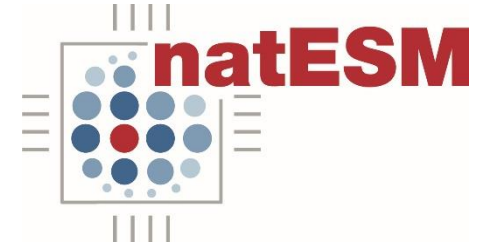# Workshop – natESM strategy
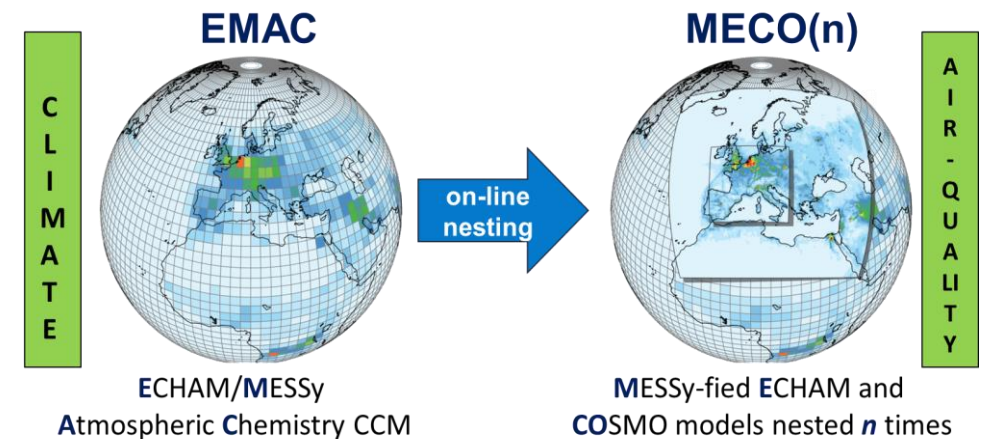

21. February 2022, virtual meeting

Request for support sprint:
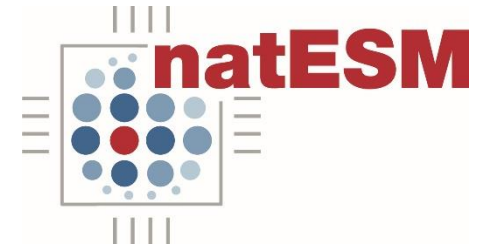## expand MESSy infrastructure for GPUs

advisory sprint: create implementation plan
MESSy (Modular Earth Submodel System)

Research Center Jülich (IEK-8) / German Aerospace Center (DLR-PA)
contact: a.kerkweg@fz-juelich.de

EMAC

CLIMATE

on-line
nesting

MECO(n)

AIR-QUALITY

ECHAM/MESSy
Atmospheric **C**hemistry CCM

MESSy-fied **E**CHAM and
COSMO models nested *n* times

© Mariano Mertens (DLR)

DKRZ
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Brief Overview of Model/Software

- ESM field:

  global and regional chemistry climate and air quality modelling
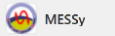
- User group: 24 MESSy consortium member institutions:

  about 200 active users (continuously increasing)

- Targeted simulations:
  - All from transient chemistry climate (≈100 years) to air quality simulations
  - global to regional/local
  - deterministic => ensembles
  - stratospheric chemistry (≈100 tracers) to detailed tropospheric organic (gas, liquid and aerosol phase) chemistry (≈2500 tracers)

- HPC usage:
  - pure MPI based parallel domain decomposition
  - HPC CPU systems (DKRZ, JSC (JUWELS cluster), LRZ, MPCDF, SARA(NL), and various university clusters),
  - first steps on GPU systems: CUDA, OpenACC (JSC: JUWELS booster)
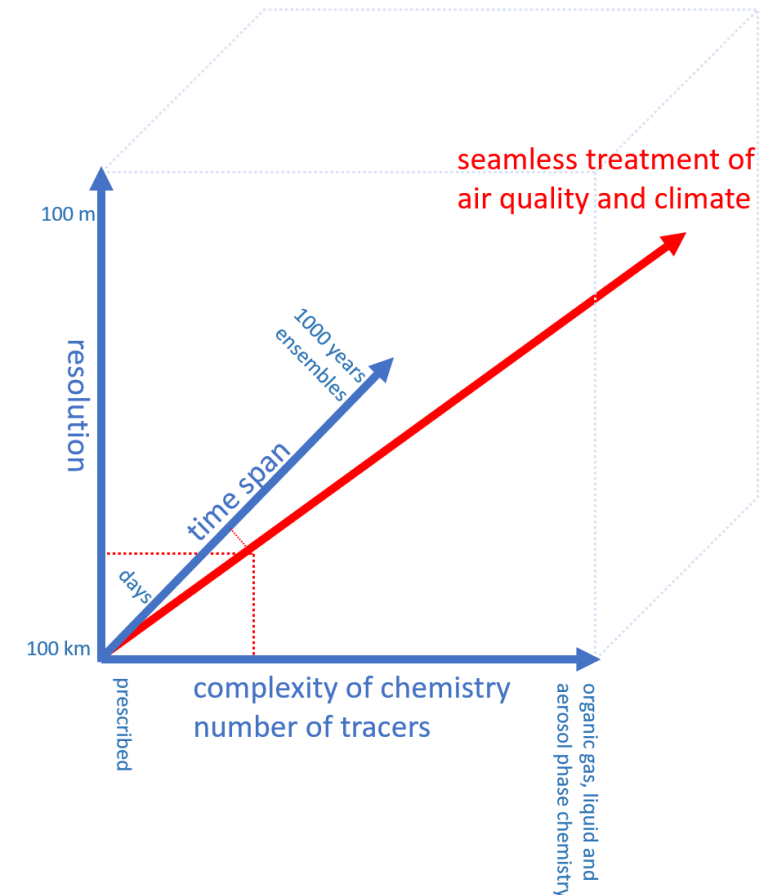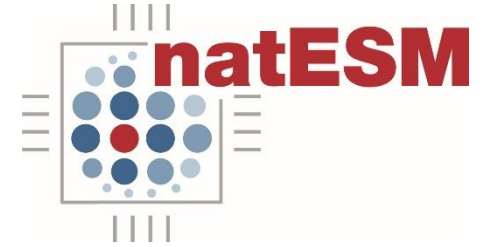
Brief Overview of Model/Software

- ## Maintenance:

  - MESSy code hosted a DKRZ GitLab

  - MESSy code parts open source / basemodels (ECHAM5, ICON, COSMO) licence restricted
    - $\Rightarrow$ the full MESSy package will be open source as soon as basemodels are open source
    - $\Rightarrow$ published and documented in GMD/ACP MESSy special issue
  - all 24 MESSy consortium institutions contribute to code development:
    - about 40 submodel and 5 infrastructure developers
  - DLR-PA and FZJ-IEK-8 provide dedicated resources for central code management

  MESSy development was started in 2001, since then the code and the number of code users and developers has grown steadily and is foreseen to continue to increase.

Model/Software Application Field
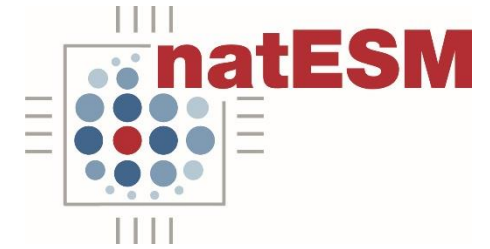
- Scientific highlights:
  - Ubiquitous atmospheric production of organic acids mediated by cloud droplets, (Franco et al., Nature, 2021)
  - Attributing ozone and its precursors to land transport emissions in Europe and Germany (Mertens et al., ACP, 2020)
  - COVID-19 induced lower-tropospheric ozone changes (Mertens et al., REL, 2020)
  - **474 scientific publications since 2005**

- Social relevance:
  - contributions to WMO/UNEP Ozone Assessment report (CCMI) and IPCC (CMIP)
  - impact of anthropogenic emissions on air quality and climate (e.g., DLR, TU Delft, NLR)
  - health impact and hazard studies (MPI for Chemistry)
  - basic research on air quality and chemistry climate interactions

- Plans for further use and dissemination:
  - improved air quality and chemistry climate research (seamless)
  - transition to ICON as basemodel
  - open source (where possible)

Fig. 1: Formic acid abundance from satellite and model.
From: Ubiquitous atmospheric production of organic acids mediated by cloud droplets
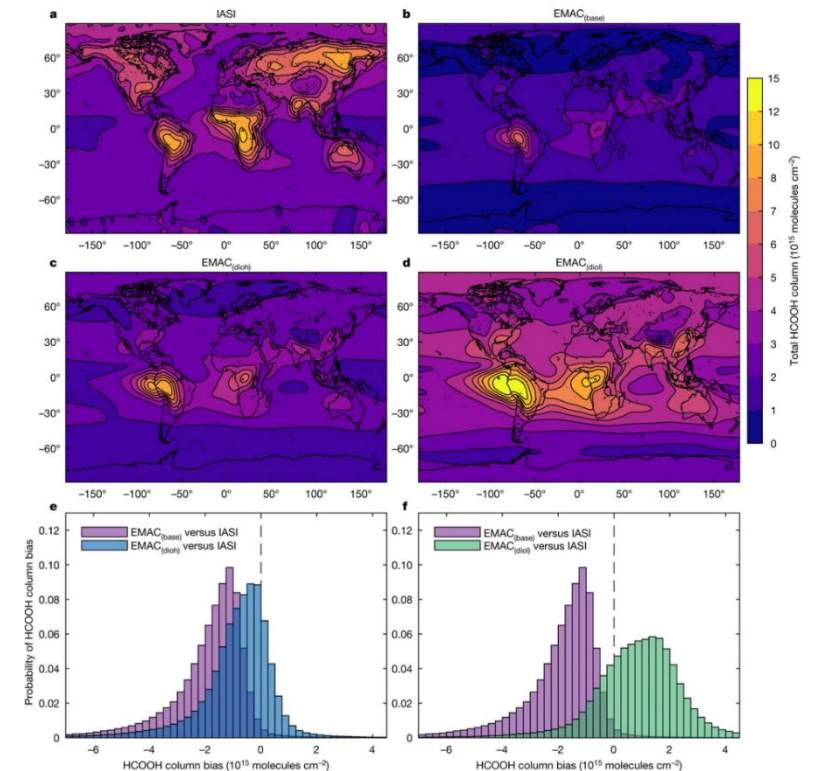
Franco et al., Nature, 2021

Description of Planned Work

- Expected scientific and/or performance improvements:
  - <u>performance</u>:   optimise data management between CPU and GPU
      (i.e., optimised for variable complexity of MESSy configurations)
      => speed up / efficient use of GPUs
      => run MESSy on GPU architectures => exascale computing
  - <u>scientifically</u>:   ensembles of CCMI type simulations at 10km resolution with detailed organic chemistry (≈3000 tracer)
      => improved transport
      => explicit treatment of organics
      => Exascale vision:
         Seamless simulations of Air Quality and Climate!

- Scope of Request:
  - duration: 4 weeks (introduction MESSy, evaluate different approaches)
  - methods to be used: OpenACC
  - targeted systems: GPU based HPC systems (JUWELS booster => exascale system

- Criteria for fulfilment:
  - Implementation plan ready for realisation