconditioner for General Matrices", *SIAM J. Matrix Anal. Appl.*, vol. 58, no. 1, pp. 1-15, 2016.
 - V. Alexandrov, "A New Sparse Monte Carlo Preconditioner for General Matrices", *SIAM J. Matrix Anal. Appl.*, vol. 58, no. 1, pp. 1-15, 2016.
 - O. Esquivel, D. Davila, V. Alexandrov, "A New Sparse Monte Carlo Preconditioner for General Matrices", *SIAM J. Matrix Anal. Appl.*, vol. 58, no. 1, pp. 1-15, 2016.

Experiments

The main program are carried out during the experimentation. Preconditioner comparison and future evaluation. In the first step, matrices are used as inputs to both the MSPAI and the Monte Carlo based preconditioners. In the last step preconditioner are used to create an equivalent SAAI which is then solved by the CGMRES implementation in ParSolvers 1.0.0 library.

Time was recorded for each of the matrices in the following set:

Matrix	Dimension	nnz	Type
Spars	14,000 x 14,000	1,802,000	non-symmetric
NaCl	5,000 x 5,000	305,000	symmetric
Number_01_011	300,000 x 300,000	10,420,000	non-symmetric
Number_01_011	3,000 x 3,000	12,000	non-symmetric
Time_01_011	20,000 x 20,000	300,000	symmetric
Time_01_011	80,000 x 80,000	2,000,000	symmetric

We compared the algorithm behavior for matrices drawn from different sets from two collections - The Matrix Market and The University of Florida Sparse Matrix Collection as well from some real life problems from our scientific collaborations. All matrices are non-diagonally dominant.

Experiments were selected to produce preconditioners with similar properties and therefore producing methods within similar ranges when used as preconditioners for CGMRES.

Statistical experiments have been carried out on the MareNostrum III supercomputer at BSC.

Results

It is evident that Monte Carlo preconditioner is faster than MSPAI and in some cases MSPAI is not converging at all for certain number of cores. (see Fig 1). Also it is important to notice the larger amount of iterations used by MSPAI to obtain similar iteration time in comparison with Monte Carlo.

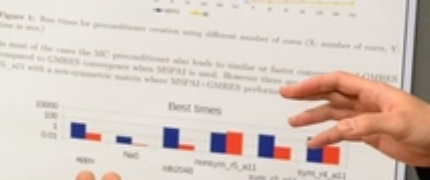


Figure 1: Run times for preconditioner creation using different number of cores (X: number of cores, Y: time in sec.)

In most of the cases the MC preconditioner also leads to similar or faster convergence compared to CGMRES convergence when MSPAI is used. However there are cases where MSPAI + CGMRES performs better than MC + CGMRES when MSPAI + CGMRES performance is used.

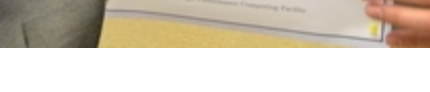


Figure 2: Dist. Times. Comparison of MSPAI times and MC times for different matrices.

Further improvements are needed by Monte Carlo for the preconditioner compared to MSPAI.

Acknowledgments

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