

Multi-Scale Computational Modeling of Chemical and Biochemical Systems

MULTIMOD



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"Info-day for the 2011 Open Calls of the PEOPLE Specific Programme – 7th Framework Programme"

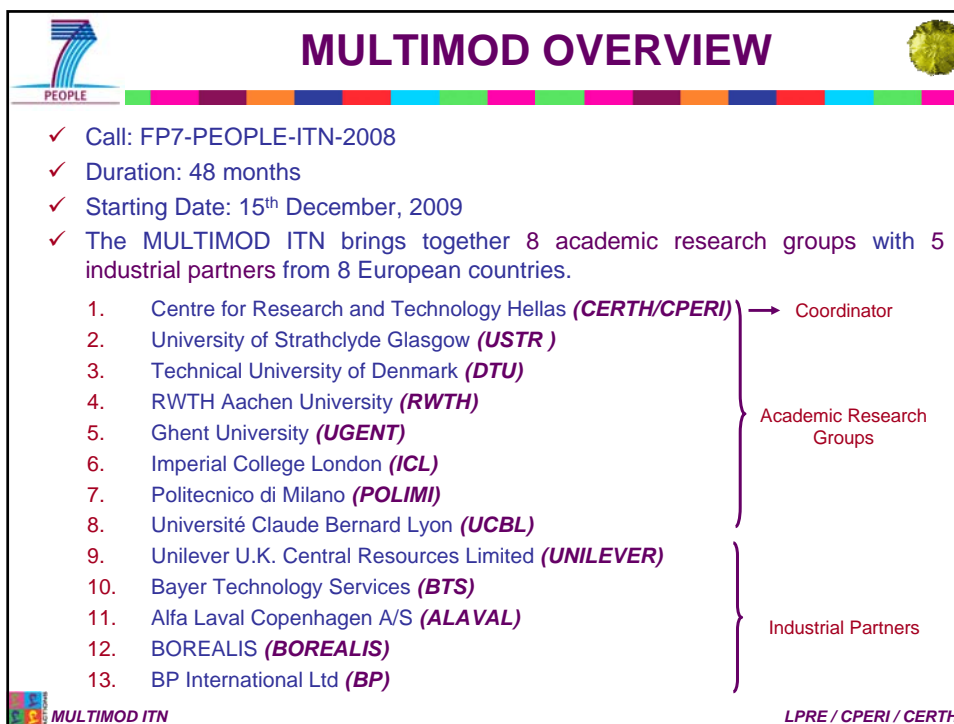
CERTH, Thessaloniki, Thursday, 21 October 2010



OUTLINE



- **MULTIMOD Overview**
- **Evaluation Summary Report – Tips**
- **How to Prepare a Successful Proposal**
- **Negotiations with EC**
- **Implementation**
- **Impact on the Organization**



MULTIMOD OVERVIEW


PEOPLE

- ✓ Call: FP7-PEOPLE-ITN-2008
- ✓ Duration: 48 months
- ✓ Starting Date: 15th December, 2009
- ✓ The MULTIMOD ITN brings together 8 academic research groups with 5 industrial partners from 8 European countries.

1. Centre for Research and Technology Hellas (CERTH/CPERI)	}	Coordinator
2. University of Strathclyde Glasgow (USTR)		
3. Technical University of Denmark (DTU)	}	Academic Research Groups
4. RWTH Aachen University (RWTH)		
5. Ghent University (UGENT)		
6. Imperial College London (ICL)		
7. Politecnico di Milano (POLIMI)	}	Industrial Partners
8. Université Claude Bernard Lyon (UCBL)		
9. Unilever U.K. Central Resources Limited (UNILEVER)		
10. Bayer Technology Services (BTS)		
11. Alfa Laval Copenhagen A/S (ALAVAL)		
12. BOREALIS (BOREALIS)		
13. BP International Ltd (BP)		

MULTIMOD ITN

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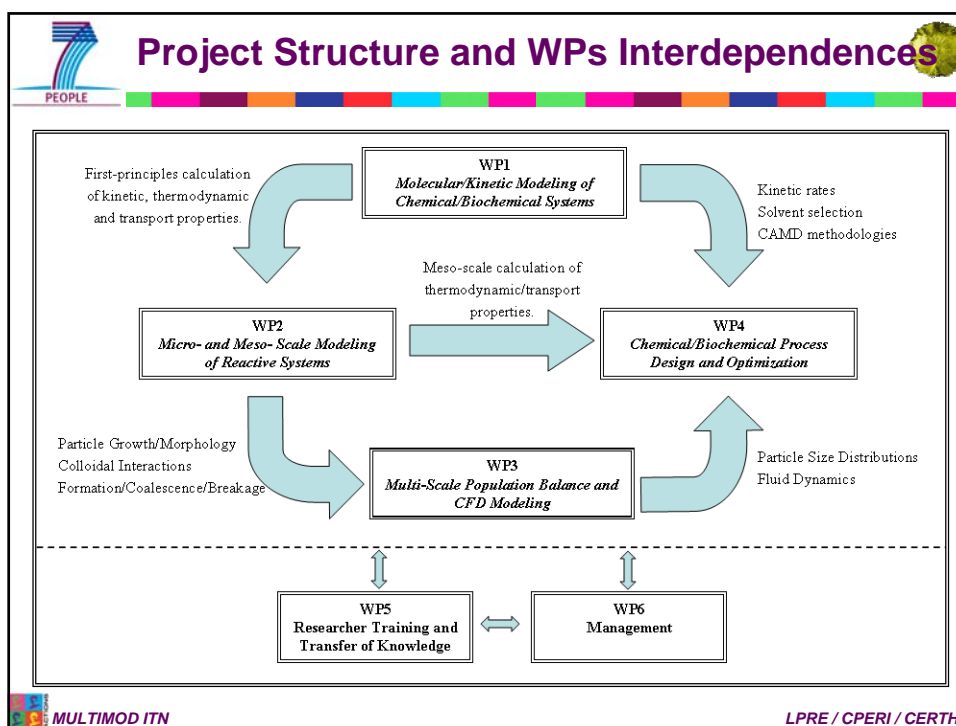
MULTIMOD OVERVIEW

PEOPLE

- The MULTIMOD ITN provides unique cross- and multi-disciplinary training opportunities for 19 ESRs (each for 3 years)
- MULTIMOD ITN aims at R&D and training of young researchers in:
 - (i) Advanced modeling and simulation of chemical/biochemical systems
 - (ii) Training and transfer of knowledge opportunities.
- The present challenge in chemical/biochemical engineering is *to bridge the gap* between the molecular, micro-, meso- and macro-scale phenomena with large-scale applications.
- The skills offered by the network are urgently required by the chemical and biochemical sectors: *the foreseen advances in modeling and simulation will have a significant impact on reducing the cost and time involved in the industrial R&D by allowing the accurate prediction of process performance and product properties during the stage of process design.*

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ESR Positions of the MULTIMOD network

Position		Host Organization(s)	Secondment Organization(s)
Position 1	Molecular Modeling of Macromolecular Systems (WP1.1)	POLIMI	UNILEVER
Position 2	Solvent Screening through Model-Based Experimental Analysis (WP1.2)	RWTH	BTS + DTU
Position 3	Chemical Synthesis with New Solvents (WP1.2)	BTS	RWTH
Position 4	Data-Driven Estimation of Reaction Kinetics (WP1.3)	RWTH	UGENT + USTR
Position 5	Data-Driven Estimation of Reaction Kinetics (WP1.3)	UGENT	RWTH + USTR
Position 6	Meso-Scale Modeling of Catalytic Processes (WP2.1)	BOREALIS + CERTH	-
Position 7	Investigation of Particle Growth and Morphology (WP2.2)	USTR	CERTH
Position 8	MD/DPD Modeling of Surfactant/Polymer Self Assembly (WP2.3)	UNILEVER	ICL + POLIMI
Position 9	Investigation of Micro-structure Phenomena in Colloidal Systems (WP2.3)	USTR + CERTH	-
Position 10	Numerical Solution of Multivariate PBMs (WP3.1)	CERTH	UCBL
Position 11	CFD Modeling of 2-Phase, Incompressible Flow Systems (WP3.2)	UNILEVER	ICL
Position 12	CFD Modeling of 2-Phase, Incompressible Flow Systems (WP3.2)	UCBL	UNILEVER
Position 13	Model-Based Integrated Process-Product Design (WP4.1)	DTU	
Position 14	Model-Based Integrated Process-Product Design (WP4.1)	ALAVAL	ALAVAL
Position 15	Incremental Refinement of Process Design (WP4.2)	DTU + ALAVAL	RWTH
Position 16	Bioprocess Design for Production of Biopharmaceuticals (WP4.3)	BTS	ICL
Position 17	Bioprocess Design for Production of Biopharmaceuticals (WP4.3)	ICL	BTS
Position 18	Bioprocess Design for Production of Biopolymers (WP4.3)	CERTH + ICL	-
Position 19	Model-Based Catalyst Design (WP4.4)	UGENT + BP	-

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Evaluation Summary Report



S&T Quality: The S&T quality is very good and the proposed project represents a composite of a number of different modeling approaches on a broad range of applications. The institutions show good complementarity, which is well exploited in the research programme. The theoretical approach complemented with experimental work is also very positive (Mark: 4.5/5.0).

Strong Points - Tips:

- ✓ Well detailed research programme with strong interactions with industry.
- ✓ Clear S&T objectives and research methodology.
- ✓ Exciting project (integrating molecular, kinetic, thermodynamic, morphological, population balance with fluid dynamics models in a unified computational approach).
- ✓ Multidisciplinary aspects of the proposal (from the molecular level to plant level).
- ✓ Validation of the Modeling results by experimental data.
- ✓ Project must be of significant value to the industry (chemical/biochemical).
- ✓ Include recent references to the advances on the topics covered on the State of the Art.
- ✓ Sufficiently demonstration of the synergy between the work packages.




Evaluation Summary Report



Training: The training programme is of very high quality and is well structured . Special care is taken in order to provide a high level of industry involvement (Mark: 4.6/5.0).

Strong Points - Tips:

- ✓ High level of Industry participation at the consortium (5 industrial partners).
- ✓ The Conference organization must be well-described.
- ✓ Network wide training (i.e., Seminar / courses / workshops).
- ✓ Ensure extra funding beyond network for PhD completion.
- ✓ Complementary skills including training on inter-cultural perception.
- ✓ Short term (1-4 weeks) exchanges.
- ✓ Annual one week "retreat" for all fellows in the network with academic and industry experts.



Training Events

➤ During the MULTIMOD ITN lifetime twenty-four (24) training events will be organized.

	Number of events	Duration (days)	Expected participation (persons)	
			Internal	External
Seminars	1	1	30	0
Courses	4	2	20	5
Workshops	3	3	20	10
Conferences	1	3	60	50
Web Seminars	12	2	30	0
Annual Retreats	3	5	30	2*

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Training Events

Courses: Four (4) courses open to both intra- and extra-network participation will be provided on the following topics:

- Course 1: Model-Based Experimental Analysis (RWTH).
- Course 2: Population Balance Modeling (CERTH).
- Course 3: Model-Based Control of Mammalian Cell Cultures (ICL).
- Course 4: Solvent Selection for Organic Synthesis (DTU).

Workshops: The network will organize three (3) workshops covering various thematic areas of the research program.

- Workshop 1: Introduction on Multi-Scale Systems Engineering (CERTH*, ICL, RWTH).
- Workshop 2: Computational Molecular Science and Engineering (POLIMI*, DTU).
- Workshop 3: Biochemical Engineering: Fundamentals and Innovations (ICL*, USTR, CERTH).

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Training Events



- ✓ The workshop's programme will include:
 - **Keynote lectures** from distinguished academic researchers and representatives from the chemical/biochemical industry,
 - **Technical presentation sessions**, focusing on the development of research themes and experience derived from interdisciplinary collaboration, in the context of the various multi-scale modeling case studies,
 - **Software demonstration sessions**, where project leaders and researchers will showcase novel and in-house computational tools with functional capabilities suitable for tackling multi-scale problems,
 - **Training on complementary skills** and
 - **Student posters** and a **plenary discussion forum** to facilitate the exchange of ideas on training and career development opportunities.

Conferences: An international conference will be organized at the end of the MULTIMOD network.



Indicative Training Event Time Schedule



Event	Host	Year 1												Year 2											
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
Seminar	USTR			■																					
Workshop 1	CERTH																						■		
Course 1	RWTH						■																		
Course 2	CERTH																		■						
Retreat 1	CERTH												■												
Retreat 2	CERTH																								■

Event	Host	Year 3														Year 4													
		25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48				
Course 3	ICL						■																						
Course 4	DTU																		■										
Workshop 2	POLIMI																												
Workshop 3	ICL																						■						
Retreat 3	CERTH																												
Conference	CERTH																								■				



Complementary Skill Training



- A series of *web seminars* will be provided for complementary skill development, targeted not only to the appointed ESRs but also to the permanent research personnel of the consortium. Recruited researchers will be encouraged to attend 12 complementary skill training events (i.e., 4 events per year) with a minimum of 8 events required throughout their recruitment period by the network.
- The list of web seminars offered will include:
 - Finding and Managing Research Information,
 - Introduction to Teaching and Mentoring,
 - Introduction to Personal Development and Career Planning,
 - Job Applications and Interviews,
 - CV's and Supporting Statements,
 - PhD Management,
 - IT for Researchers and Web Design,
 - Communication Skills, Conferencing and Poster Creation,
 - Scientific Writing,
 - Funding and Proposal Writing,
 - Entrepreneurial Skills,
 - Project Management and Strategic Planning,
 - Risk Assessment,
 - Intellectual Property and Patent Recognition,
 - Societal Impact of Advancing Technologies and
 - Research Ethics.



Life-Long Training and Technology / Expertise Transfer Activities



- Short term exchanges (i.e., 1-4 weeks) will be carried out between members of the MULTIMOD research teams **on specific areas and needs of the MULTIMOD 'Programme of Research Activities'**. In addition, **training seminars** tailored for industrial researchers and technical staff will be included on the network's activities. These activities will primarily benefit the members of the research teams of participating organizations but will **also function towards supporting the initial training of recruited ESRs through the establishment of a scientific interface for exchange of knowledge and ideas.**

Interactive Tools for Communication, Training and Transfer of Knowledge

- **MULTIMOD website:** www.multimod.eu
The website serves as to engender a community spirit and identity within the network and promote the transfer of knowledge both across and outside of it.



Evaluation Summary Report



Implementation: The implementation strategy is well defined with good details on the most important items. Plans for implementation are well-structured and credible, one concern relates to the capacity of the various hosts to train the fellows (Mark: 4.5/5.0).

Strong Points - Tips:

- ✓ Emphasize on good communication and monitoring progress.
- ✓ Recruitment plans and gender issues.
- ✓ Arrangements on Intellectual Property.
- ✓ Clear and effective dissemination strategy.
- ✓ Detailed work plan and good overview of tasks, milestones and deliverables.
- ✓ Very good management strategy (incl. Researchers Board Advisory Council, Recruitment Committee and Supervisory board).
- ✓ Good facilities for the training programme for both theoretical and experimental work.
- ✓ Provide information on the available scientific staff, for each partner, to coach the fellows.
- ✓ Emphasize on the experience of the coordinating to host EC programs.



Evaluation Summary Report



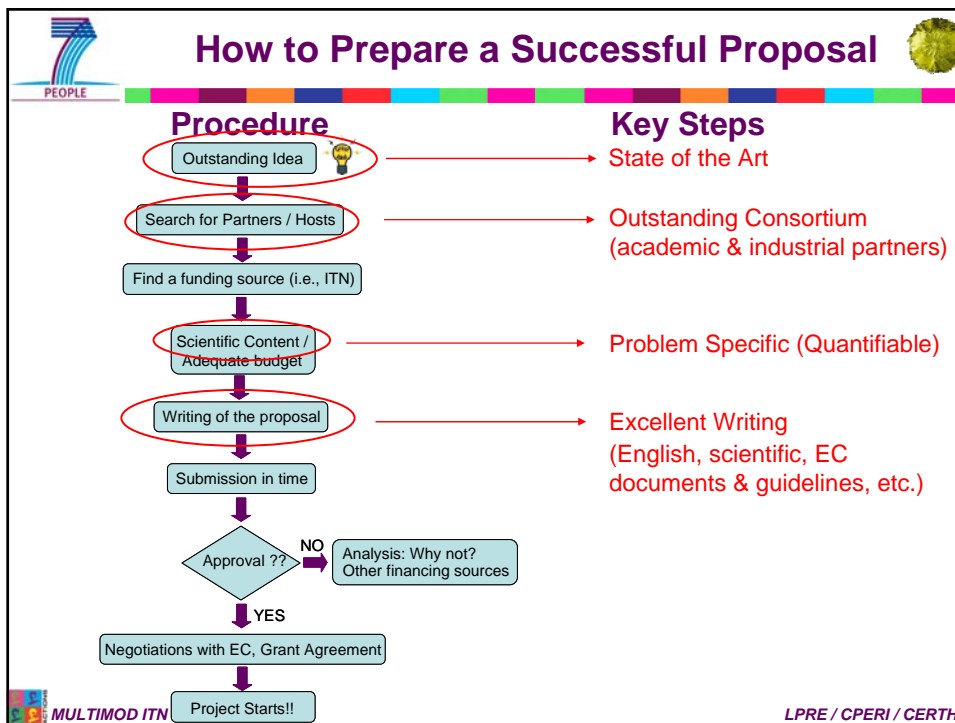
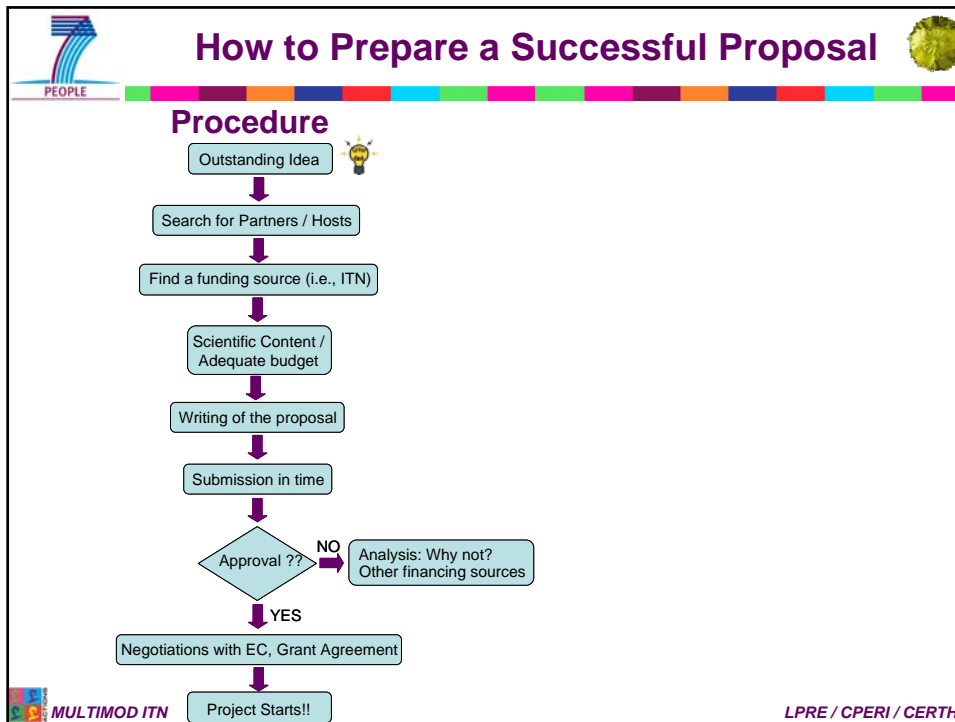
Impact: It can be expected that the career prospects of the fellows will substantially be improved as a result of their participation in this project, especially because of the direct interactions with the industry partners. (Mark: 4.4/5.0).

Strong Points - Tips:

- ✓ Emphasize on that the ESRs will both be exposed to high quality academic training as well as direct industrial exposure.
- ✓ There is a clear need in industry for researchers that have a deep understanding of the dynamics of complex systems at different scales.
- ✓ The planned training has great potential to enhance the researchers' career prospects.
- ✓ Establishment of long term relations between the partners and interaction of the partners in future projects.
- ✓ The network based training with secondments, workshops, short visits and interconnected WPs will create a good foundation for future collaboration among the partners.

Ethical Issues : No

TOTAL MARK : 90.2 / 100





How to Prepare a Successful Proposal



You have to Consider:

- If all the partners have the capacity to carry out their duties.
- Which training activities will be carried out (i.e., courses, conferences, workshops, etc.) during the project lifetime and where?
- Collaborations among the partners (secondment periods, who and where)
- If the project raise sensitive ethical issues.
- What will be the management scheme?

Tips:


- Pay attention to the "Guide for Applicants"
- Surprise the evaluators with innovative ideas
- Explain the impact of your project for Europe
- Use the same terms as they appear in the evaluation criteria
- **Do NOT promise too much. Be Reliable!!**




Negotiations with EC




- All comments/weaknesses by the evaluators were taken into consideration when preparing the Annex I (Description of work).
- Negotiations through NEF portal → submission of Forms
- Very good collaboration with Project Officer.
- Minor problems on communication with the partners.



Implementation



- The implementation strategy is well defined with good details on the most important items.
- Plans for implementation are well-structured and credible.
- Experience of the coordinating host on EC programs.
- All partners have the capacity to host and train the fellows.
- Very good management strategy (incl. Researchers Board Advisory Council, Recruitment Committee and Supervisory board).
- The most difficult stage is the Recruitment.
 - ✓ The recruitment procedure is well defined in Annex I.
 - ✓ Recruitment Committee.
 - ✓ Advertisement of the positions on EURAXESS, MULTIMOD Website, partner's websites.
 - ✓ Development of a Recruitment Database available to all partners.
- Recruitment of women.



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Impact on the Organization



- Foster co-operation between public research organizations & private commercial enterprises on joint research projects (common know-how).
- Stimulate long-term collaboration between sectors through secondment of researchers between the public & private research domains.
- Allow CERTH to hire early stage researchers (ESRs) with different backgrounds (i.e., chemical engineering, biological engineering, mechanical engineering etc.).
- Diverse career possibilities & research experience for ESRs, knowledge sharing/cultural exchange.
- Promotion and enhancement of publicity of CERTH in Europe through the participation of the ESRs in social & scientific events (i.e., coordination days, celebration days, conferences, workshops).
- Contribute to achieving the goals of Lisbon Strategy for growth and jobs: *"To make EC the most competitive and dynamic knowledge-based economy in the world capable of sustainable economic growth with more and better jobs and greater social cohesion"*



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