

Global chemistry-climate modelling with EMAC

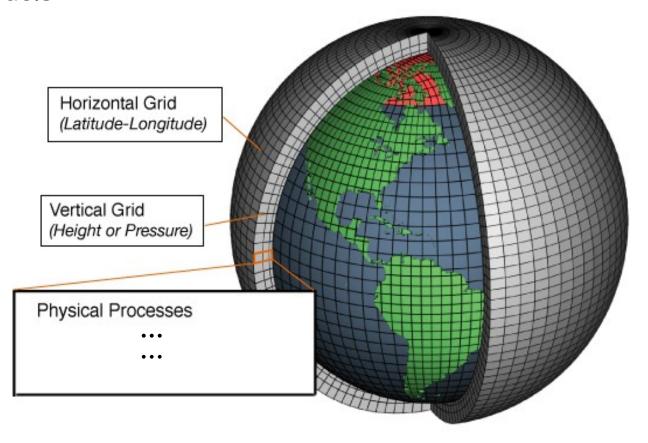
R. Deckert, R. Sausen, P. Jöckel, V. Aquila, S. Brinkop, U. Burkhardt, I. Cionni, M. Dall'Amico, M. Dameris, S. Dietmüller, V. Eyring, K. Gottschaldt, V. Grewe, J. Hendricks, M. Ponater, and M. Righi

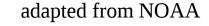
Deutsches Zentrum für Luft- und Raumfahrt Institut für Physik der Atmosphäre Oberpfaffenhofen

High Performance Computing in Science and Engineering Garching, 8 - 9 December 2009

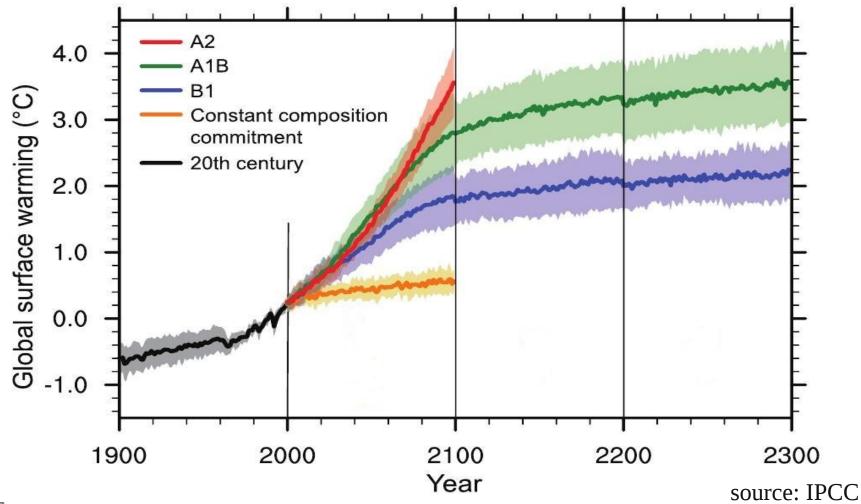


Global climate models



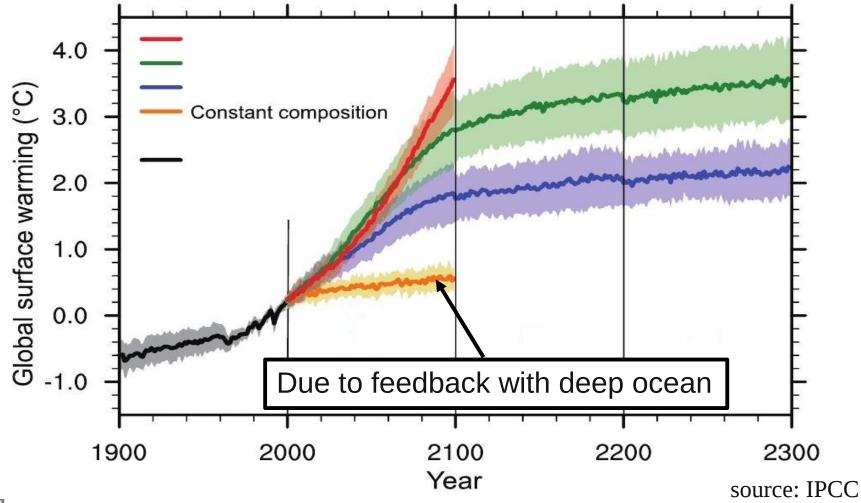


Global climate models: climate projections





Global climate models: climate projections



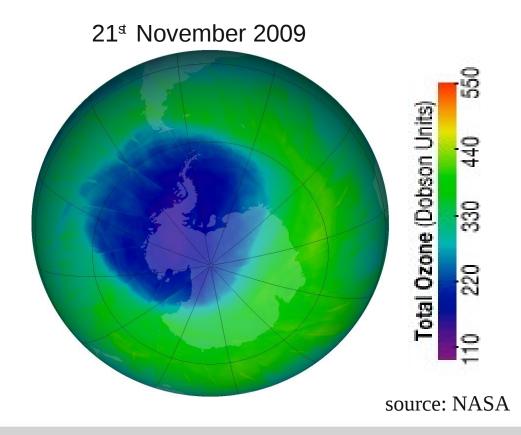


Global climate models: no atmospheric chemistry



Global climate models: no atmospheric chemistry

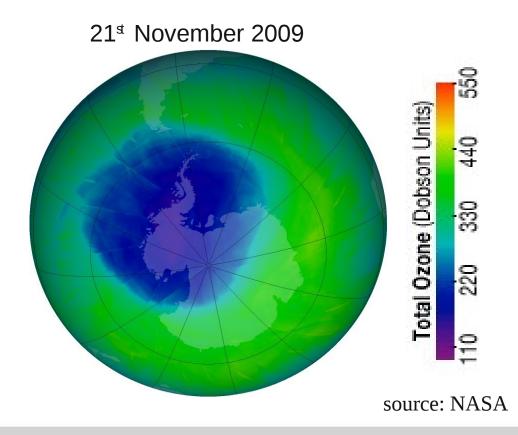
Future ozone layer?





Global climate models: no atmospheric chemistry

- Future ozone layer?
- Chemically triggered climate modifications?





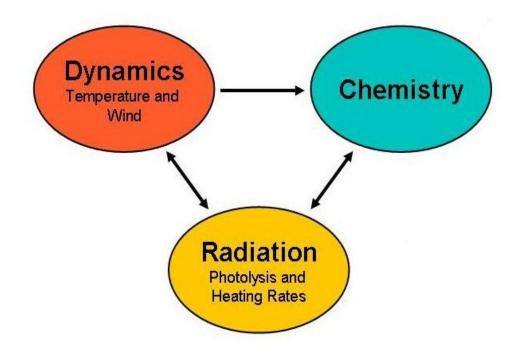
Global chemistry-climate models (CCMs)

> Atmosphere // deep ocean



Global chemistry-climate models (CCMs)

- Atmosphere deep ocean
- ➤ Atmospheric physics ↔ atmospheric chemistry

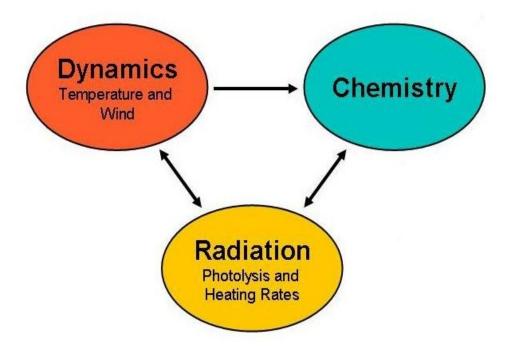




Global chemistry-climate models (CCMs)

- Atmosphere deep ocean
- ➤ Atmospheric physics ↔ atmospheric chemistry

We use and refine a CCM





Outline

- Model description
- Performance on LRZ/ALTIX
- Modelling activities on LRZ/ALTIX



CCM system EMAC (ECHAM/MESSy Atmospheric Chemistry)

- Overall system by MPI for Chemistry, Mainz
- Fluid dynamics by MPI for Meteorology, Hamburg



CCM system EMAC (ECHAM/MESSy Atmospheric Chemistry)

- Overall system by MPI for Chemistry, Mainz
- Fluid dynamics by MPI for Meteorology, Hamburg

EMAC follows standards → easily portable

- Fortran95 (ISO/IEC-1539-1)
- Message Passing Interface (MPI-2)
- NetCDF data format



CCM system EMAC (ECHAM/MESSy Atmospheric Chemistry)

- Overall system by MPI for Chemistry, Mainz
- Fluid dynamics by MPI for Meteorology, Hamburg

EMAC follows standards → easily portable

- Fortran95 (ISO/IEC-1539-1)
- Message Passing Interface (MPI-2)
- NetCDF data format

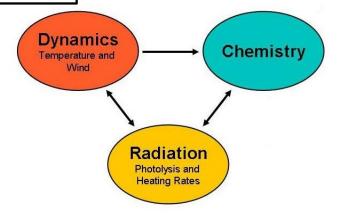
EMAC is flexible

- Selectable spatial resolution
- Configurable chemistry scheme
- Modular structure (see http://www.messy-interface.org)



Atmospheric primitive equations – spectral representation

- Spectral transformation (horizontal)
- Finite differences (vertical)
- Semi-implicit leap frog (time)

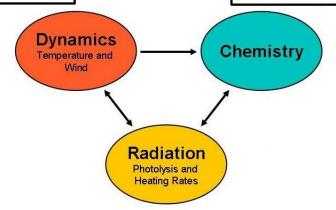


Atmospheric primitive equations – spectral representation

- Spectral transformation (horizontal)
- Finite differences (vertical)
- Semi-implicit leap frog (time)

Stiff system of ordinary differential equations – gaussian grid

Rosenbrock sparse-matrix technique with adaptive time step

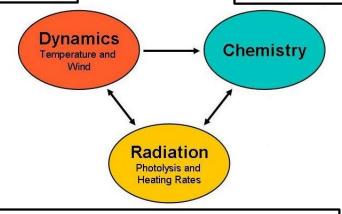


Atmospheric primitive equations – spectral representation

- Spectral transformation (horizontal)
- Finite differences (vertical)
- Semi-implicit leap frog (time)

Stiff system of ordinary differential equations – gaussian grid

Rosenbrock sparse-matrix technique with adaptive time step



Radiative transfer, tracer transport, other sub-models – gaussian grid

Miscellaneous techniques



Diverse demands on hardware architecture ...

Various numerical techniques

Diverse demands on hardware architecture ...

- Various numerical techniques
- Distributed-memory domain decomposition
 - Spectral representation: spherical
 - Gaussian grid: latitude-longitude, ping-pong blocks
 - Tracer advection: vertical and latitude-longitude



Diverse demands on hardware architecture ...

- Various numerical techniques
- Distributed-memory domain decomposition
 - Spectral representation: spherical
 - Gaussian grid: latitude-longitude, ping-pong blocks
 - Tracer advection: vertical and latitude-longitude
- Vectorisation of latitude-longitude blocks
 - To exploit cache sizes

Diverse demands on hardware architecture ...

- Various numerical techniques
- Distributed-memory domain decomposition
 - Spectral representation: spherical
 - Gaussian grid: latitude-longitude, ping-pong blocks
 - Tracer advection: vertical and latitude-longitude
- Vectorisation of latitude-longitude blocks
 - To exploit cache sizes
- → EMAC valuable for benchmarking

Good performance, but gain limited

vertical layers	CPUs	CPU time	wall time
		[kh/model year]	[days/model year]
L41	64	5.4	3.5
L41	128	7.9	2.6
L90	64	12.0	7.9
L90	128	12.1	4.0
L90	256	poor	poor



Good performance, but gain limited

Communication between nodes (hardware specific)

vertical layers	CPUs	CPU time	wall time
		[kh/model year]	[days/model year]
L41	64	5.4	3.5
L41	128	7.9	2.6
L90	64	12.0	7.9
L90	128	12.1	4.0
L90	256	poor	poor



Good performance, but gain limited

- Communication between nodes (hardware specific)
- Load imbalance from photo-chemistry (being tackled)

vertical layers	CPUs	CPU time [kh/model year]	wall time [days/model year]
L41	64	5.4	3.5
L41	128	7.9	2.6
L90	64	12.0	7.9
L90	128	12.1	4.0
L90	256	poor	poor



Good performance, but gain limited

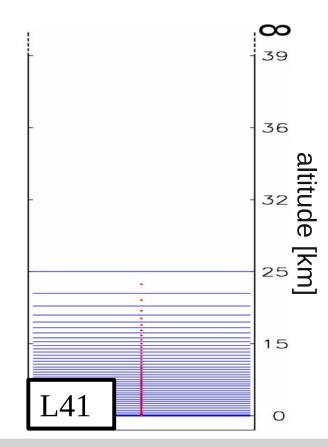
- Communication between nodes (hardware specific)
- Load imbalance from photo-chemistry (being tackled)

L41 version: multi-decadal simulations sensible

vertical layers	CPUs	CPU time	wall time
		[kh/model year]	[days/model year]
L41	64	5.4	3.5
L41	128	7.9	2.6
L90	64	12.0	7.9
L90	128	12.1	4.0
L90	256	poor	poor



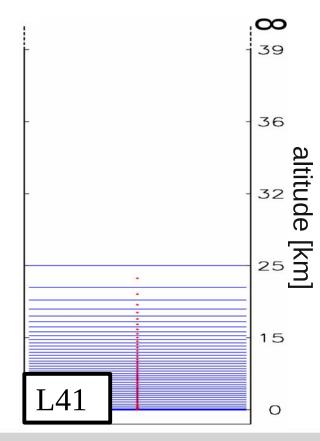
L90 expensive → our L41 version





L90 expensive → our L41 version

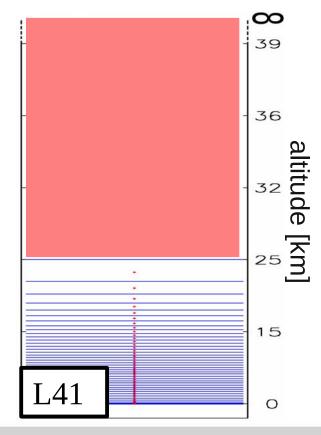
Appropriate for our purposes





L90 expensive → our L41 version

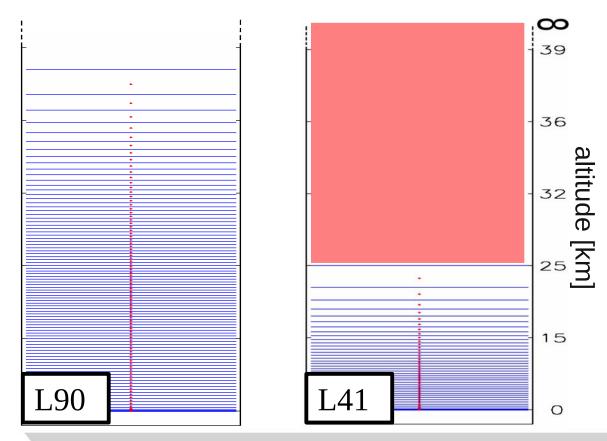
- Appropriate for our purposes
- But: single layer for whole atmosphere above 25 km
- → Impact on chemistry below





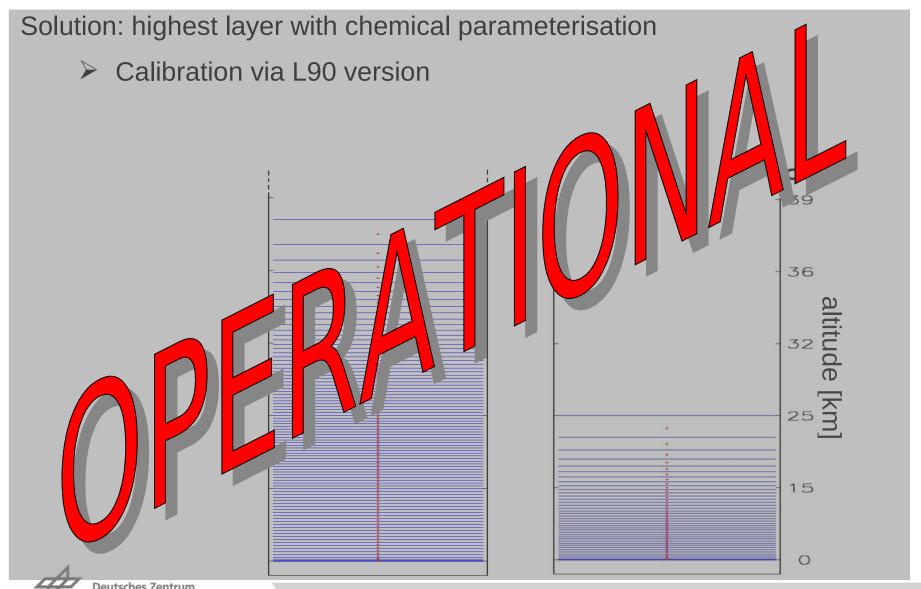
Solution: highest layer with chemical parameterisation

Calibration via L90 version



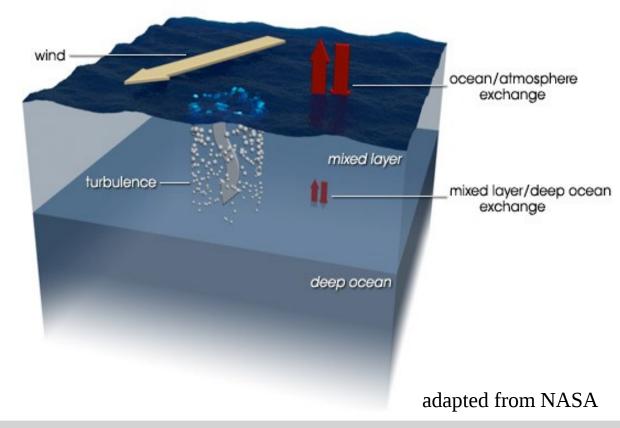


für Luft- und Raumfahrt e.V. in der Helmholtz-Gemeinschaft



Implementation of mixed-layer ocean

- ➤ Feedback: atmosphere ↔ mixed-layer ocean
- No feedback: mixed-layer ocean ↔ deep ocean





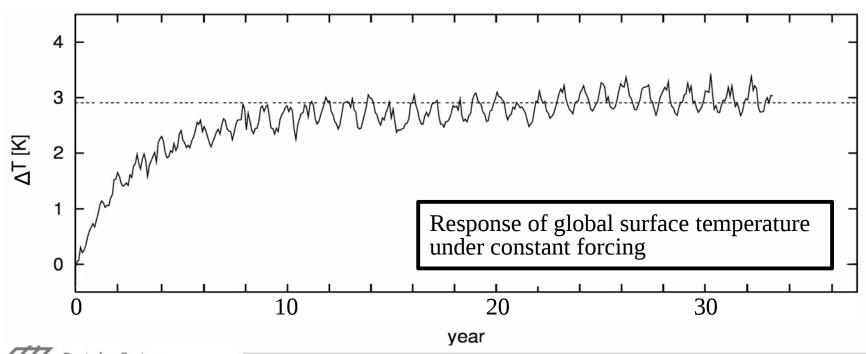
Mixed-layer ocean – additional computational demands

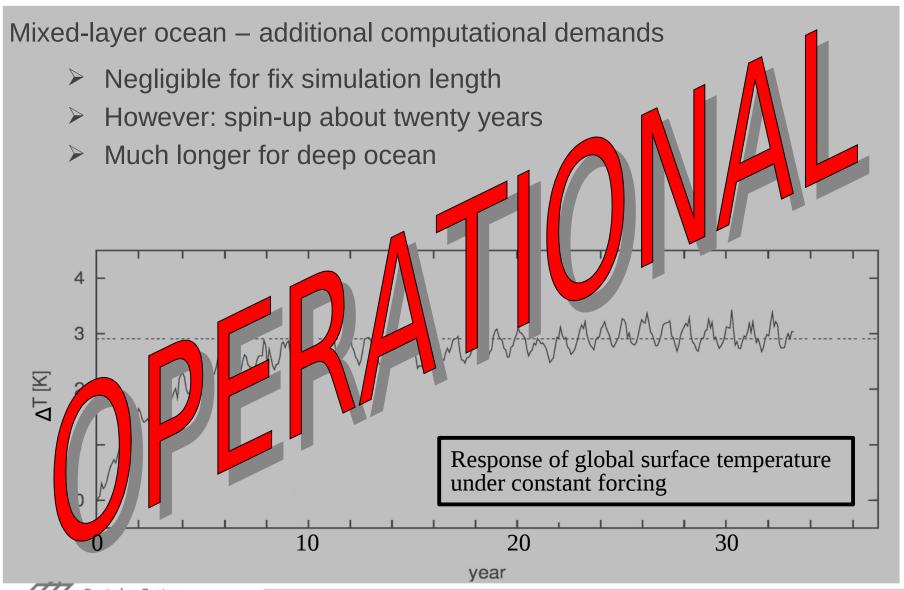
Negligible for fix simulation length



Mixed-layer ocean – additional computational demands

- Negligible for fix simulation length
- However: spin-up about twenty years
- Much longer for deep ocean





Development: Lagrangian formulation

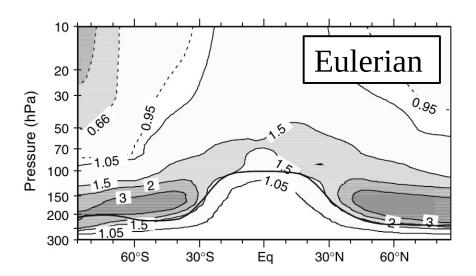
Standard formulation of fluid dynamics: Eulerian

- Separate schemes for dynamics and tracer transport
- Tracer transport numerically diffusive

Development: Lagrangian formulation

Standard formulation of fluid dynamics: Eulerian

- Separate schemes for dynamics and tracer transport
- Tracer transport numerically diffusive





Water vapour: ratio EMAC/satellite

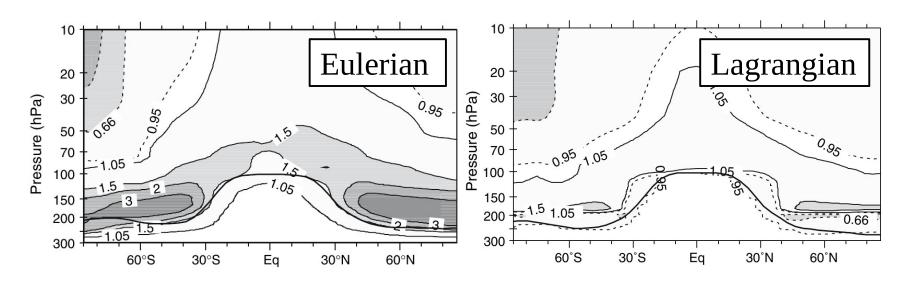
Development: Lagrangian formulation

Standard formulation of fluid dynamics: Eulerian

- Separate schemes for dynamics and tracer transport
- Tracer transport numerically diffusive

Implementation of full-Lagrangian tracer transport

No numerical diffusion



Water vapour: ratio EMAC/satellite



Development: Lagrangian formulation

Standard formulation of fluid dynamics: Eulerian

- Separate schemes for dynamics and tracer transport
- Tracer transport numerically diffusive

Implementation of full-Lagrangie: 10 cm en sport



Development: Lagrangian formulation

Standard formulation of fluid dynamics: Eulerian

- Separate schemes for dynamics and tracer transport
- Tracer transport numerically diffusive

Implementation of full-Lagrangian tracer transport

No numerical diffusion

In development: full-Lagrangian dynamical core

- > Finite-mass method (Gauger et al., 2000)
- > Lagrangain air parcels with variable spatial extent
- Completely new approach in climate modelling

Important question

- Impact of disturbed emission rates on atmospheric composition and climate
- \triangleright E.g. human-made nitrogen oxide \rightarrow near-surface ozone

Important question

- Impact of disturbed emission rates on atmospheric composition and climate
- ➤ E.g. human-made nitrogen oxide → near-surface ozone

Usually: difference of CCM simulations with un-/disturbed emission rates

- ➤ Noise from dynamical-chemical feedback
- Poor signal/noise ratio



Important question

- Impact of disturbed emission rates on atmospheric composition and climate
- ➤ E.g. human-made nitrogen oxide → near-surface ozone

Usually: difference of CCM simulations with un-/disturbed emission rates

- ➤ Noise from dynamical-chemical feedback
- Poor signal/noise ratio

Our solution: switch off feedback

- Dynamics binary identical despite chemistry unequal
- Main challenge: polar stratospheric clouds

Important question Impact of disturbed emission rates on atmospheric composition \triangleright E.g. human-made nitrogen oxide \rightarrow near-surface ozone Usually: difference of CCM simulation mission rates Noise from dynamical-chemin fee Poor signal/noise at Our sol ນເກສ**ອ**່າ cical despite chemistry unequal enge: polar stratospheric clouds

Production simulations

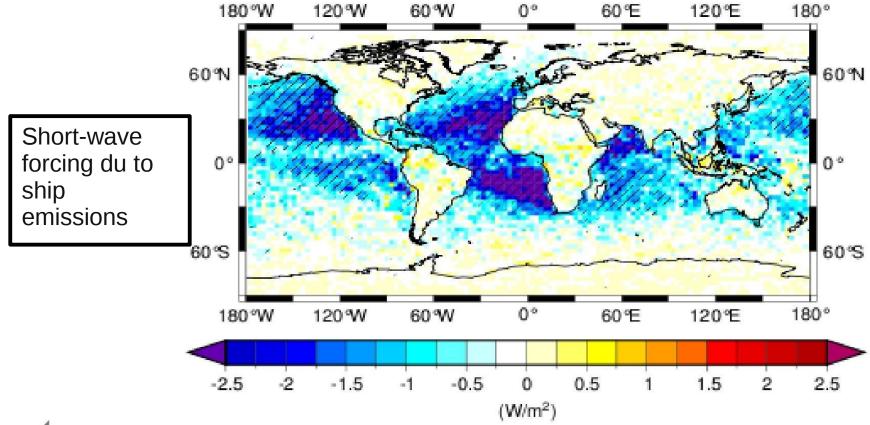
Focus on model development: prerequisite for production simulations

→ Now feasible and going to start

Production simulations

Climate impact of nitrogen oxide and sulfur dioxide from shipping

- Affects optical and microphysical cloud properties
- Mostly cooling

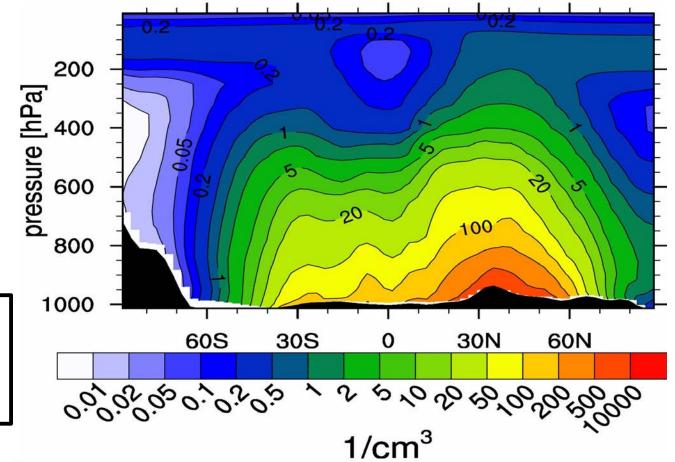




Production simulations

Aerosol aging

- > Can result in ice nuclei
- → Affects cirrus clouds



Number concentration of potential ice nuclei

Summary

We use a chemistry-climate model (CCM)

- Diverse numerics / types of domain decomposition
- Good performance on LRZ/ALTIX
- But: gain limited due to communication between nodes



Summary

We use a chemistry-climate model (CCM)

- Diverse numerics / types of domain decomposition
- Good performance on LRZ/ALTIX
- But: gain limited due to communication between nodes

Model development ...

- New upper boundary
- Mixed-layer ocean
- Lagrangian transport
- Chemistry-transport mode

Summary

We use a chemistry-climate model (CCM)

- Diverse numerics / types of domain decomposition
- Good performance on LRZ/ALTIX
- But: gain limited due to communication between nodes

Model development ...

- New upper boundary
- > Mixed-layengues
- > Lagragiantal sport
- Chernistry-transport mode
 - → Production going to start