



Computación de altas prestaciones en bioinformática estructural y su transferencia tecnológica al sector farmacéutico

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Bioinformatics and High Performance Computing Research Group (BIO-HPC)

- **Workshop – 1st Novel High Performance Computing algorithms and platforms in Bioinformatics (BIOHPC'17)**
 - <http://bio-hpc.eu/BIOHPC2017>
- Organised within **46th International Conference on Parallel Processing (ICPP, <http://www.icpp-conf.org/2017/index.php>), August 14, 2015, Bristol, UK**
- **Special Issue: Briefings in Bioinformatics (tentative)**

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Bioinformatics and High Performance Computing Research Group

BIO-HPC Website



- 2 Full time researchers
- 7 Professors
- 4 PhD Theses defended
- 10 PhD students being supervised
- Scientific output since May 2013
 - Journals: 80
 - Conference proceedings: 36
 - Contracts: 4
 - Projects (PI): 14
 - Funding attracted: ca. 600.000€
- NVIDIA Teaching and Research Center

TECHNOLOGY TRANSFER

- 2 international patents (licensed)
- Nanomatch.de
- Talentum-biotech.com
- Blind Docking Server
- Md.use
- 2016 HiPEAC Tech Transfer Award
- Participation in CDTI projects

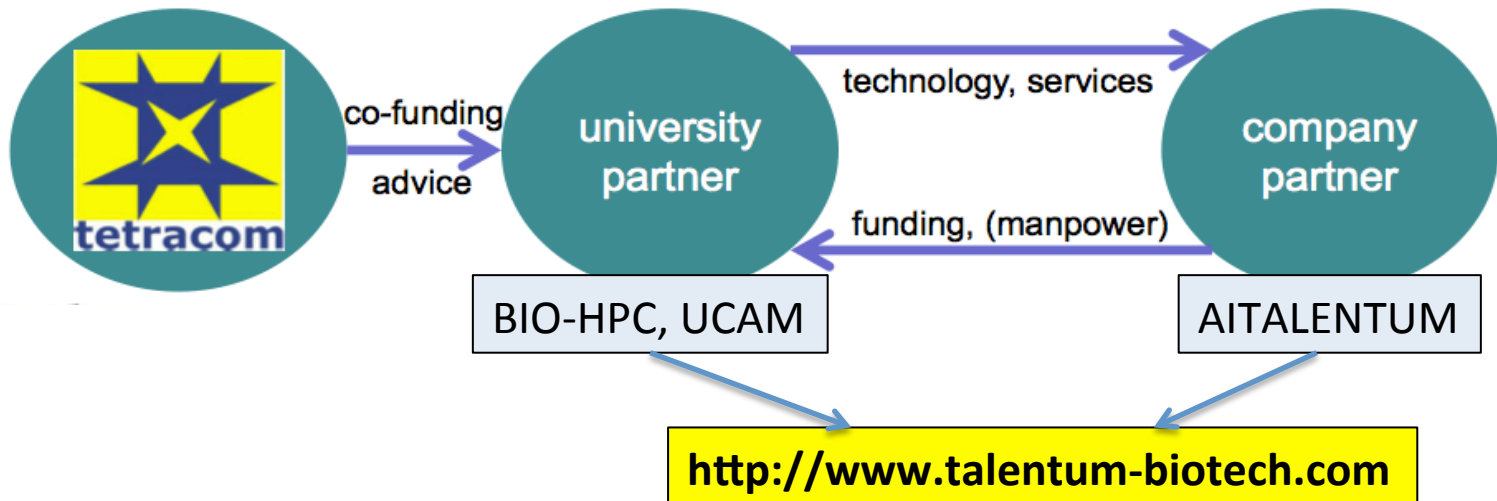
MAIN ACHIEVEMENTS

- **GPU codes developed**
 - Ant Colony Optimization for Travelling Salesman Problem
 - Biomolecular simulation kernels
 - Molecular surface
- **Web servers**
 - DIA-DB: prediction of diabetes drugs
 - Blind Docking Server: advanced blind docking
- **Novel bioactive compounds and drugs discovered**
 - Anticoagulants, Parkinson, Alzheimer, Fabry, anti-inflammatories, Zika, etc
- **LANZADOR: Efficient computational pipeline for running drug discovery calculations in clusters**
- **Parallel fuzzy clustering**
- **Extreme machine learning**
- **Technology transfer**

■ **Coordination action** in EU FP7 (grant agreement no. 609491)

Technology transfer projects (TTPs)

- TETRACOM's **major new instrument**
- TTP model:
 - **Bilateral project** between a university partner U and a company partner C
 - Typical **duration**: 3-12 months
 - C intends to purchase or license **a particular existing technology** (e.g. a SW tool or a HW IP block) from U, normally along with some **services** (porting, training,)
 - TETRACOM provides **partial funding**





EUROLAB-4-HPC

EUROLAB-4-HPC BUSINESS PROTOTYPING



INVITED TALK to HiPEAC 2017 "Transfer to Industry" Workshop

<p>Problem</p> <p><u>Accuracy of docking</u></p> <p><u>CPU-expensive calculations</u></p> <p><u>HPC is complex for bio- people</u></p>	<p>Solution</p> <p><u>Blind Docking (BD) vs docking</u></p> <p><u>Fully automated BD pipeline</u></p> <p><u>HPC/Cloud enabled</u></p> <hr/> <p>Key Metrics</p> <p>Signups</p> <p>Submission frequency</p> <p>Jobs volume</p>	<p>Unique Value Proposition</p> <p>Exhaustive docking made easy</p>	<p>Unfair Advantage</p> <p><u>Own technology</u></p> <hr/> <p>Channels</p> <p><u>Cold mailing researchers</u></p> <p><u>Research papers & presence at events</u></p>	<p>Customer Segments</p> <p><u>Researchers in bio- fields</u></p> <p><u>Biotech companies in Pharma / Cosmetics / Agro / Food industry</u></p>
<p>Cost Structure</p> <p><u>Hosting</u></p> <p><u>HPC/Cloud costs</u></p> <p><u>System administration & development</u></p>		<p>Revenue Streams</p> <p>Per usage payment, problem-size dependant size (roughly CPU-time proportional)</p>		

PhD and Postdoc positions: looking for candidates

- **Background sought**
 - Computer Engineering: High Performance Computing
 - Machine Learning, Data Science
 - Computational Chemistry
 - Structural Biology and Bioinformatics
 - Business development
- **Ongoing projects**
 - Development on GPU codes
 - Acceleration on GPU of existing codes
 - Development of computational chemistry and bioinformatics codes in HPC environments (Clusters, Grids, etc)
 - Drug Discovery
- **Potential calls**
 - MINECO FPU
 - Fundación Séneca Región de Murcia
 - Marie Curie 2017
 - Own projects from BIO-HPC group

Looking for partners for joint applications to national and international grant calls

- **Partner profiles sought**
 - Fields: HPC, Computational Chemistry, Structural Bioinformatics
 - Research groups with previous application experience or grant track record
 - Small and Medium Enterprises (SMEs)
- **Potential projects subjects**
 - Centered on
 - HPC developments
 - Drug Discovery, Structural Bioinformatics, most “bio” fields
 - Joint technology transfer projects
 - Business prototyping projects
- **Potential calls**
 - H2020
 - MINECO
 - Industry based funding
 - Selected list of international project calls curated by BIO-HPC group