egee

Estimating the Performance of BLAST runs on the EGEE Grid

Abel Carrión

Ignacio Blanquer

Vicente Hernández

www.eu-egee.org

Information Society
and Media

**Enabling Grids for E-sciencE**

- **The problem.**

- **Factors affecting the performance.**

- **Experiments on the grid.**

- **The Performance.**

- **Execution model.**

- **Conclusions and further work.**

Enabling Grids for E-sciencE
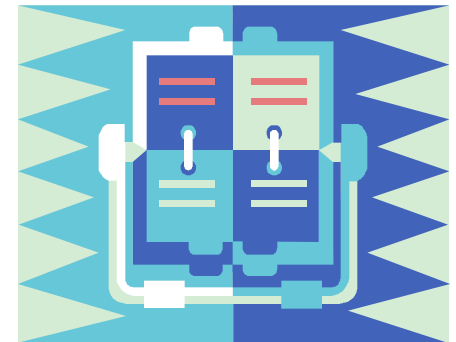
- **Sequence alignment is an key operation in Bioinformatics**
  - It involves computing the comparison of proteomic and genomic samples with respect to annotated databases.
- **It is a part of many Bioinformatics pipelines**
  - Used to search for homologous in the study the functionality of different genes and regions.
  - Used in the phylogenetic taxonomy.
- **There are many tools developed in the literature**
  - Based on the Smith-Waterman transform (e.g. BLAST).
  - Based on Hash Tables (e.g. SSAHA, BLAT).
  - Based on Burroughs-Wheeler Transform (e.g. BWA, Bowtie).
  - And combinations of them (e.g. SSAHA2).

Enabling Grids for E-sciencE

- **BLAST (Basic Local Alignment Search Tool) is the most widely used tool for performing the alignment of any length novel sequences against the ones contained in a determined database.**

  – Although it could be inefficient for many cases, It has a proven reputation.

- **Because a normal use case entails the alignment of millions of sequences, this kind of experiments are very computationally intensive (it demands years of CPU computation).**

Enabling Grids for E-sciencE

- **Problem is massive parallel and fits the requirements for using efficiently Grid infrastructures.**

- **The parallelization process follows the High-Throughput paradigm:**
  - Segmenting the input data file into several chunks which are aligned in independent computation nodes.

nr

Enabling Grids for E-sciencE
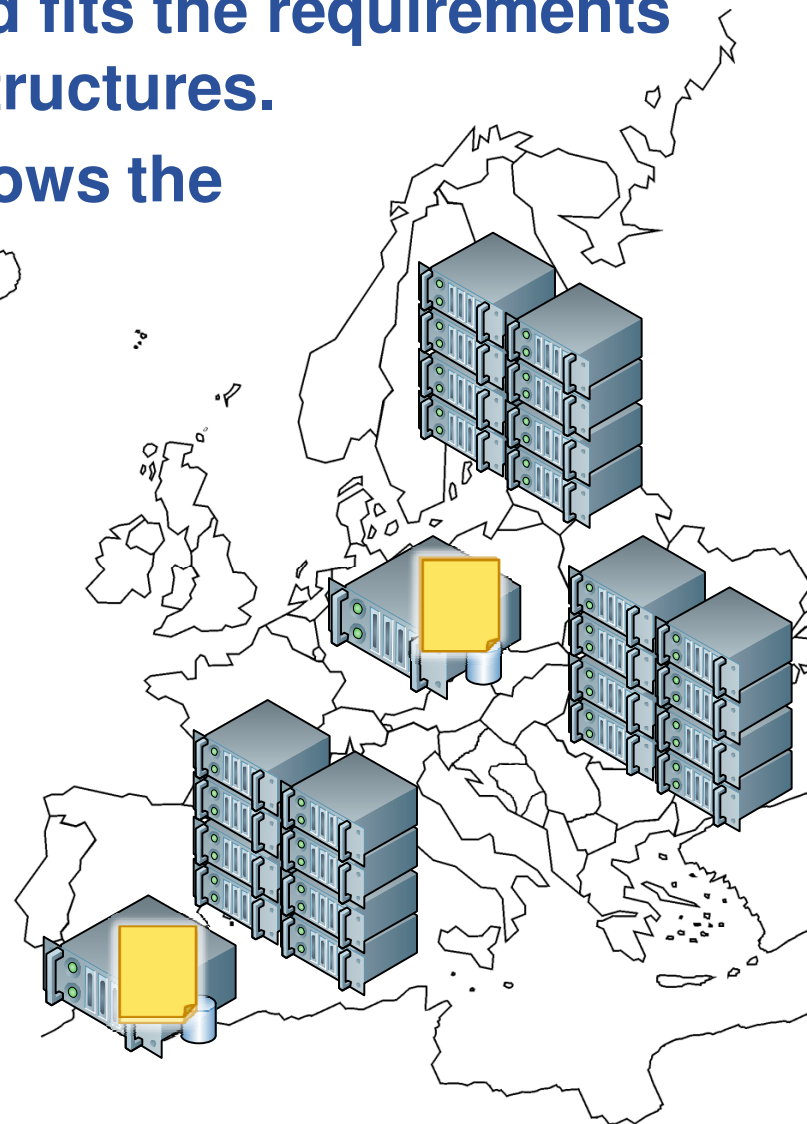
- **Two factors are key for the general performance**
  - A good selection of the resources for computing and storage.
  - A good partition strategy.
- **This not only affects the response time, but also the failure ratio**
  - Queues have a limitation in the maximum job executing time.
  - Fault-tolerance automatic resubmission also needs to know if a job is executing slowly or simply it is blocked.
- **Thus, a key issue when performing the scheduling of thousands of jobs is estimating the response time of the tasks.**
  - Create a model to estimate the execution time of a job.

Enabling Grids for E-sciencE

- **Quasi-Deterministic Factors**
  - Application dependant.
    - Input data file size.
    - DB file size.
    - Similarity.
    - Number of hits.
  - Resource dependant.
    - SPECint (SI00).
   - SPECfp (SF00).
    - Memory.

  Obtained through experiments

- **Undetermisitic Factors**
  - Load dependant
    - Queue size
    - Average waiting time
  - Site dependant
   - Site availability.
    - Specific job failure rates.

  Not yet covered in the study

Enabling Grids for E-sciencE

- **The purpose of this experiment was to analyse the influence of the data size (input file and database).**

- **Using the UniProt database, several files with different sizes were generated and executed in the same machine.**
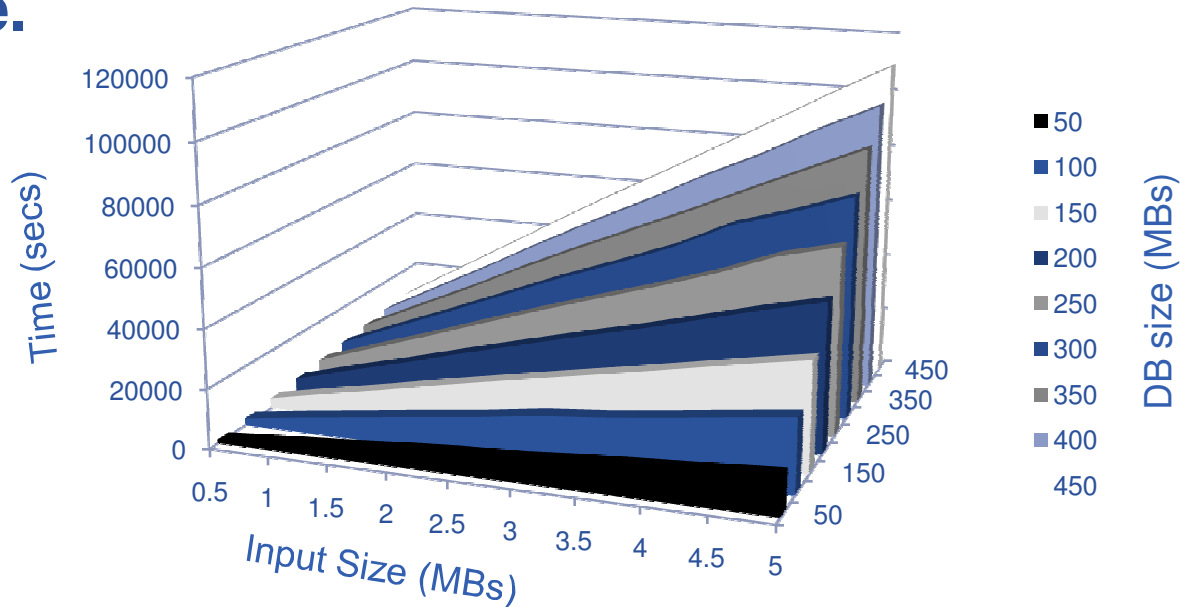

- **The results show that the input file size and database size have a direct linear impact on the response time.**

- **The heuristic nature of BLAST accelerates the comparison of two clearly unrelated sequences**
- **To check the influence of the similarity on the searches, three new versions of the UniProt database were produced, replacing 1%, 5% and 10% of their contents respectively.**
- **As it can be seen, the response time is independent from the similarity between sequences.**
  - This factor will not be considered in the final performance model.

Enabling Grids for E-sciencE
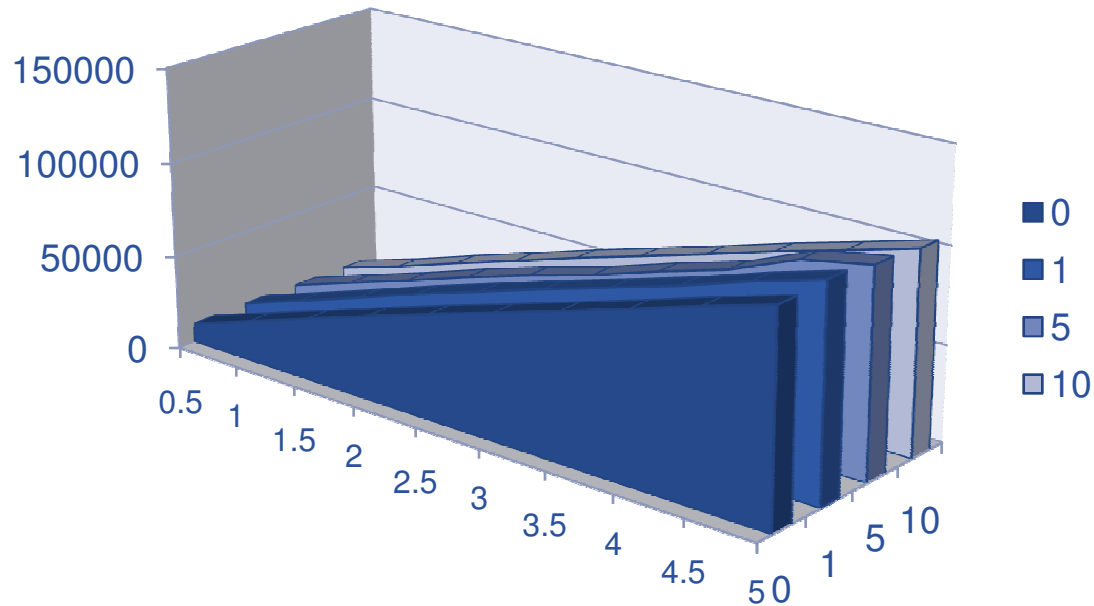
- **An experiment has been executed in different computers for different values of the "BLAST Hits" argument**
  - Values range from 5000 to 25000 (step of 2500) in 30 CEs
    - Soil NCBI Metagenome.
    - 270 Jobs with a duration from 130 to 200 minutes.
  - Although the output increases accordingly, no effect is observed on the response time nor the failure rate.

Enabling Grids for E-sciencE
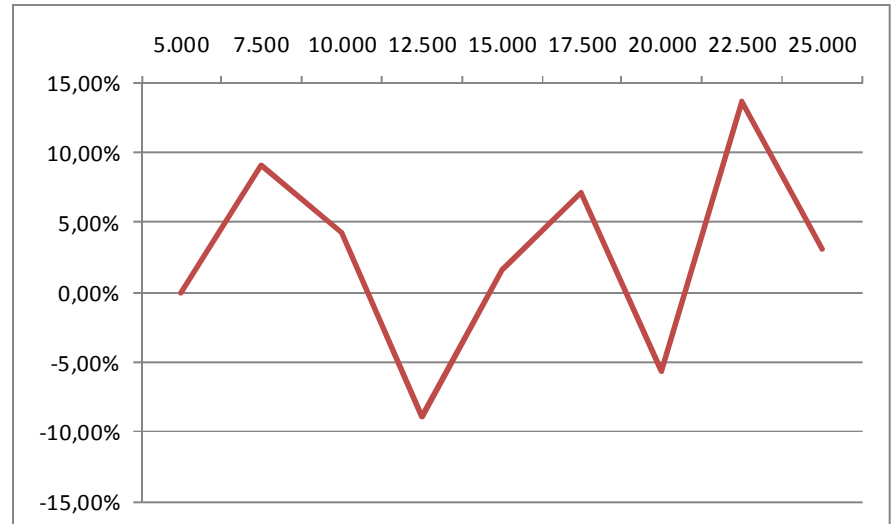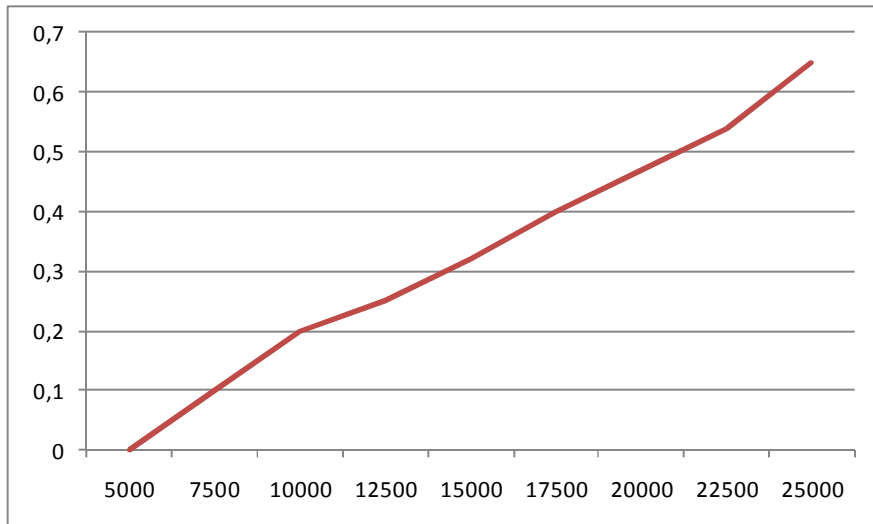
- **The GlueSchema includes the values of Benchmarks SpecInt 2000 and SpecFloat 2000.**

- **9 Different job types have been executed on 19 sites where this information was published.**
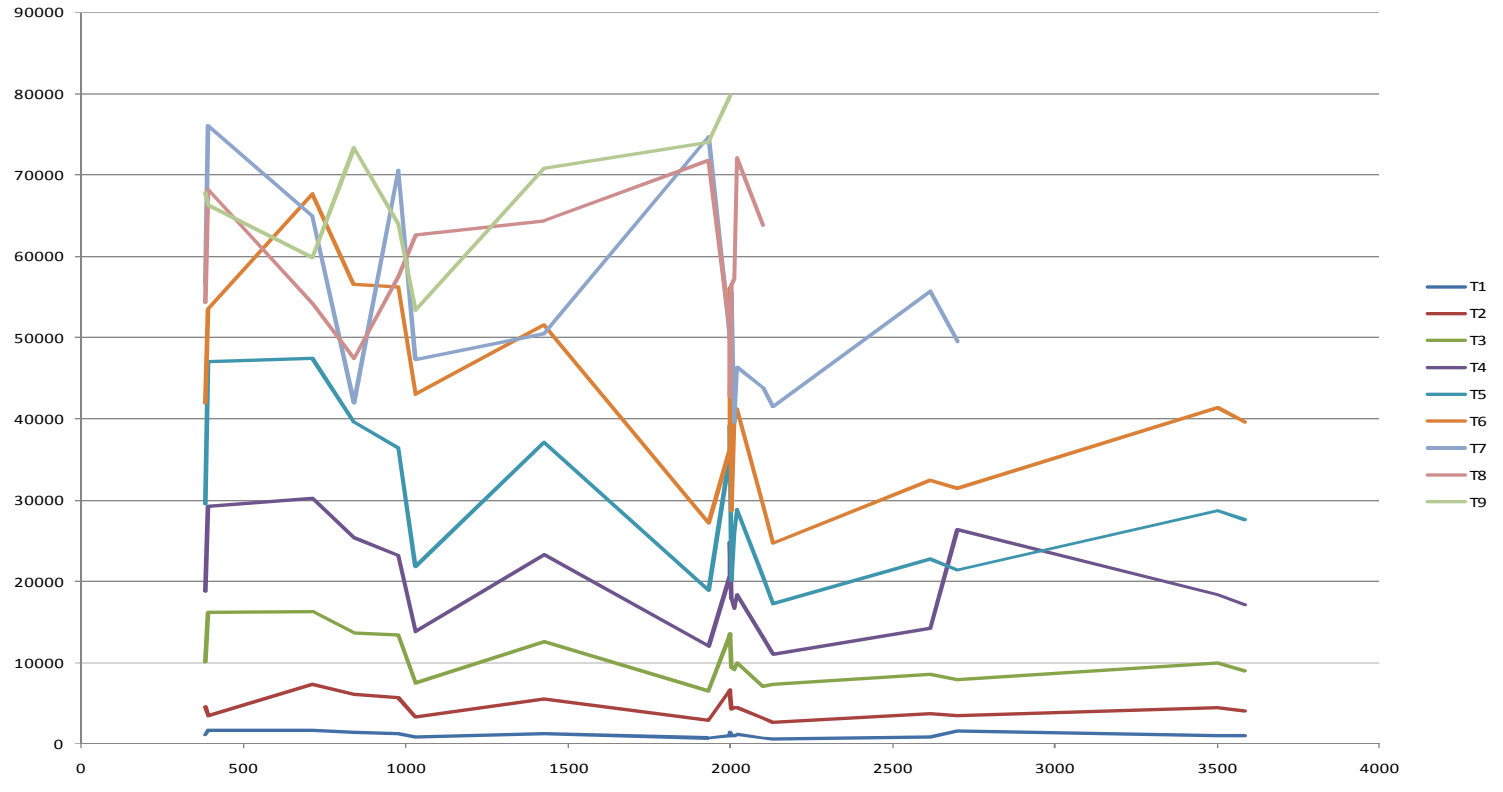
- **The SpecInt and SpecFloat benchmarks do not seem to be correlated with actual performance for BLAST**
  - Correlation index ranges from 0.08 to 0.55 with poor values of significance (up to 77% of randomness).

	T1	T2	T3	T4	T5	T6	T7	T8	T9
Pearson	-0,433	-0,309	-0,533	-0,42	-0,521	-0,549	-0,413	0,079	0,55
p	0,052	0,175	0,014	0,06	0,017	0,011	0,081	0,772	0,089

- **This might be caused by different factors**
  - Unsuitability of the benchmark for BLAST.
  - Lack of accuracy of the benchmark, which is not computed in many sites but obtained from tables.

- **Moreover, the values of the benchmarks are not always published.**

- **A new estimator is needed.**

Enabling Grids for E-sciencE

- **Ratio of average performance with respect to a fixed node**
  - Same tests are repeated in all nodes for different data sizes and speed-ups/downs are computed.
  - A single coefficient is obtained from the sum of all the computing times of all (the same number and type) of jobs.
- **Obviously, much more correlation is shown (high significance, always above 98%, but generally above 99,99%).**

	T1	T2	T3	T4	T5	T6	T7	T8	T9
Pearson	0,888	0,788	0,957	0,897	0,978	0,96	0,889	0,691	0,73
p	1,86E-07	3,33E-05	6,65E-11	8,72E-08	2,10E-13	3,12E-11	8,33E-07	0,004	0,015

Enabling Grids for E-sciencE
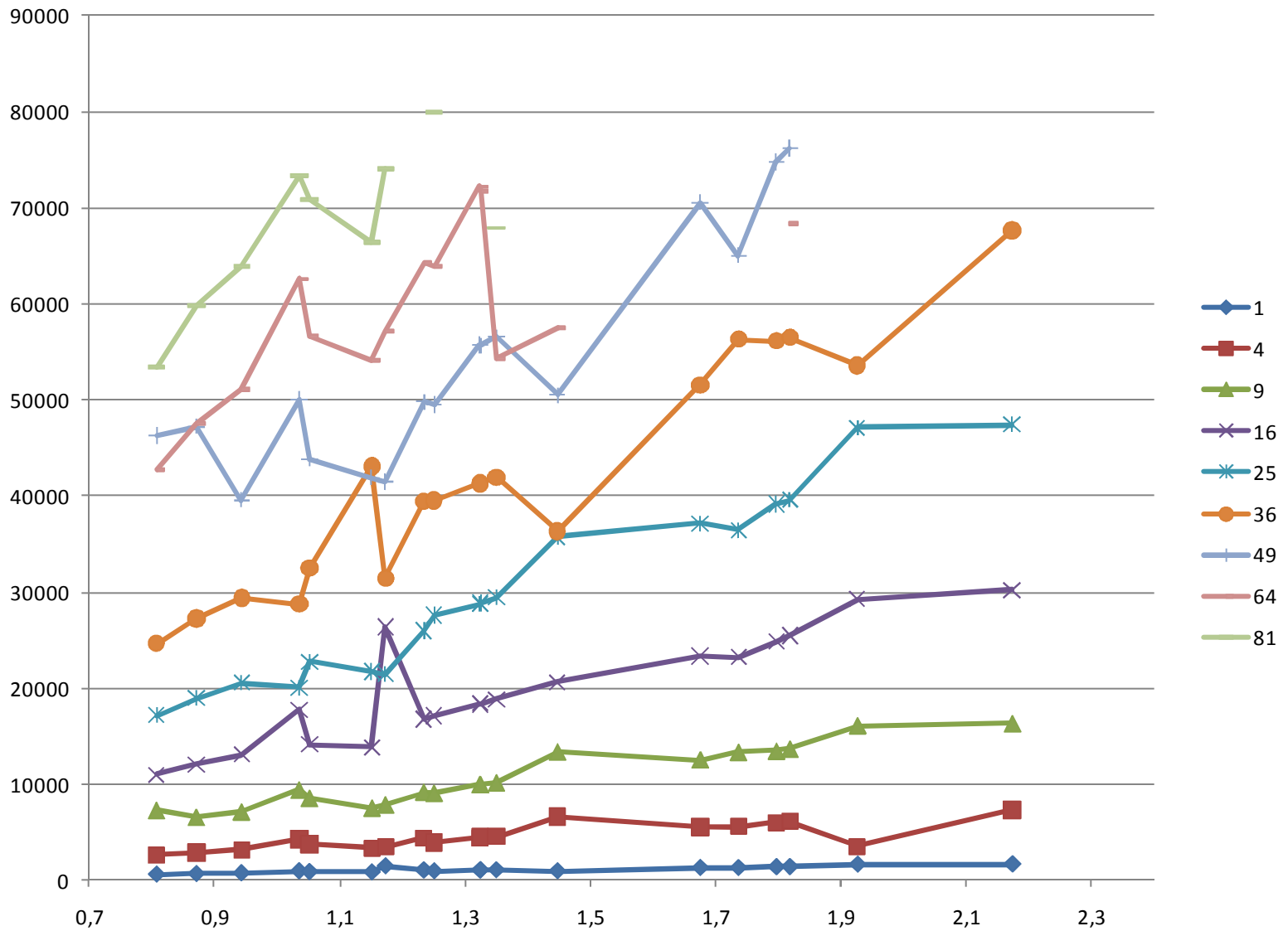
- **Current conclusions**

  - Direct dependence on the Input data size.

  - Direct dependence on the database size.

  - Direct dependence on the inverse of the process speed factor.

  - No dependency on the similarity or number of hits.

 - Low dependence on the memory, except for saturations.

- **Proposed model**

- **Where**

$$T = \frac{P_{Sp}}{Sp} P_{Tm} \left(\frac{T_{inp}}{T_{inp\_basal}} \frac{T_{BD}}{T_{BD\_basal}} \right) + K$$
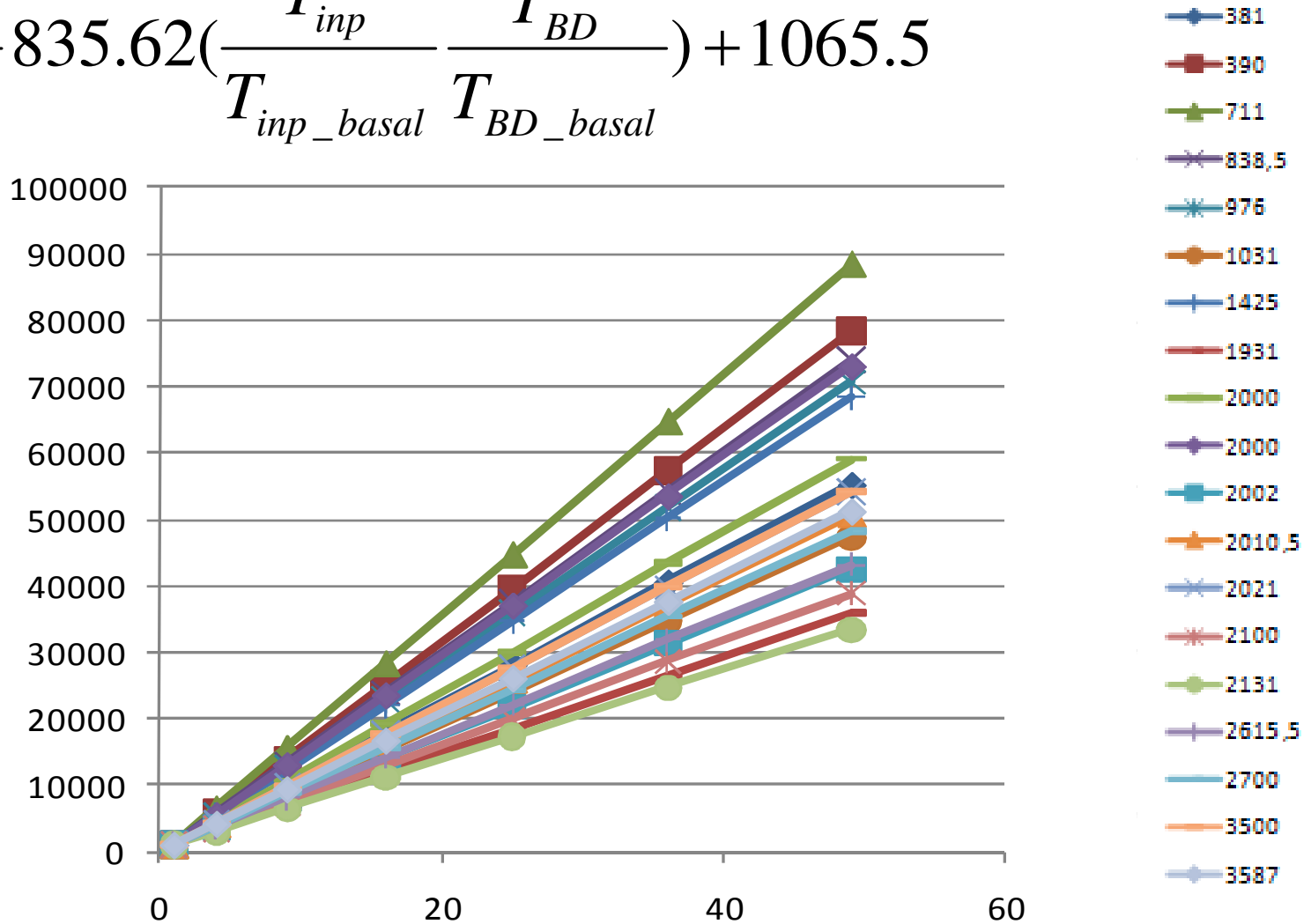
  - P_{Sp}, P_{Tm} and K are the unknown parameters of the regression model.

  - T_{inp} and T_{BD} are the fixed values for the size of data and database.

  - Sp is the ratio between the response time in a reference site and each other site.

  - T_{inp_basal} is 0,5 y T_{BD_basal} is 50.

Enabling Grids for E-sciencE
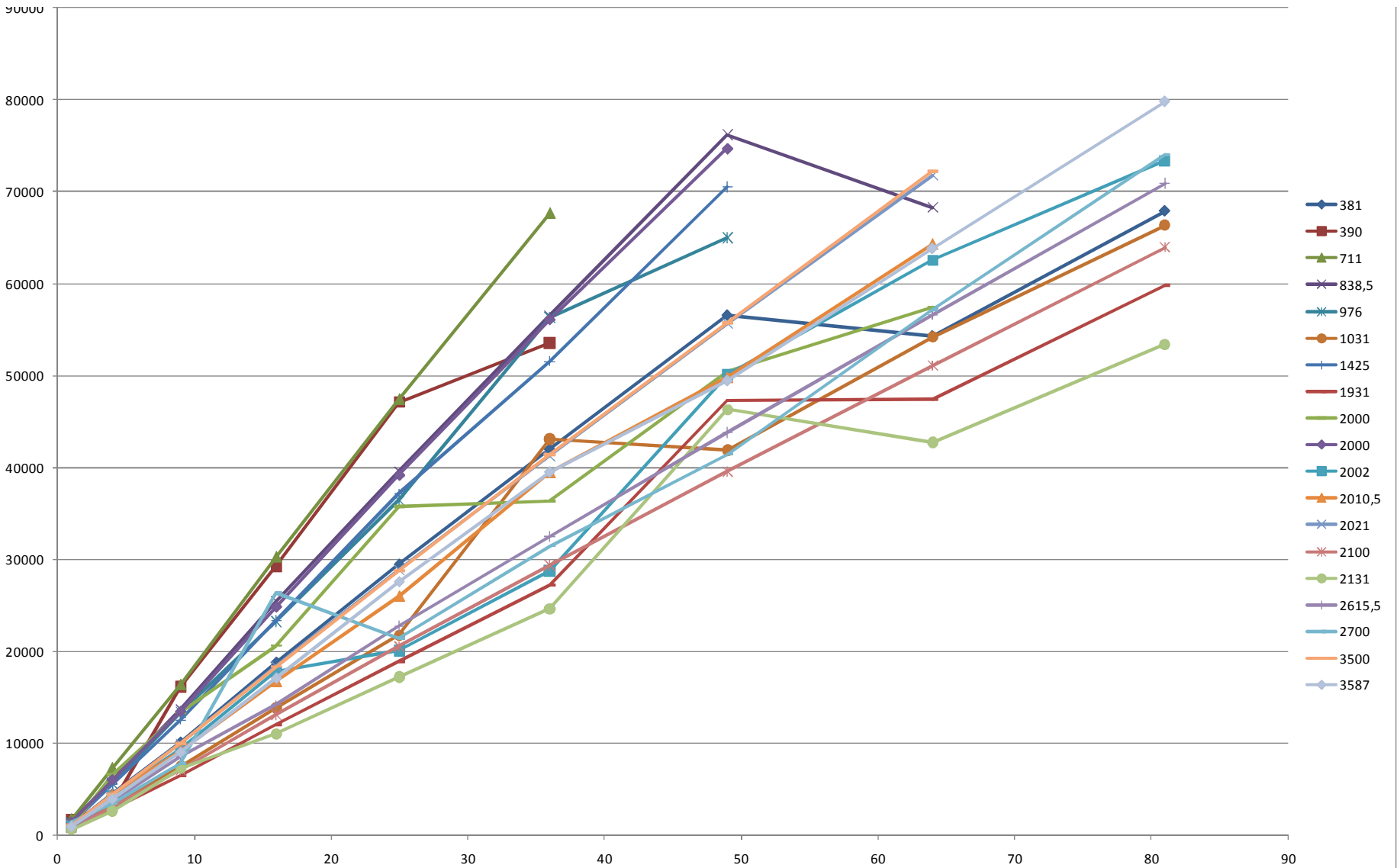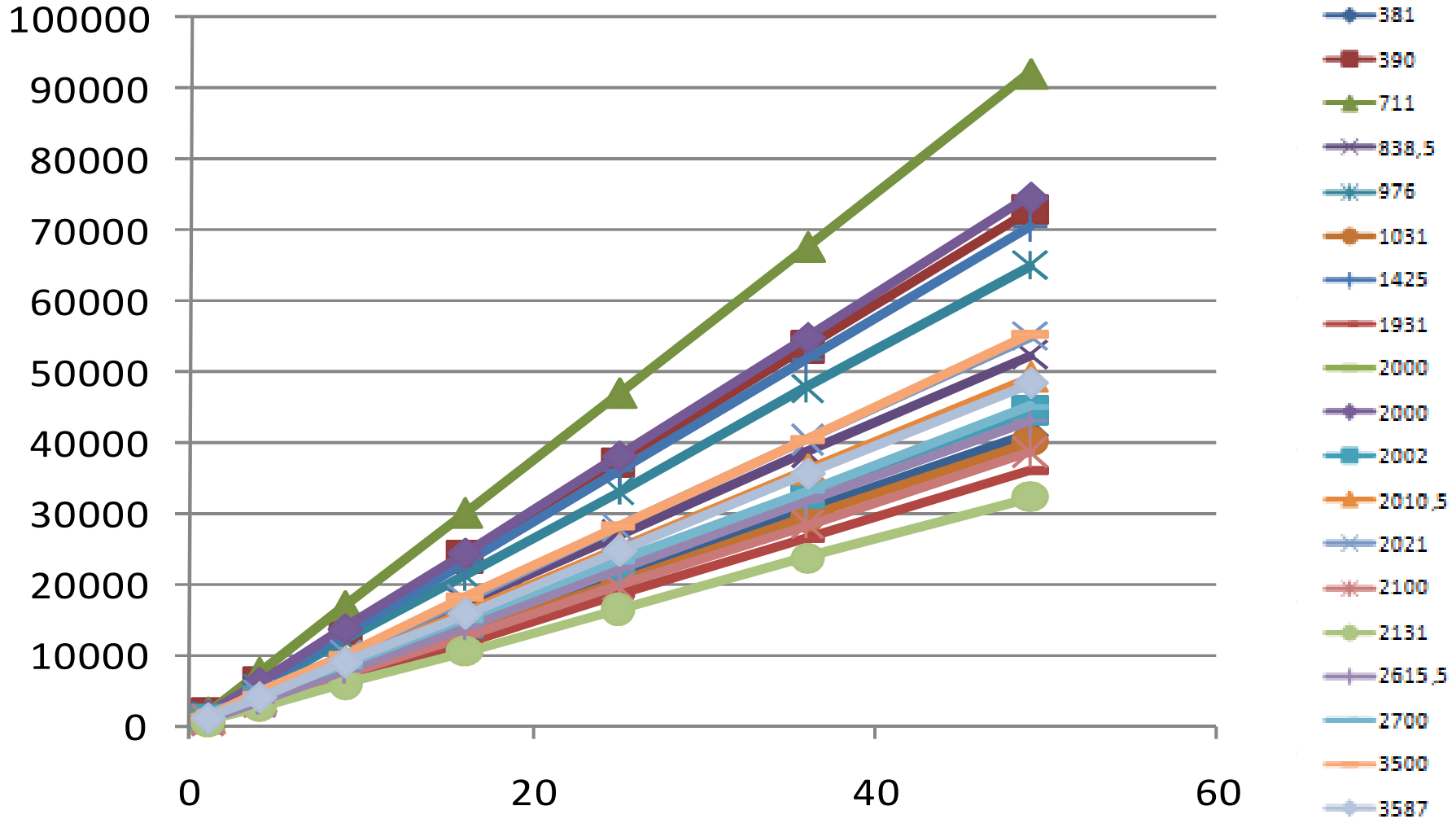
$$T = \frac{1.35}{Sp} 835.62 \left(\frac{T_{inp}}{T_{inp\_basal}} \frac{T_{BD}}{T_{BD\_basal}} \right) + 1065.5$$

egee

Enabling Grids for E-sciencE

- **This work presents a performance model for estimating the response time of BLAST runs in the EGEE grid**
  - Direct dependence with the performance indicator and the data size of input and reference database.
  - No direct dependence with memory or blast hits.
- **Very important parameter for load balancing and pre-emptive resubmission.**
- **The work will be extended, introducing new parameters from other components**
  - Workload Manager System.
  - Local Resource Management Systems.
  - Bandwidth between CEs y SEs.