



**SEVENTH FRAMEWORK PROGRAMME  
Research Infrastructure**

**FP7-INFRASTRUCTURES-2010-2 – INFRA-2010-1.2.3:  
Virtual Research Communities**

**Combination of Collaborative Project and  
Coordination and Support Actions (CP- CSA)**



**LinkSCEEM-2  
Linking Scientific Computing in Europe and  
the Eastern Mediterranean – Phase 2**

**Grant Agreement Number: RI-261600**

**D10.1  
Scalable, optimised cluster computer code**

*Final*

Version: 1.0  
Author(s): Hendrik Merx, MPG  
Date: 31/08/2012

## Project and Deliverable Information Sheet

<b>LinkSCEEM Project</b>	<b>Project Ref. No.:</b>	<b>RI-261600</b>	
	<b>Project Title:</b>	<b>LinkSCEEM-2</b>	
	<b>Project Web Site:</b>	<a href="http://www.linksceem.eu/">http://www.linksceem.eu/</a>	
	<b>Deliverable ID:</b>	<b>D10.1</b>	
	<b>Deliverable Nature:</b>	<b>Other</b>	
	<b>Deliverable Level:</b> RE*	<b>Contractual Date of Delivery:</b> 31 / 08 / 2012	
		<b>Actual Date of Delivery:</b> 12 / 09 / 2012	
<b>EC Project Officer:</b>	<b>Sonia Spasova</b>		

\* - The dissemination level are indicated as follows: **PU** – Public, **PP** – Restricted to other participants (including the Commission Services), **RE** – Restricted to a group specified by the consortium (including the Commission Services). **CO** – Confidential, only for members of the consortium (including the Commission Services).

## Document Control Sheet

<b>Document</b>	<b>Title:</b>	<b>Scalable, optimised cluster computer code</b>	
	<b>ID:</b>	<b>D10.1</b>	
	<b>Version:</b> 0.1	<b>Status:</b> Final	
	<b>Available at:</b>	<a href="http://www.eniac.cyi.ac/">http://www.eniac.cyi.ac/</a>	
	<b>Software Tool:</b>	Microsoft Word 2011	
	<b>File(s):</b>	emac.linksceem.tar.gz	
<b>Authorship</b>	<b>Written by:</b>	Hendrik Merx, MPG	
	<b>Contributors:</b>	Klaus Klingmüller, CyI-CaSToRC	
	<b>Reviewed by:</b>		
	<b>Approved by:</b>	Jens Wiegand, CyI-CaSToRC	

## Document Status Sheet

<b>Version</b>	<b>Date</b>	<b>Status</b>	<b>Comments</b>
0.1	31/08/2012	Draft	
0.2	12/09/2012	Draft	
1.0	12/09/2012	Final version	approved

## Document Keywords

<b>Keywords:</b>	LinkSCEEM-2, Computational Science, HPC, e-Infrastructure, Eastern Mediterranean
------------------	--

## Executive Summary

The ECHAM/MESSy Atmospheric Chemistry (EMAC) model is used by the European climate and atmospheric chemistry modelling community to simulate the Earth's atmosphere and its interactions with land, ocean, and space. It is based on the general circulation climate model European Centre/HAMburg (ECHAM) that has been extended by the Modular Earth Submodel System (MESSy) to include a variety of atmospheric processes such as homogeneous and heterogeneous chemistry, photochemistry, and aerosols. Some of these processes require computationally complex calculations that are unequally distributed over the simulated atmosphere.

Running the EMAC model requires large amounts of computing resources and is usually performed on parallel supercomputers. While the climate model ECHAM provides the simulations with a parallelisation that has been tailored to the computational load distribution of a standard climate model, the distribution of computational complexity of an atmospheric chemistry model differs markedly creating a load imbalance that wastes valuable computing resources. Furthermore, the load imbalance problem worsens with increasing numbers of processors of future computer architectures that due to limitations in semiconductor physics rely on higher parallelisation rather than faster single processors. Thus, the simulations do not scale well to higher numbers of processors.

The load imbalance and its consequent reduction in effective computer performance required a re-evaluation of the load balancing strategies in EMAC and lead to a different parallelisation strategy of the model space for physically local processes. Moreover, the implementation also provided for higher allowed numbers of processors for low-resolution simulations that had been limited by neighbourhood relations for the exchange of data between simulation cells. The new, highly-scalable load distribution policy was implemented in the EMAC model and has been made available to the climate and atmospheric modelling community of the Eastern Mediterranean on BA and CaSToRC systems.

Deliverable D10.1 comprises all three parts of the EMAC model source code packed in one compressed archive. The archive can be unpacked on any UNIX system using the

```
gzip -dc emac.linksceem.tar.gz | tar xf -
```

command. The unpacked directory contains one directory with the combined source code of the ECHAM5.3.01 and MESSy1.9 models and one directory with the source code of the UniTrans library.