Vi-SEEM
Virtual Research Environment Portal

Meteo
All about weather

The WRF-Chem model

Overview, capabilities, examples

Theodore M. Giannaros

Post-doc Researcher

National Observatory of Athens

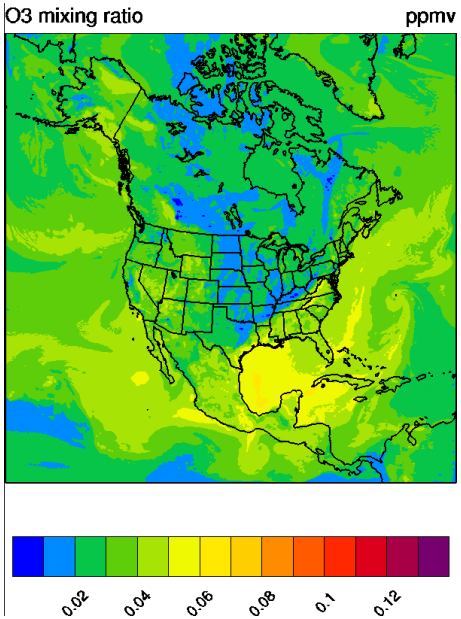
Institute for Environmental Research and Sustainable Development

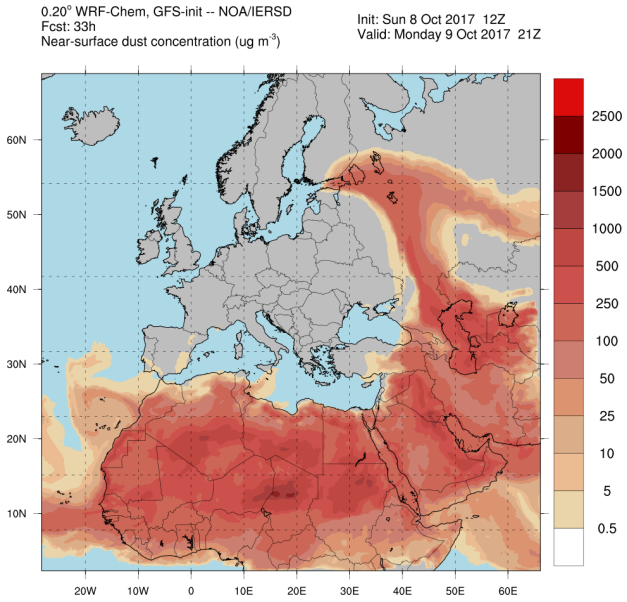
Email: thgian@noa.gr

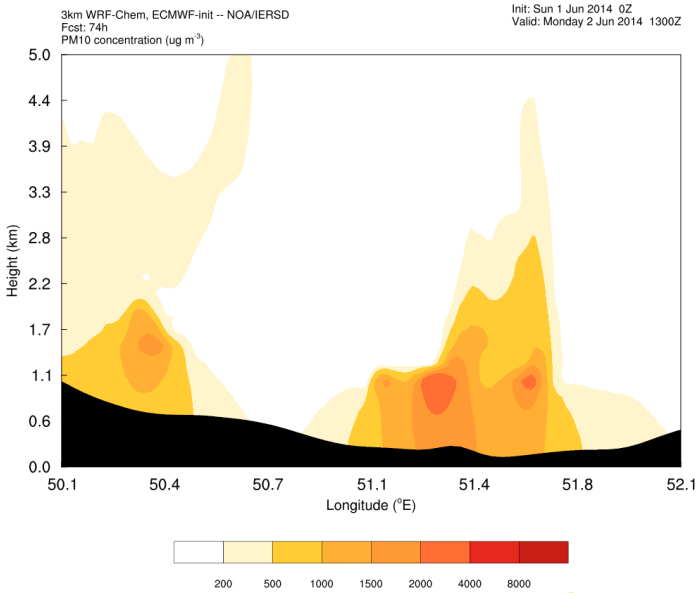
What is it?

A version of the **WRF** model that can be used for the simulation of **trace gases** and **particulate matter** simultaneously with the meteorology (Grell *et al.*, 2005)

- **Online** chemistry, fully embedded within the WRF
- **Consistency**: same grid structure (vertical, horizontal), same physics for sub-grid scale transport, no time interpolations
- Perfectly suited for examining **meteorology-chemistry feedbacks** on local to global scales (climate change)
- Suitable for operational **air quality forecasting** on regional to cloud-resolving scales







Why ‘online’ is important?

Atmospheric Environment
Volume 45, Issue 38, December 2011, Pages 6845-6851

Integrated modeling for forecasting weather and air quality: A call for fully coupled approaches

Georg Grell [a], Alexander Baklanov [b]

“Eventually though, a migration to an integrated modeling system will provide new opportunities for weather prediction modelers as well. The simulation of chemical species will allow identification of shortcomings in currently used forecast models as well as lead to better use of meteorological data assimilation”

- More **realistic representation** of the atmosphere: the offline approach introduces errors that increase with increasing grid resolution
- **Numerically** more **consistent**: same grid structure (horizontal, vertical), no time interpolation
- Proven **improvements** in medium-range weather **forecasts**

Nevertheless:

- Computationally very **expensive**
- **Less** flexibility for conducting **ensemble** modeling

How does the 'coupling' work?

- **Advection** and **diffusion** provided by WRF
- Sub-grid scale **transport** carried out by WRF **physics** parameterizations, **PBL** schemes and **convective** parameterization schemes
- Chemical processes carried out by WRF-Chem, dependent on meteorological input: **emissions** (anthropogenic, biogenic, fire, dust, sea salt, volcanic), dry **deposition**, wet **scavenging**
- Chemical reactions carried out by WRF-Chem: **aqueous** and **gas** phase chemistry, **aerosols**
- Chemical radiation processes carried out by WRF-Chem: computation of **photolysis** rates
- Chemistry-meteorology **feedback** carried out by coupling interface: **radiation**, **microphysics**, **convection**

Installation

Similar procedure and dependencies as for installing the WRF model

export WRF_CHEM=1

./configure

./compile em_real

50+ compilation options: Serial, DM, SM, Hybrid (DM+SM), numerous compilers and architectures

```
 1. (serial)   2. (smpar)   3. (dmpar)   4. (dm+sm)   PGI (pgf90/gcc)
 5. (serial)   6. (smpar)   7. (dmpar)   8. (dm+sm)   PGI (pgf90/pgcc): SGI MPT
 9. (serial)  10. (smpar)  11. (dmpar)  12. (dm+sm)   PGI (pgf90/gcc): PGI accelerator
13. (serial)  14. (smpar)  15. (dmpar)  16. (dm+sm)   INTEL (ifort/icc)
                                        17. (dm+sm)   INTEL (ifort/icc): Xeon Phi (MIC architecture)
18. (serial)  19. (smpar)  20. (dmpar)  21. (dm+sm)   INTEL (ifort/icc): Xeon (SNB with AVX mods)
22. (serial)  23. (smpar)  24. (dmpar)  25. (dm+sm)   INTEL (ifort/icc): SGI MPT
26. (serial)  27. (smpar)  28. (dmpar)  29. (dm+sm)   INTEL (ifort/icc): IBM POE
30. (serial)               31. (dmpar)               PATHSCALE (pathf90/pathcc)
32. (serial)  33. (smpar)  34. (dmpar)  35. (dm+sm)   GNU (gfortran/gcc)
36. (serial)  37. (smpar)  38. (dmpar)  39. (dm+sm)   IBM (xlf90_r/cc_r)
40. (serial)  41. (smpar)  42. (dmpar)  43. (dm+sm)   PGI (ftn/gcc): Cray XC CLE
44. (serial)  45. (smpar)  46. (dmpar)  47. (dm+sm)   CRAY CCE (ftn/gcc): Cray XE and XC
48. (serial)  49. (smpar)  50. (dmpar)  51. (dm+sm)   INTEL (ftn/icc): Cray XC
52. (serial)  53. (smpar)  54. (dmpar)  55. (dm+sm)   PGI (pgf90/pgcc)
56. (serial)  57. (smpar)  58. (dmpar)  59. (dm+sm)   PGI (pgf90/gcc): -f90=pgf90
60. (serial)  61. (smpar)  62. (dmpar)  63. (dm+sm)   PGI (pgf90/pgcc): -f90=pgf90
```

Quick how-to

Procedure similar to a meteorological WRF simulation

1. Setup your modeling domain as you do for a typical WRF simulation

./geogrid.exe

2. Decode forcing data

./ungrib.exe

3. Horizontally interpolate forcing data on your modeling domain

./metgrid.exe

Chemistry 'part'

1. Select chemistry option

chem_opt = ??

2. Prepare emissions (users' 'job from scratch') ** will not be covered in this talk
3. Generate initial and boundary conditions (optionally also lower boundaries) for both meteorology and chemistry

./real.exe

4. Run your simulation!

./wrf.exe

Getting started: Read - Think - Design

Define your objectives

What are your **scientific** and/or **practical objectives**? **Why** do you need to run WRF-Chem? **How** will you know that your simulations are successful?

You and your scientific problem: 'to know us better'

Review literature! What are the **atmospheric and chemical processes** involved? Which are the most **important** (clouds, radiation, convection, aerosols, etc.)? **What** is known? Is anything **missing**? **Judge** the **efficacy** of your "simulations-to-do".

Determine available observational datasets

What **observations** are available? Again, become familiar with the **processes** that you want to study. How will the observations be used for **verifying** and/or **complementing** your simulations? **Judge** the **adequacy** of your "simulations-to-do".

Prepare your strategy

Are you going to focus on a **case study**? If yes, **which** one and **why**? Are there adequate **observations** for verifying your "simulations-to-do"? Will you set up an **operational** weather and air quality forecasting service? What are the practical **requirements**?

Setting up domains

First things, first

- **Target** horizontal grid spacing
- Resolution of **initialization** data

Most often, you will need to adopt a **nesting** strategy.

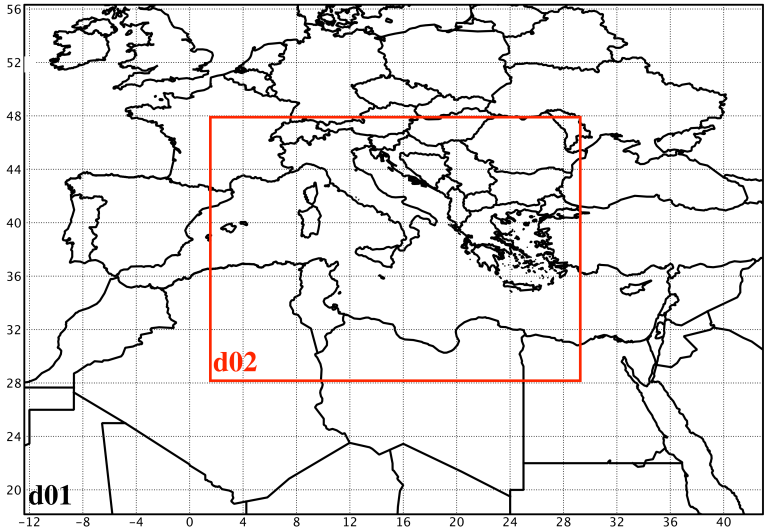
Hints

- Place domain **boundaries away** from each other, and away from **steep** topography
- Odd parent-child ratios are preferred (e.g. **3:1, 5:1**)
- Higher **horizontal** resolution will also require higher **vertical** resolution
- Use at least **30-35** vertical levels; larger density closer to the ground and to the model top to avoid numerical instability (aka 'CFL violation')
- **Lambert**: mid-latitudes, **Mercator**: low-latitudes, **Lat-Lon**: global, **Rotated lat-lon**: regional
- Start **inside-out** (first the nest, then move up)

Never forget!

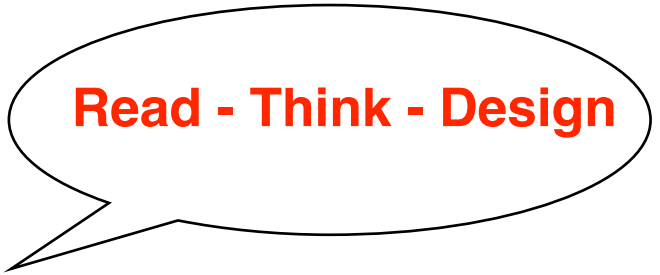
Avoid the "grey zone" (**4-10 km**)

What about **computational** requirements?



Forcing data

Garbage in, garbage out (GIGO)



General questions:

- Do the **static** data (topography, land use, etc.) represent my study area adequately?
- How 'good' are the **meteorological** forcing data? Does their **resolution** (temporal, spatial) fit my domain setup?
- Do I need **lower boundary** conditions (e.g. SST)?

WRF-Chem specific questions:

- Do I need an **emission inventory**? Do I have one? Does it **represent** well my study area? Does it have adequate **resolution** (temporal and spatial) and fit the purposes of my simulation?
- What kind of **chemistry** do I need? **Gas** phase only? Do I need to include **aerosols**?

Physics

Too many options! Where to start from?

- Back to basics: Which processes are important? **Review literature**. What others did?
- Consider first well documented (**extensively tested**) schemes

Hints

- Convective schemes are generally not required at **dx<4 km**
- Sophisticated microphysics schemes (double-moment, detailed species) may not be necessary at **dx>>10 km**
- Try to have **consistent physics** between the domains or use 1-way nesting
- If your simulation spans more than **5 days**, you could start thinking to adopt the **SST update** option

What about the meteorology-chemistry feedback?

- Certain physics parameterizations may be required to account for e.g. **aerosol-radiation** and **aerosol-microphysics** interactions

Chemistry (1)

```
&chem
 kemit                  = 1,
 chem_opt               = 10, 10,
 bioemdt                = 0, 0,
 photdt                 = 0, 0,
 chemdt                 = 0, 0,
 io_style_emissions     = 0,
 emiss_opt              = 0, 0,
 emiss_opt_vol          = 0, 0,
 emiss_ash_hgt          = 20000.,
 chem_in_opt            = 0, 0,
 phot_opt               = 0, 0,
 gas_drydep_opt         = 0, 0,
 aer_drydep_opt         = 201, 201,
 bio_emiss_opt          = 0, 0,
 ne_area                = 0,
 dust_opt               = 2,
 dmsemis_opt            = 0,
 seas_opt               = 0,
```

Chemistry option

Timesteps

Input emissions options

Anthro/volcanic emissions

Input emissions options

Photolysis option

Dry deposition

Biogenic, dust, sea salt

Chemistry (2)

```
depo_fact                 = 0.25, 0.25,
gas_bc_opt                = 0, 0,
gas_ic_opt                = 0, 0,
aer_bc_opt                = 0, 0,
aer_ic_opt                = 0, 0,
gaschem_onoff             = 0, 0,
aerchem_onoff             = 0, 0,
wetscav_onoff             = 1, 1,
cldchem_onoff             = 0, 0,
vertmix_onoff             = 1, 1,
chem_conv_tr              = 1, 0,
conv_tr_wetscav           = 1, 0,
conv_tr_aqchem            = 0, 0,
biomass_burn_opt          = 0, 0,
plumerisefire_frq         = 0, 0,
have_bcs_chem             = .false., .false.,
aer_ra_feedback           = 0, 0,
aer_op_opt                = 0, 0,
opt_pars_out              = 0,
diagnostic_chem           = 1, 1,
```

Gas/aerosols ICBC

Gas/aerosols chemistry switches

Wet scavenging

Aerosol effects

Sub-grid scale processes

Biomass burning options

Gas/aerosols ICBC

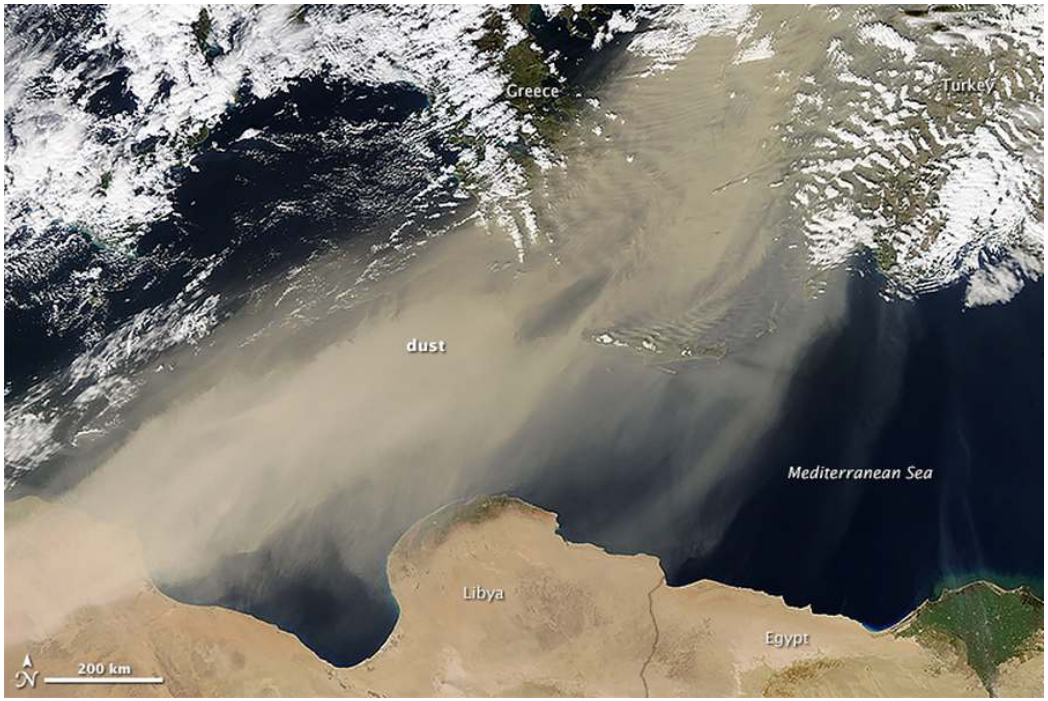
Aerosol effects

Dust in WRF-Chem

Why dust?

- Large **uncertainty** in estimating global dust emissions: 514 - 4313 Tg/yr
- Emissions depend heavily on surface wind speed and soil properties: high spatial and temporal **variability**
- Incomplete **understanding** of the processes that lead to dust emission: threshold friction velocity, horizontal saltation flux, vertical flux

Understanding changes in dust emissions is of paramount importance for both interpreting **past** and predicting **future climate change**



Dust emissions options

Available dust emission schemes (version 3.9)

All schemes are founded on the GOCART mechanism:

1. **GOCART** (**dust_opt = 1**)

module_gocart_dust.F

2. **AFWA** (**dust_opt = 3**)

module_gocart_dust_afwa.F

3. **UoC** (**dust_opt = 4**) with either **dust_schme=1** (Shao, 2001) or **dust_schme = 2** (Shao, 2004) or **dust_schme = 4** (Shao, 2011)

module_uoc_dust.F

module_uoc_dustwd.F

module_qf03.F

Always, examine code!

Required input

Dust source function: **Ginoux erodibility** (default, provided via WPS)

Dust emissions are computed **online** using surface **wind speed** and **soil** properties; no need for any emission inventory

Advice: Adopt a sufficiently long spin-up period for building up emissions

(Dust) aerosol models

Available aerosol models (version 3.9)

1. **Modal** (MADE/SORGAM, MADE/VBS, MAM)

Size distribution of aerosols represented by several overlapping intervals (**modes**), assuming a **log-normal distribution** within each mode

- Computationally efficient
- Less accurate

2. **Sectional** (MOSAIC)

Size distribution of aerosols represented by several discrete **size bins**, specified by the upper and lower dry **particle diameters**

- Computationally expensive
- More accurate

3. **Bulk** (**chem_opt = 401**)

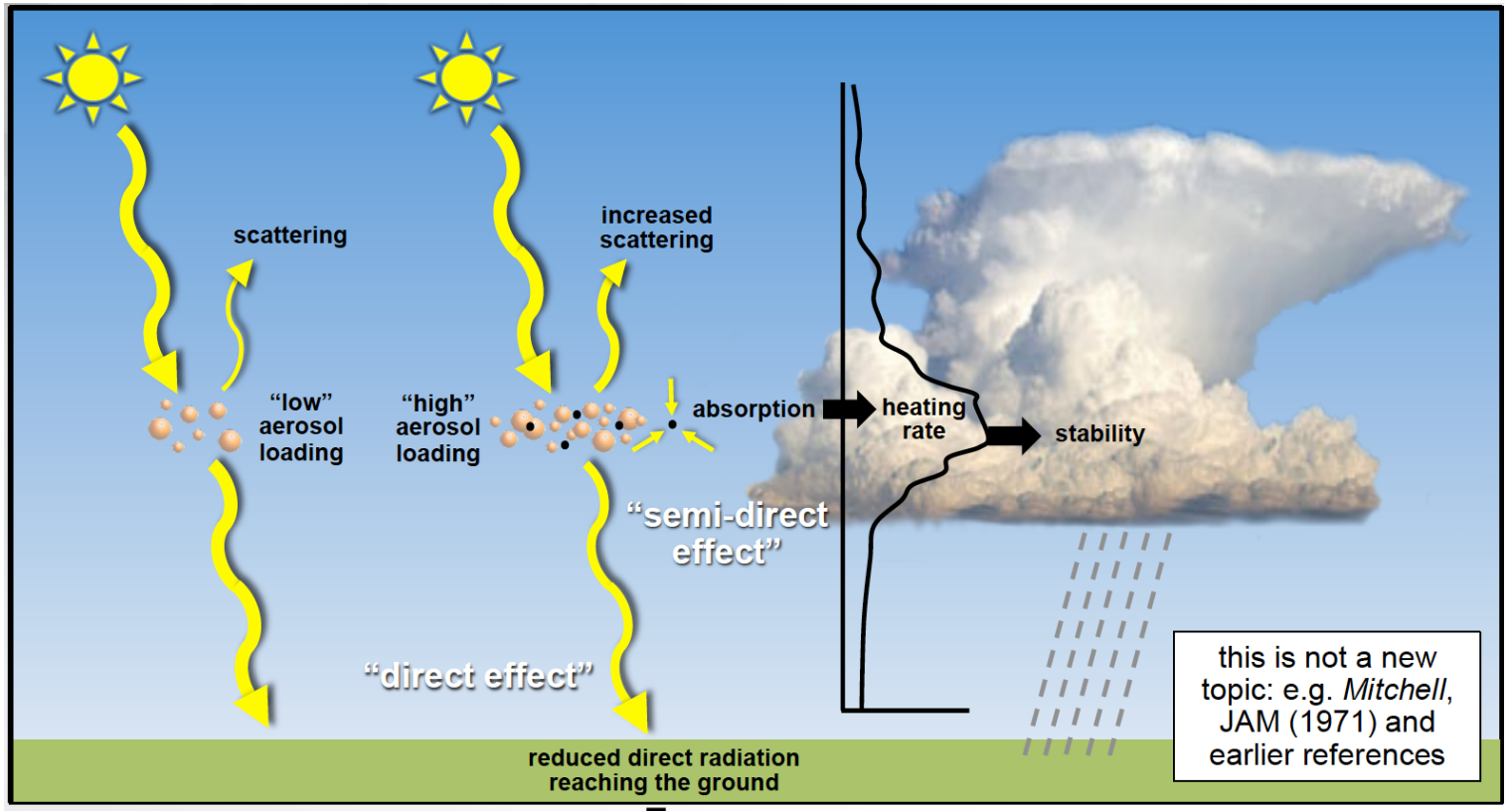
Provides only dust concentration, assuming 10 ash size bins

- Computationally fast
- Dust is treated as a passive tracer

When do I need to use an aerosol model for dust?

Necessary to account for aerosol **direct** and **indirect** effects

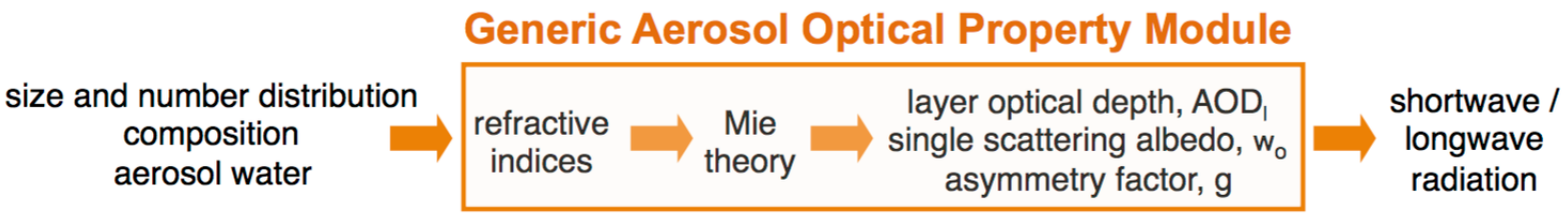
(Dust) aerosol direct (radiative) effects (1)



Direct effect: Solar/IR **scattering** & **absorption** → Modification of the **radiative balance**

Semi-direct effect: Modification of **heating rates**, surface fluxes (**sensible**, **latent**), static **stability**

(Dust) aerosol direct (radiative) effects (2)



- Aerosol optical properties (**AOD, asymmetry factor, SSA**) computed for **4 SW** and **16 LW** wavelengths: large uncertainty in determining dust refractive indices!
- Compatible **aerosol models**: Bulk, MADE/SORGAM, MAM, MOSAIC
- Compatible **radiation schemes**: Goddard, RRTMG

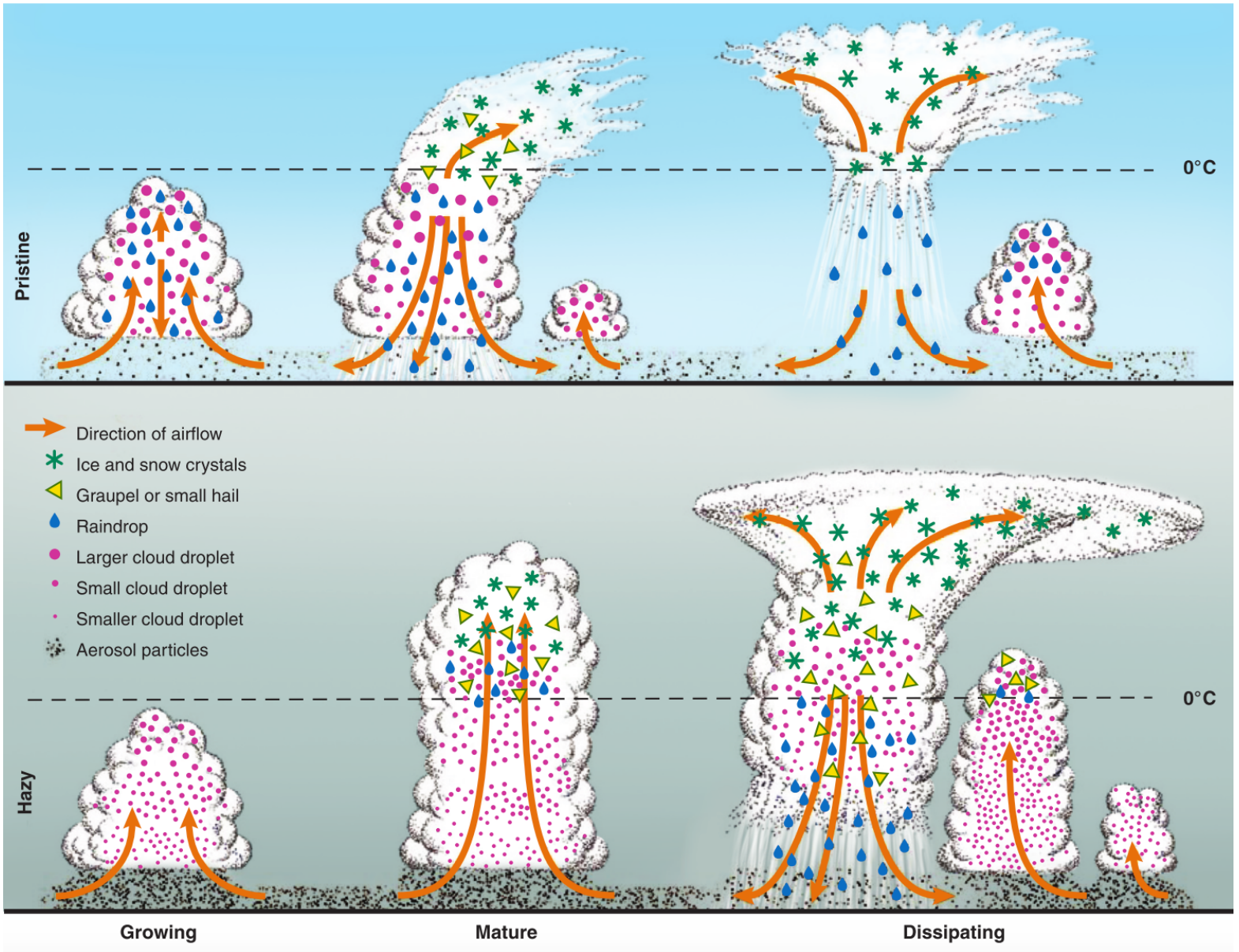
Setting up your namelist

ra_sw_physics = 2 or 4
ra_lw_physics = 4
aer_ra_feedback = 1
aer_op_opt > 0 (select mixing rule for Mie calculations)
cu_rad_feedback = .true. (account for sub-grid scale cloud effects)
chem_opt = any (except for 401 - 'dust-only')

Evaluate direct effects

Compare simulations with aer_ra_feedback = 0 (OFF) and 1 (ON) but consider semi-direct effects (changes in clouds induced by radiative effects)

(Dust) aerosol indirect effects (1)



When activated, they are effective cloud condensation nuclei (**CCN**) and ice nuclei (**IN**), thus **modifying the microphysical properties** of clouds.

(Dust) aerosol indirect effects (2)

- Prognostic aerosol **number concentrations** influence **cloud albedo** and **rain mixing ratio**
- Compatible **chemistry options**: any with aqueous reactions
- Compatible **aerosol models**: Bulk, MADE/SORGAM, MAM, MOSAIC
- Compatible **radiation schemes**: Goddard, RRTMG
- Compatible **microphysics schemes**: Lin, Morrison

Setting up your namelist

progn = 1 (enable prognostic number concentrations for microphysics species)
mp_physics = 2 or 10
cldchem_onff = 1 (turn on cloud chemistry)
wetscav_onff = 1 (turn on wet scavenging)
chem_opt = any that supports aqueous chemistry (suggested 10-MOSAIC, 11-MADE/SORGAM)

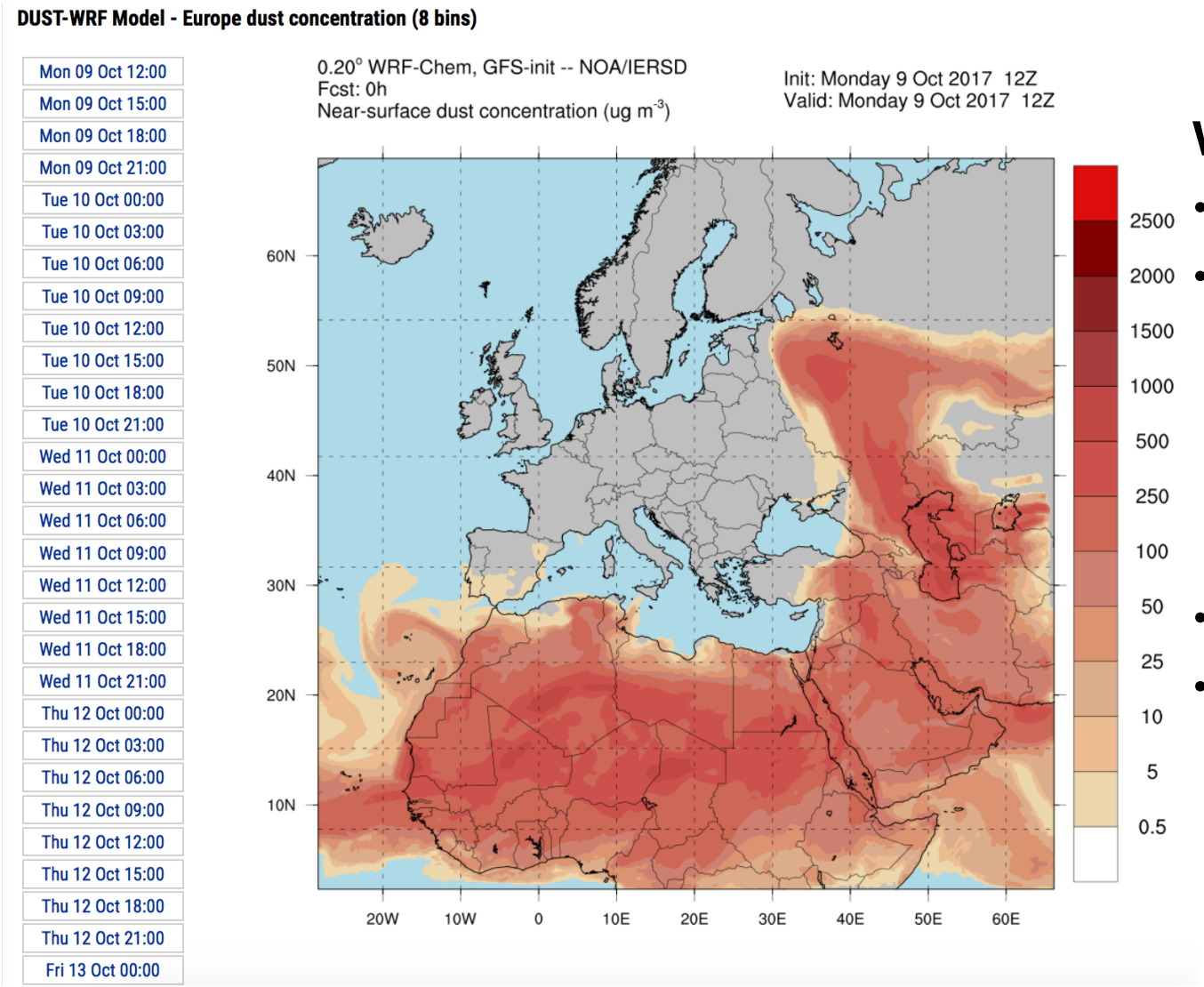
Evaluate indirect effects

- 1 control simulation (CNTL)
- 1 radiative experiment (RAD)
- 1 experiment with radiative and indirect effects (TOT)

indirect effects = TOT - RAD

WRF-Chem application examples (1)

Operational dust forecasting system for Europe



WRF-Chem v3.6.1

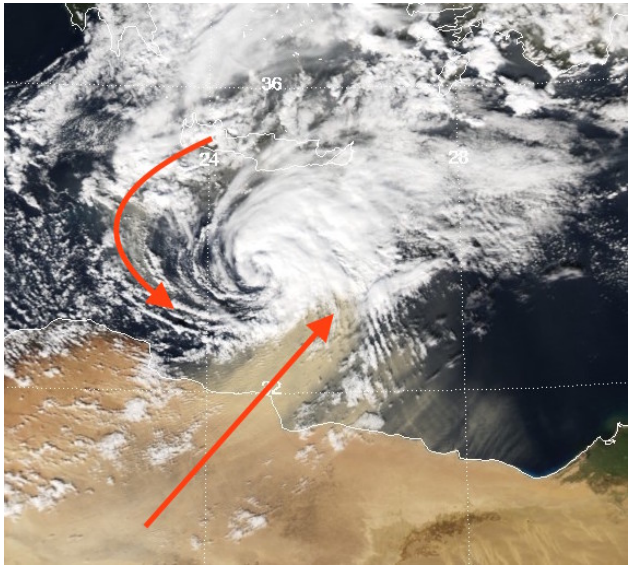
- 'Dust-only'
- Modified GOCART scheme (**chem_opt=401**) to use 8-bin size distribution following DREAM (Flaounas et al., 2017 GMD)
- Daily, 84-h forecasts
- Part of WMO SDS-WAS for NA-ME-E

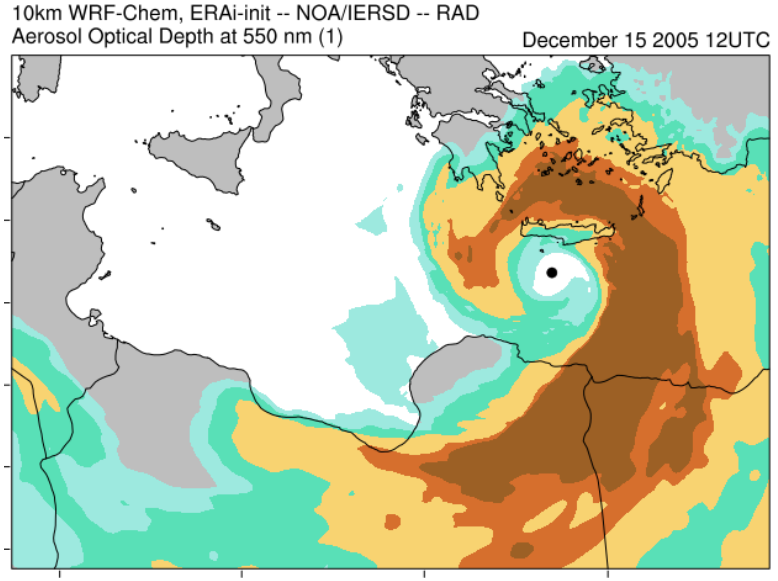
http://meteo.gr/meteomaps/wrf_dust.cfm

WRF-Chem application examples (2)

Work in progress!

Dust-cyclones interactions





Application on ARIS HPC in the frame of VI-SEEM

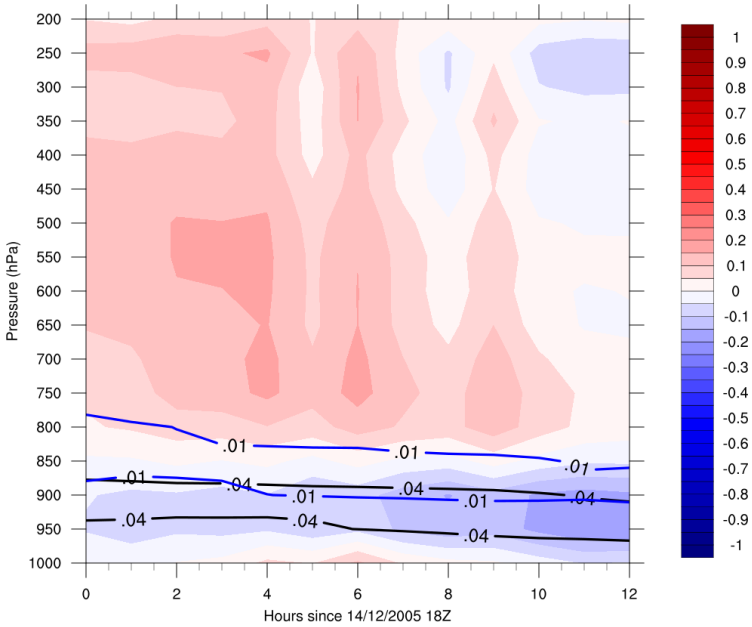
WRF-Chem v3.7.1

Study direct/indirect effects of dust on a Medicane

- GOCART/MOSAIC (Zhao et al., 2010)

chem_opt=10, **dust_opt=2**

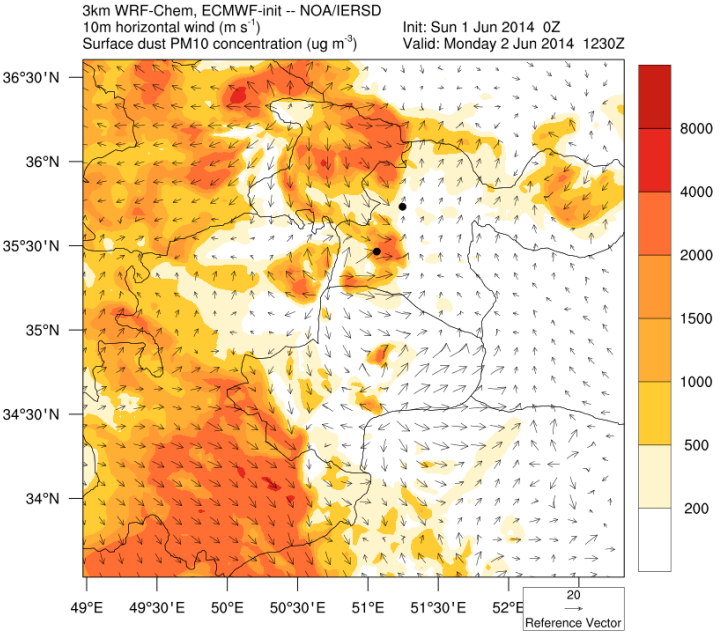
- Nested modeling: **10, 3.333 km**

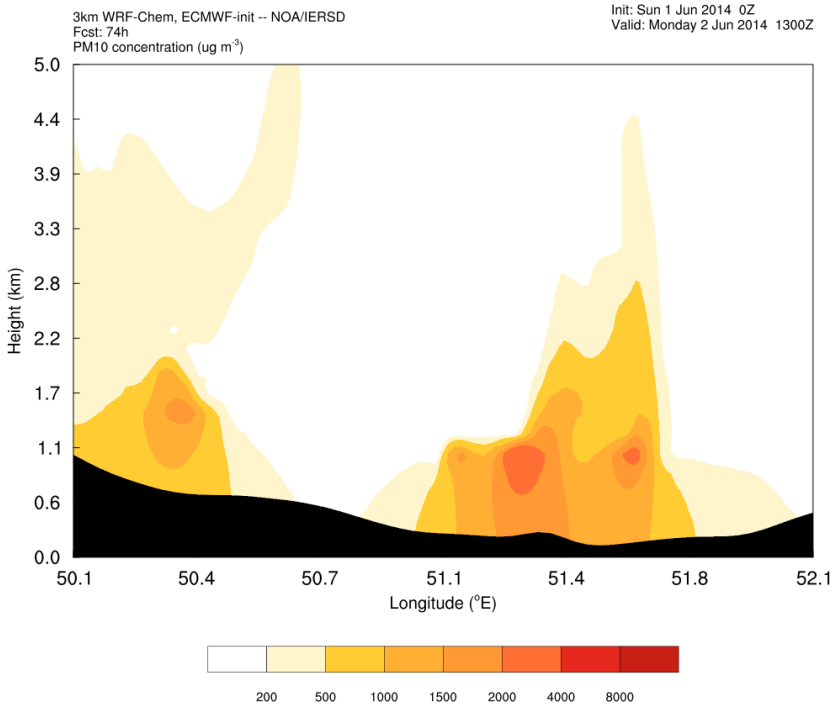


WRF-Chem application examples (3)

Work in progress!

Dust storms - Haboob in Iran





Application on ARIS HPC in the frame of VI-SEEM

WRF-Chem v3.7.1

Numerical simulation of an intense, short-lived dust storm (haboob) in Iran

- GOCART/MOSAIC (Zhao et al., 2010)

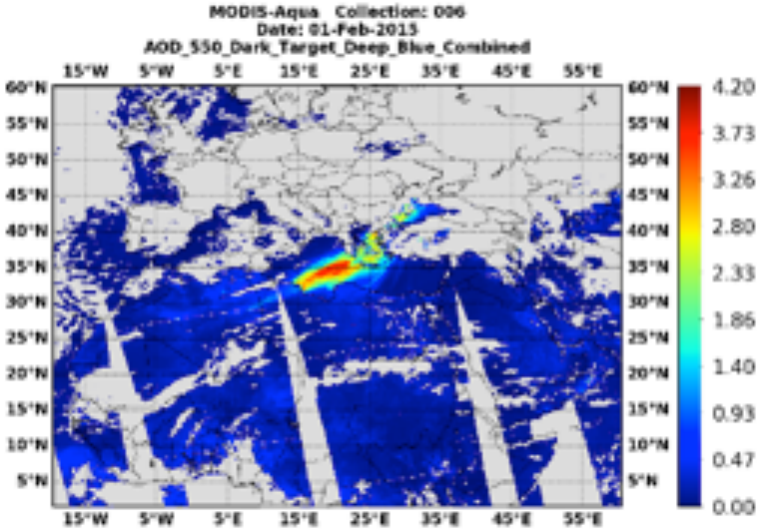
chem_opt=10, dust_opt=2

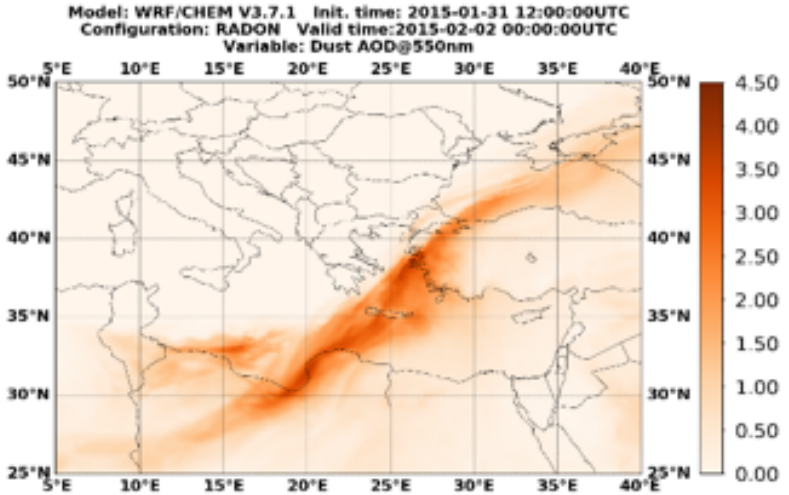
- Nested modeling: **9, 3 km**

WRF-Chem application examples (4)

Work in progress!

Dust outbreak in the Mediterranean





Application on ARIS HPC in the frame of VI-SEEM

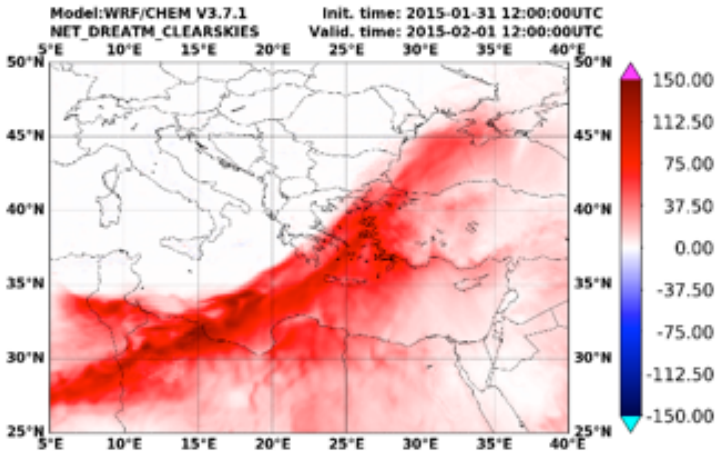
WRF-Chem v3.7.1

Numerical simulation of an intense dust outbreak in SE Med

- GOCART/MOSAIC (Zhao et al., 2010)

chem_opt=10, **dust_opt=2**

- 1 domain: **10 km**



Summary

WRF-Chem is a powerful **integrated** modeling system that can support a wide range of applications including:

- air quality **forecasting** services
- case study modeling of **chemistry-meteorology** feedbacks (e.g. aerosols)
- **climate change** assessment studies focusing on chemistry (e.g. aerosols)

Take-aways & Hints

- **R**ead - **t**hink - **d**esign
- Get your hands dirty - **dig into the code**!
  There are some '**hidden**' schemes and options, and **bugs** as well
- WRF-Chem is a really **heavy** model
  Consider carefully the scope of your application, its adequacy and its efficiency

Resources (not the wealth you may be used to for WRF)

https://ruc.noaa.gov/wrf/wrf-chem/ (main WRF-Chem page)

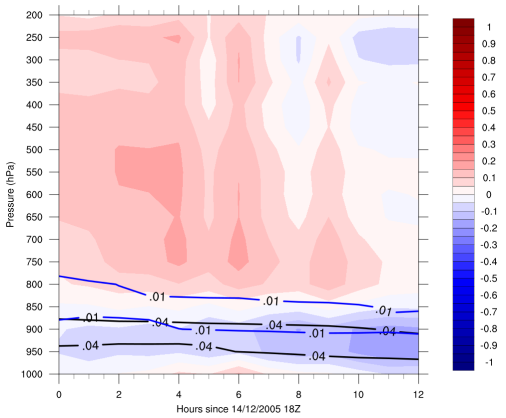
Tutorials, user manuals, references for chemistry options, papers using the model for various purposes

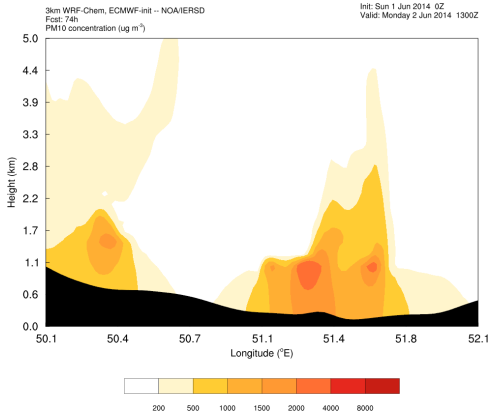
Vi-SEEM
Virtual Research Environment Portal

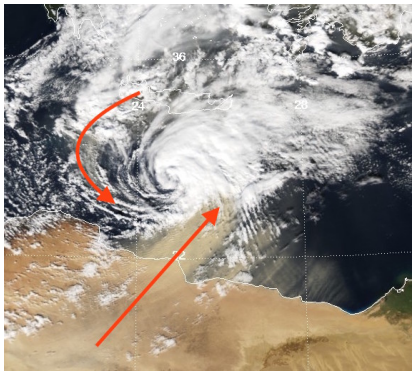
Meteo
All about weather

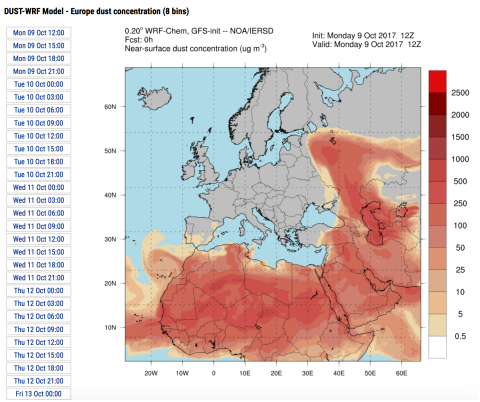
Thank you!

Questions? Comments?









Contact: Theodore M. Giannaros, thgian@noa.gr