Innovations in dispersion modeling using FALL3D and operations at the Buenos Aires VAAC

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WORLD METEOROLOGICAL ORGANIZATION (WMO)
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Anchorage, Alaska, October 19-23

- **FALL3D**: An Eulerian model for emission, transport, deposition and re-suspension of tephra.
  - Community of users.
  - Experimental operational setup at the Buenos Aires VAAC based on coupling WRF/ARW with FALL3D-7.0 (http://www.smn.gov.ar/).

- **This talk** overviews different innovations implemented in the model (at a research level yet):
  1. Coupling with FPLUME-1.0 (a new BPT model considering wet aggregation).
  2. Ensemble forecast strategies using the Dakota toolkit.
  3. WARIS-Transport: a framework for HPC code optimization and porting to accelerator-based architectures.
  4. ZEN-ATM: an air traffic impact evaluation tool.
  5. Re-suspension (not today).

1. FPLUME-1.0

- Model forecasts strongly depend on the **source term**. Approaches to quantify the source term include:

1. Empirical relationships between plume height and MER.
    - Good from the operational point of view.

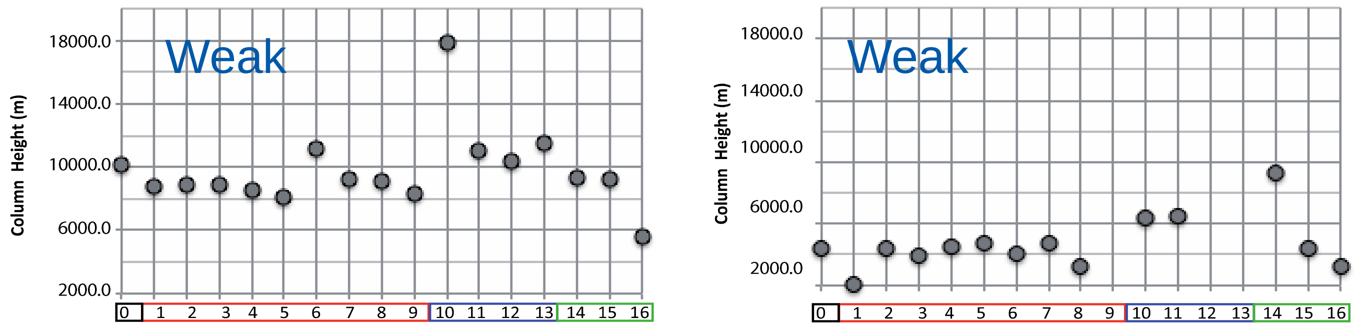
2. Assimilation of satellite retrievals trough model inversion.
    - Virtual source.
    - Only for fine ash.

3. *Coupling with 1D BPT models to simulate the source term.*

1. FPLUME-1.0

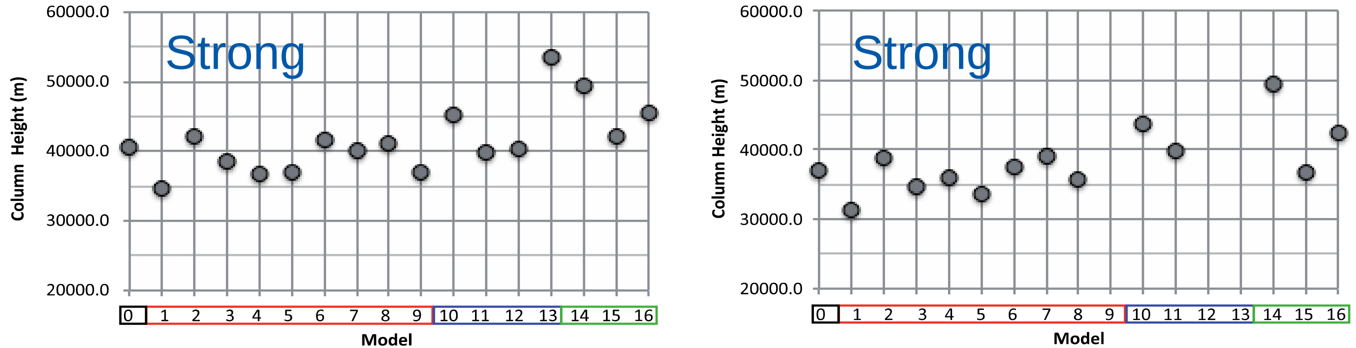
- Plume model **inter-comparison exercise** promoted by IAVCEI (Costa et al., submitted; more on Yujiro's talk later on):
  - Blind test for strong and weak plumes.
  - Similar results for weak plumes, larger model discrepancies for strong plumes.
  - 1D models oversimplify wind entrainment coefficients.

column heights given the MER at the vent



a) Weak plume no wind

b) Weak plume with wind



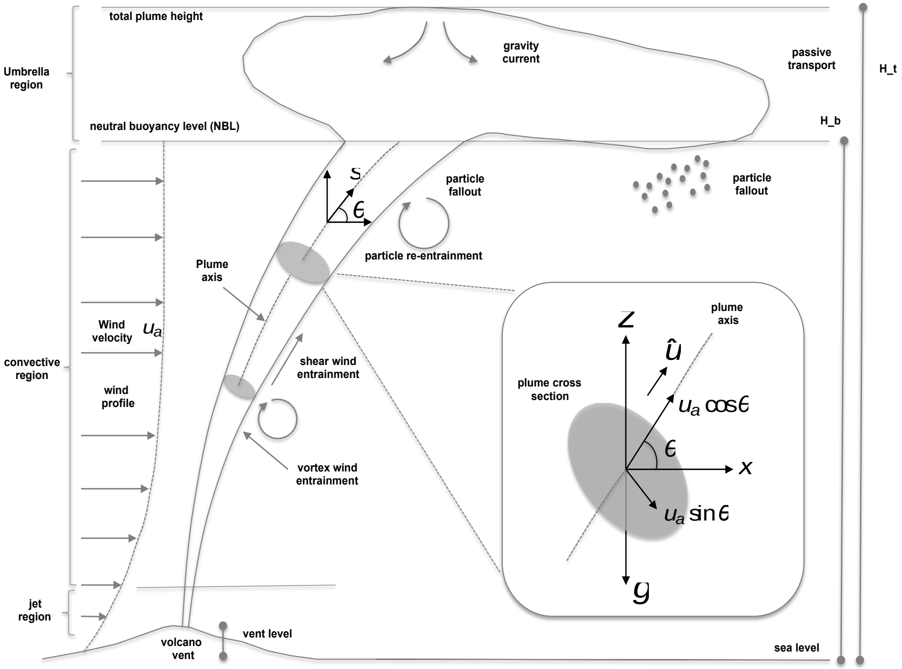
c) Strong plume no wind

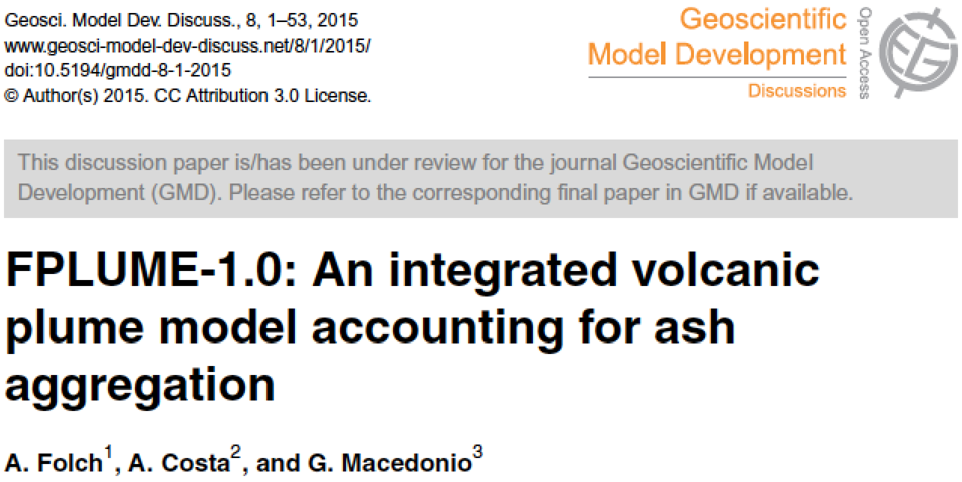
d) Strong plume with wind

1. FPLUME-1.0

FPLUME-1.0: a new steady-state 1-D cross-section averaged model based on the BPT that accounts for:

- Plume bent over by wind.
- Entrainment of ambient moisture.
- Water phase changes.
- Particle fallout.
- Particle re-entrainment.
- **Variable wind entrainment coefficients.**
- **Wet aggregation.**

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www.geosci-model-dev-discuss.net/8/1/2015/
doi:10.5194/gmdd-8-1-2015
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Geoscientific Model Development Discussions

Open Access

This discussion paper is/has been under review for the journal Geoscientific Model Development (GMD). Please refer to the corresponding final paper in GMD if available.

FPLUME-1.0: An integrated volcanic plume model accounting for ash aggregation

A. Folch[1], A. Costa[2], and G. Macedonio[3]

1. FPLUME-1.0

- **Wind entrainment coefficients** are typically assumed constant by BPT models:

$$u_\varepsilon = \alpha_s|\hat{u} - u_a\cos\theta| + \alpha_v|u_a\sin\theta|$$

↓ Shear coefficient (stream-wise)

$$\alpha_s \approx 0.1 - 0.17$$

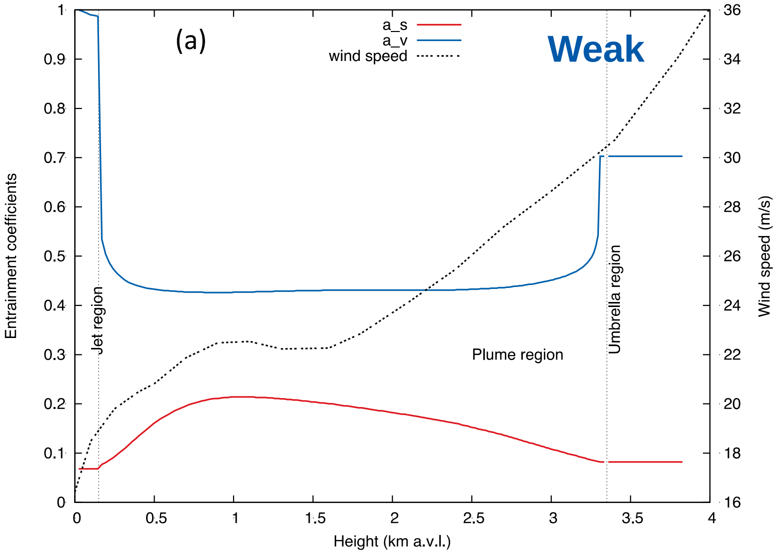
↓ Vortex coefficient (cross-flow)

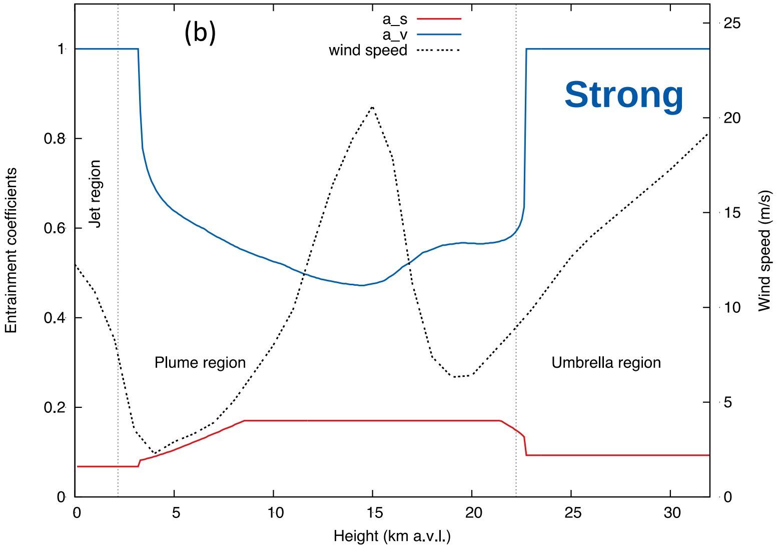
$$\alpha_v \approx 0.3 - 1.0$$

- FPLUME-1.0 assumes parameterizations depending on the local *Ri* number:

$$\alpha_s = 0.0675 + \left(1 - \frac{1}{A(z_s)}\right) Ri\,\sin\theta + \frac{r}{2}\frac{1}{A(z_s)}\frac{dA}{dz}$$

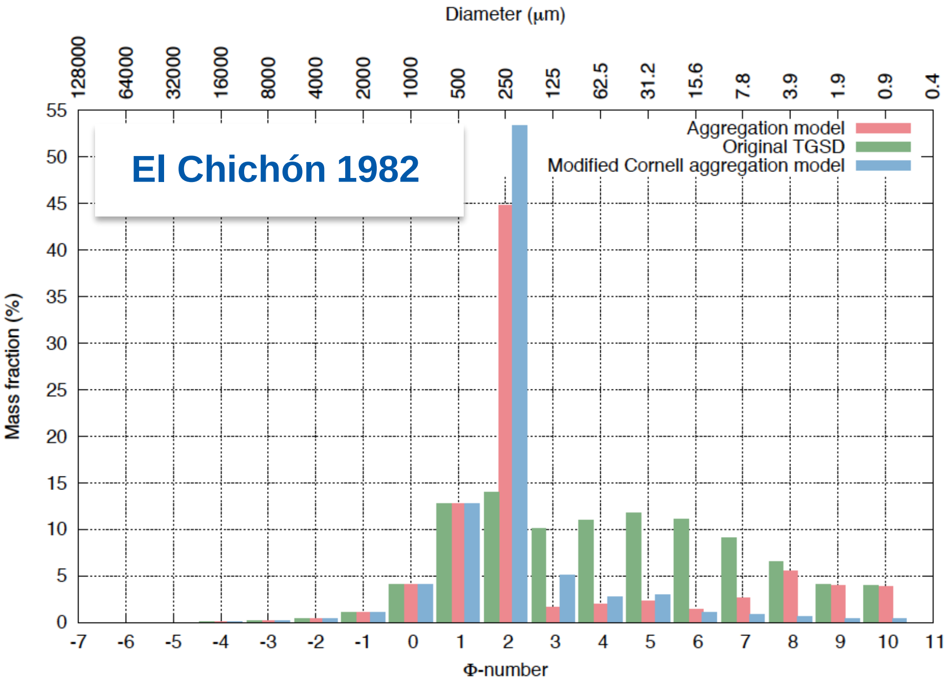
$$\alpha_v = 0.34\left(\sqrt{2|Ri|}\frac{\bar{u}_a}{\hat{u}_o}\right)^{-0.125}$$

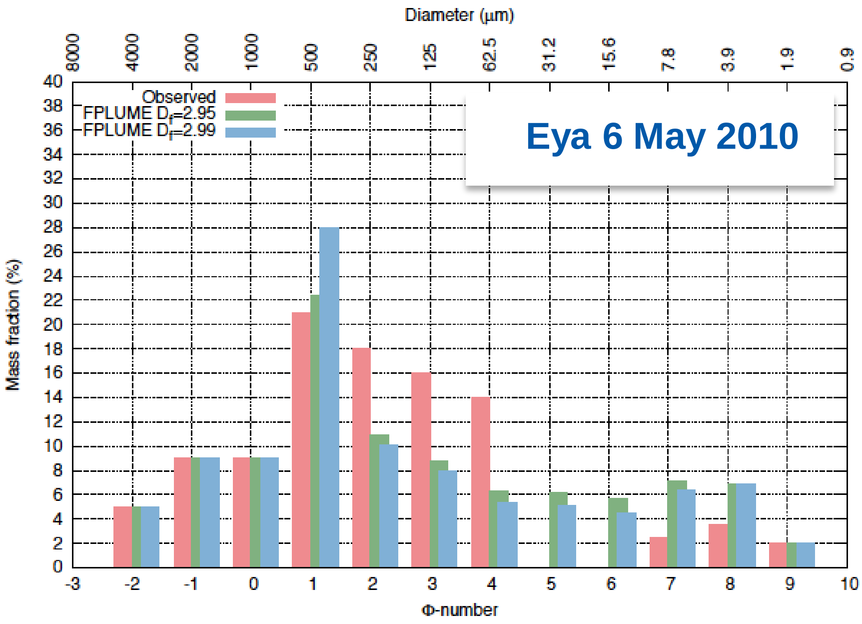




1. FPLUME-1.0

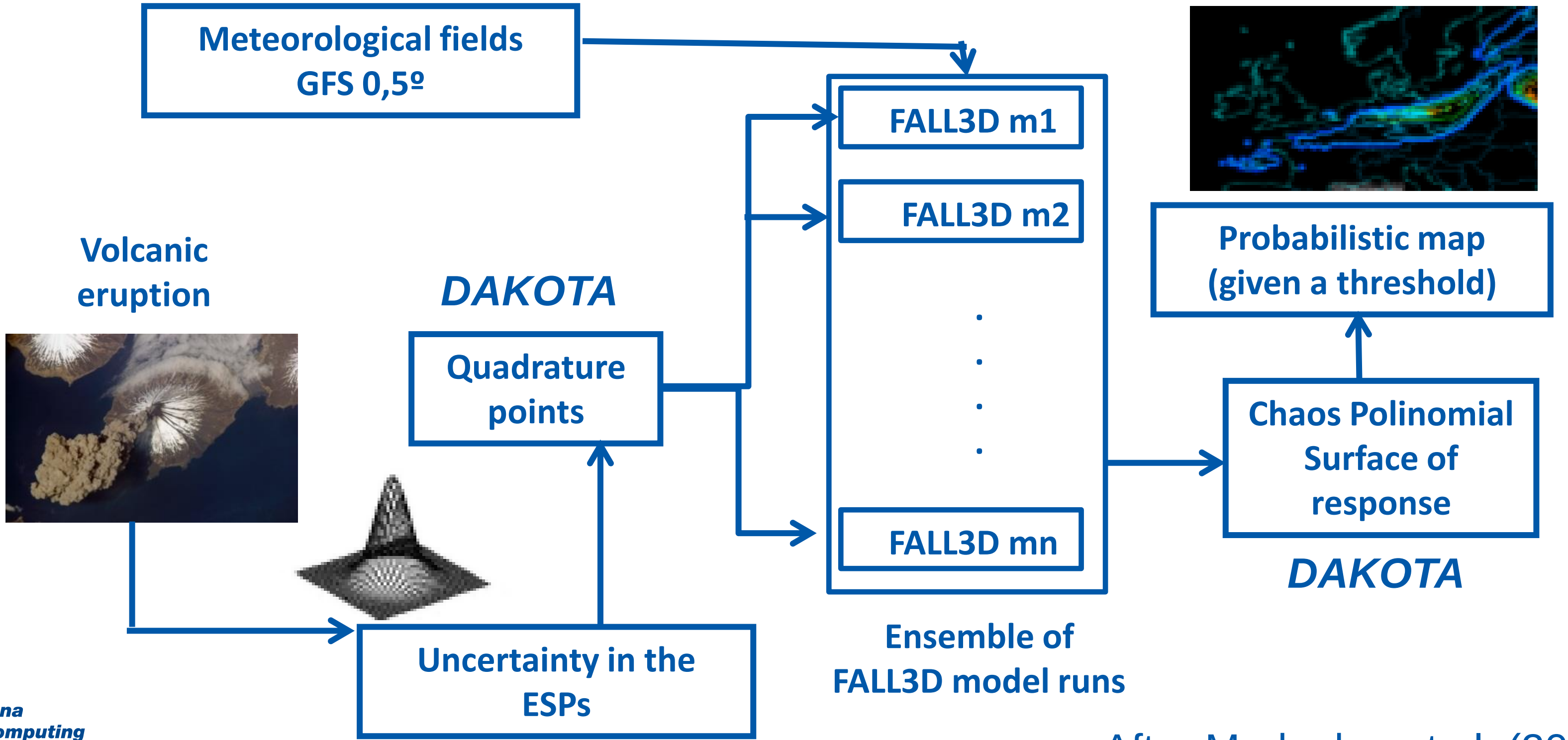
- A model for **wet aggregation** in the plume (Costa et al., 2010; Folch et al., 2010):
  - Ash aggregation by liquid water and ice.
  - One single aggregated class assumed.
  - Aggregates follow a fractal relationship.
  - Particle decay based on 4 collision kernels: Brownian motion, turbulent inertial effects, fluid shear and differential sedimentation.
  - The model predicts an “effective” TGSD: fraction of fine ash can be estimated.





2. Ensemble forecast

- PhD under development at the UBA/SMN (S.Osores).
- **Objectives**:
  1. To develop, implement and validate an operational ensemble forecast strategy for ash dispersal and fallout at the Buenos Aires VAAC.
  2. To account for uncertainties in the source term (and driving meteorology).



Meteorological fields
GFS 0,5º

Volcanic eruption

DAKOTA

Quadrature points

Uncertainty in the ESPs

FALL3D m1

FALL3D m2

. . . .

FALL3D mn

Ensemble of FALL3D model runs

Chaos Polinomial Surface of response

DAKOTA

Probabilistic map (given a threshold)

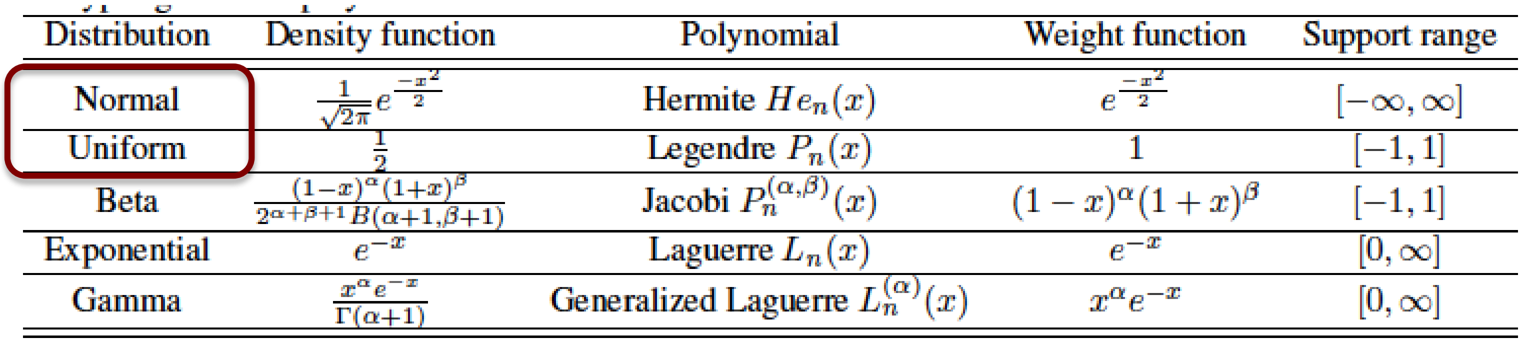
After Madankanet al. (2013)

2. Ensemble forecast

DAKOTA-v6.1.0:

- A Sandia National Laboratories open source toolkit (https://dakota.sandia.gov).
- DAKOTA contains algorithms for optimization, uncertainty quantification, parameter estimation and sensitivity/variance analysis.
- We use the stochastic expansion using the polynomial chaos expansion (*i.e.* bases of orthogonal polynomials are used to interpolate solutions at collocation points).

Basis for different types of PDFs



Distribution	Density function	Polynomial	Weight function	Support range
Normal	$\frac{1}{\sqrt{2\pi}}e^{\frac{-x^2}{2}}$	Hermite $He_n(x)$	$e^{\frac{-x^2}{2}}$	$[-\infty, \infty]$
Uniform	$\frac{1}{2}$	Legendre $P_n(x)$	1	$[-1, 1]$
Beta	$\frac{(1-x)^\alpha(1+x)^\beta}{2^{\alpha+\beta+1}B(\alpha+1,\beta+1)}$	Jacobi $P_n^{(\alpha,\beta)}(x)$	$(1-x)^\alpha(1+x)^\beta$	$[-1, 1]$
Exponential	e^{-x}	Laguerre $L_n(x)$	e^{-x}	$[0, \infty]$
Gamma	$\frac{x^\alpha e^{-x}}{\Gamma(\alpha+1)}$	Generalized Laguerre $L_n^{(\alpha)}(x)$	$x^\alpha e^{-x}$	$[0, \infty]$

Methodology:

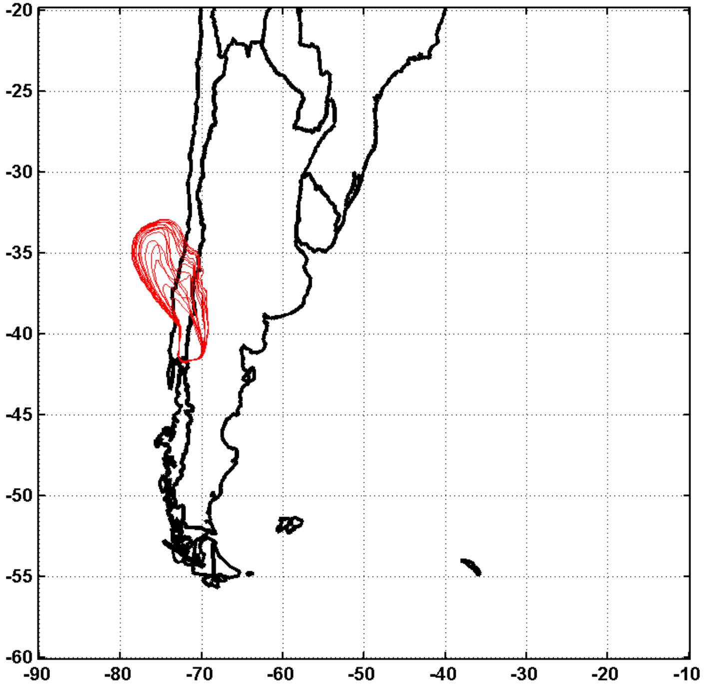
1. Obtain the collocation points for all PDFs (depending on polynomial order).
2. Perform one run (ensemble member) for each set of values of the collocation points.
3. Obtain the stochastic response at each node of the output grid and time step.

2. Ensemble forecast

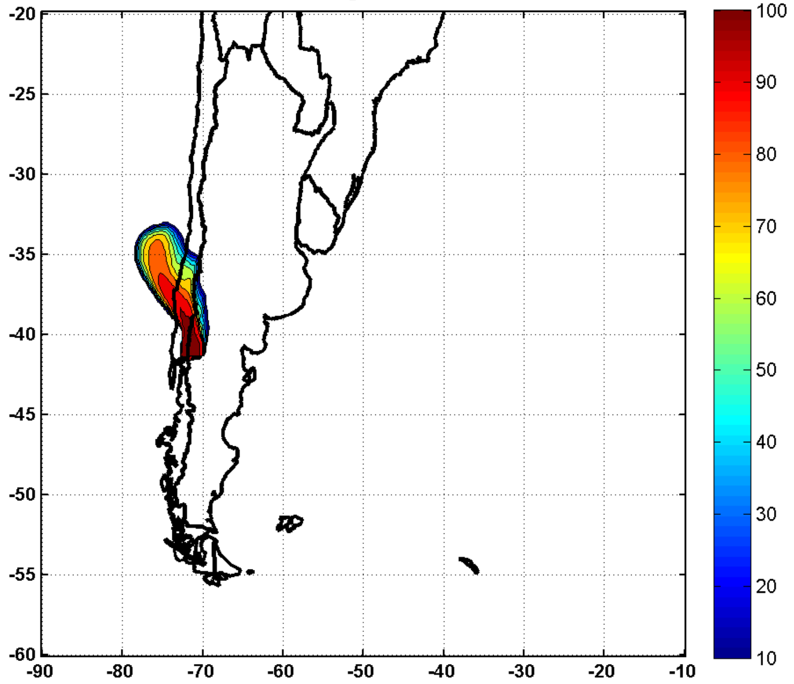
Application to the 2015 Calbuco eruption (Chile)

- We considered 3 uncertain ESPs with uniform PDFs.
    1. Column height: 13-17 km a.v.l. (constant in time; 15 km reported).
    2. Mean TGSD: 3-4 ϕ
    3. Sigma TGSD: 0.5-1.5 ϕ
- MER is related to column height using Degruyter and Bonadonna (2012).
- Collocation using (Legendre) polynomials of 4th order (4^3 = 64 ensemble members).

Gauss Quadrature Points Ensemble
CON FL300>2 mg/m3, Valid for 23-04-2015 15 UTC

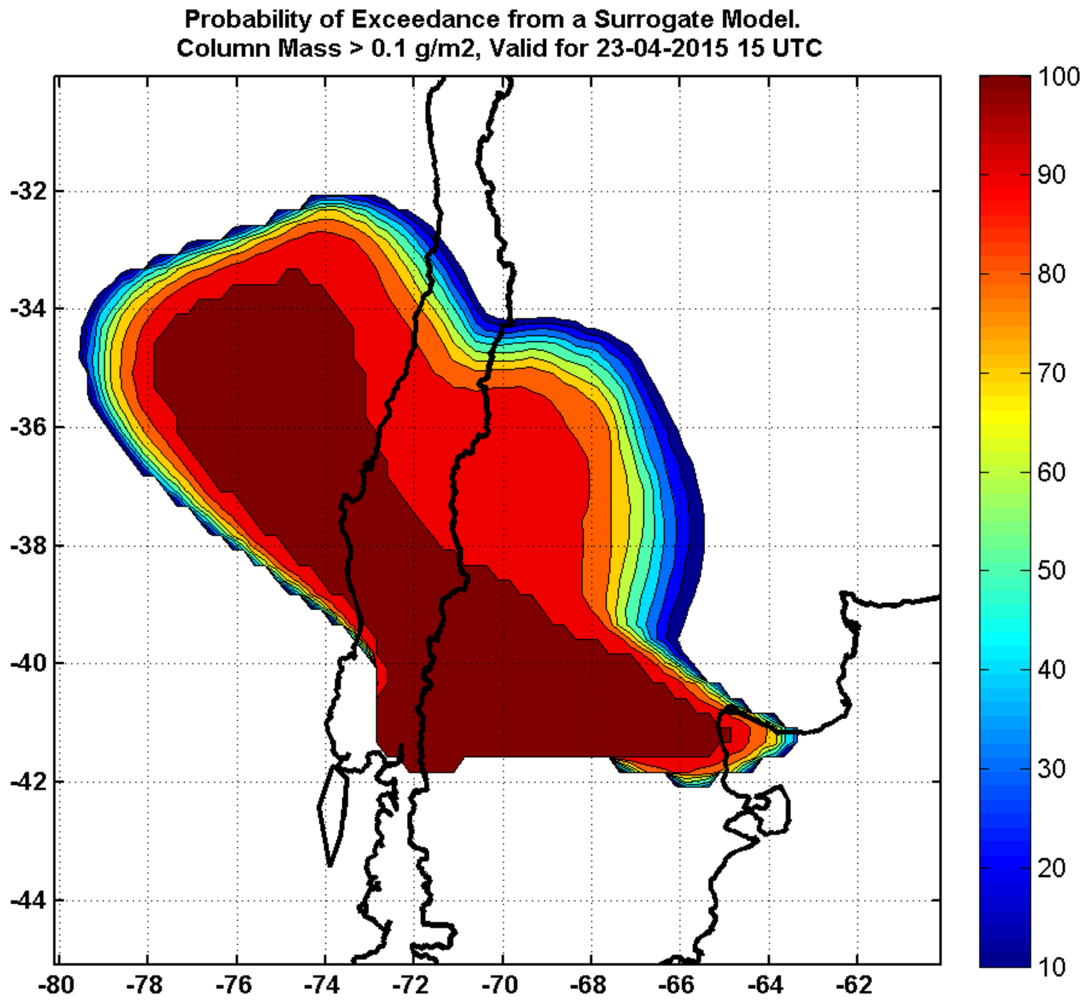


Probability of Exceedance using a Surrogate Model.
Concentration at FL300 > 2 mg/m3, Valid for 23-04-2015 15 UTC

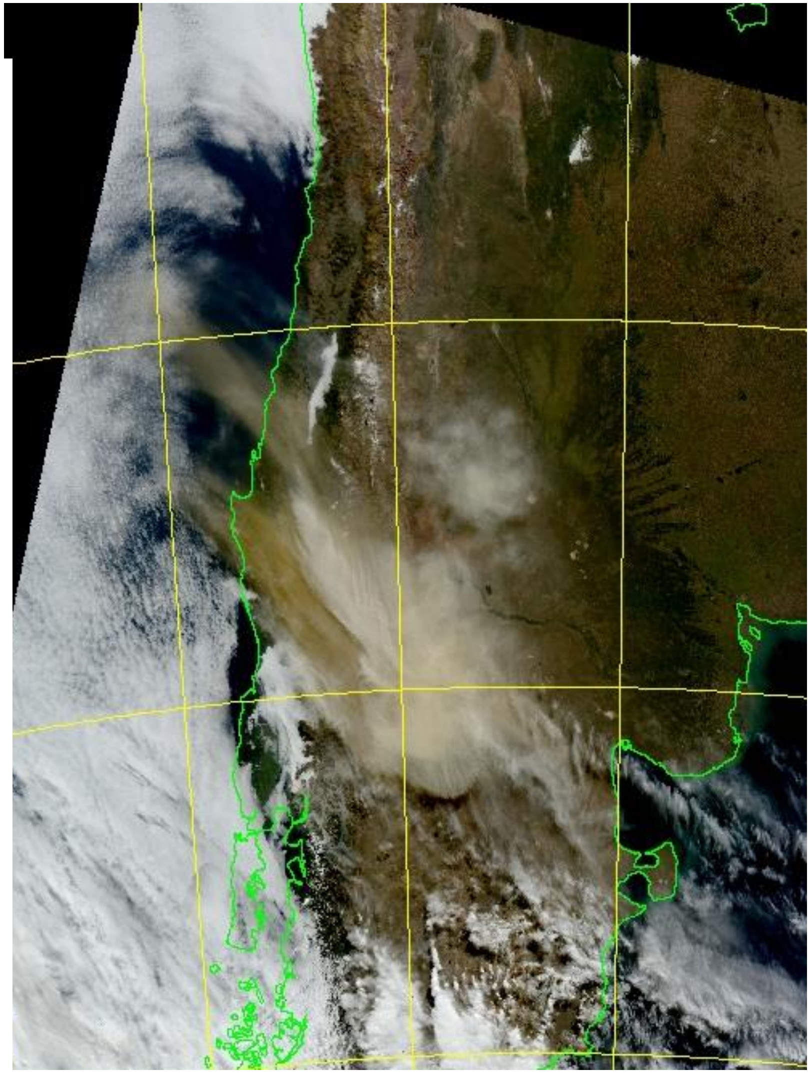


2. Ensemble forecast

Probability to exceed 0.1 g/m^2
23-04-2015 at 15 UTC



MODIS composite 23-04-2015 15-18 UTC



3. Code optimization and porting

- Ensemble forecast strategies may require several **tens of model runs**...
  - Is this feasible at operational level given the computational resources available?
  - Codes (FALL3D and others) are typically written and maintained by atmospheric scientists.
  - What a smart software engineer can do for you?

- For **FALL3D** we have done the following (de la Cruz et al., submitted):
  1. Software optimization:
     - FALL3D re-implemented in the BSC in-house WARIS framework.
     - Further WARIS-Transport improvements.
  2. Code porting to 2 accelerator-based architectures:
     - Intel Xeon Phi 5110P (60 cores, 240 threads).
     - Tesla K40 NVIDIA GPU card.
  3. Analysis of code performance and strong scalability.
  4. 2011 Cordón Caulle simulation: 3 days of forecast, 8 particle bins, very high-resolution computational domain (4km, 601 x 601 x 64 = 23M nodal points).

3. Code optimization and porting

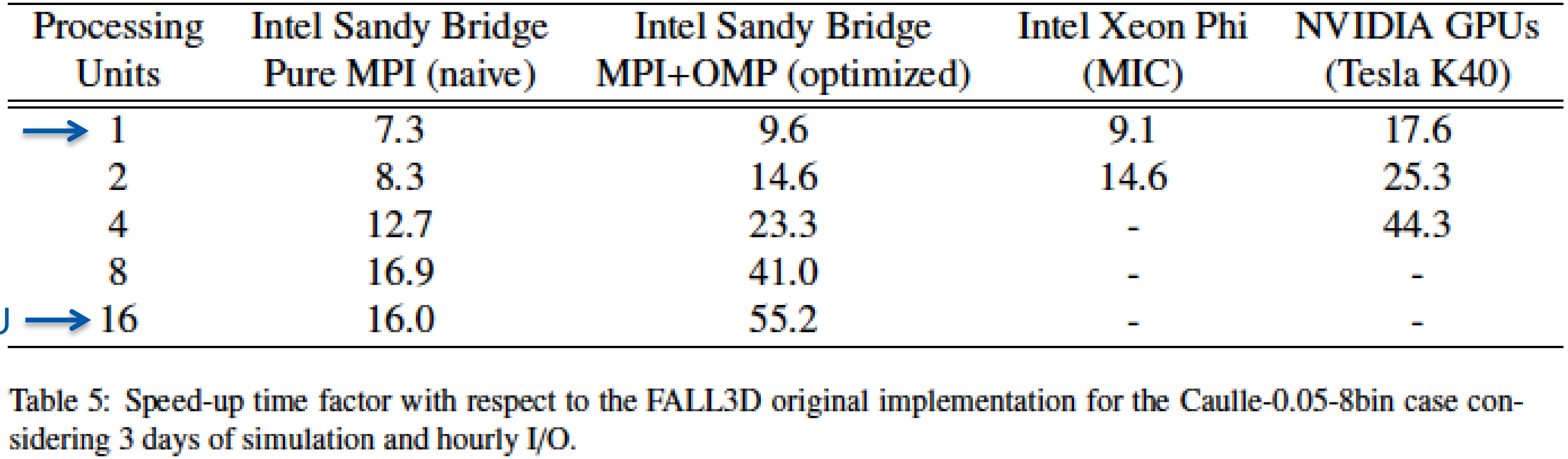
Software optimizations considered in WARIS-Transport:

- Parallel I/O (HDF5).
- Asynchronous MPI communications.
- Hybrid MPI-OpenMP parallelization.
- Thread scheduler for optimal work balance.
- Minimize memory access latency.
- Spatial blocking (data reuse by traversing data in a specific order).
- Thread affinity (avoid memory access disruption and interferences across threads).

After that, porting to accelerator-based hardware architectures:

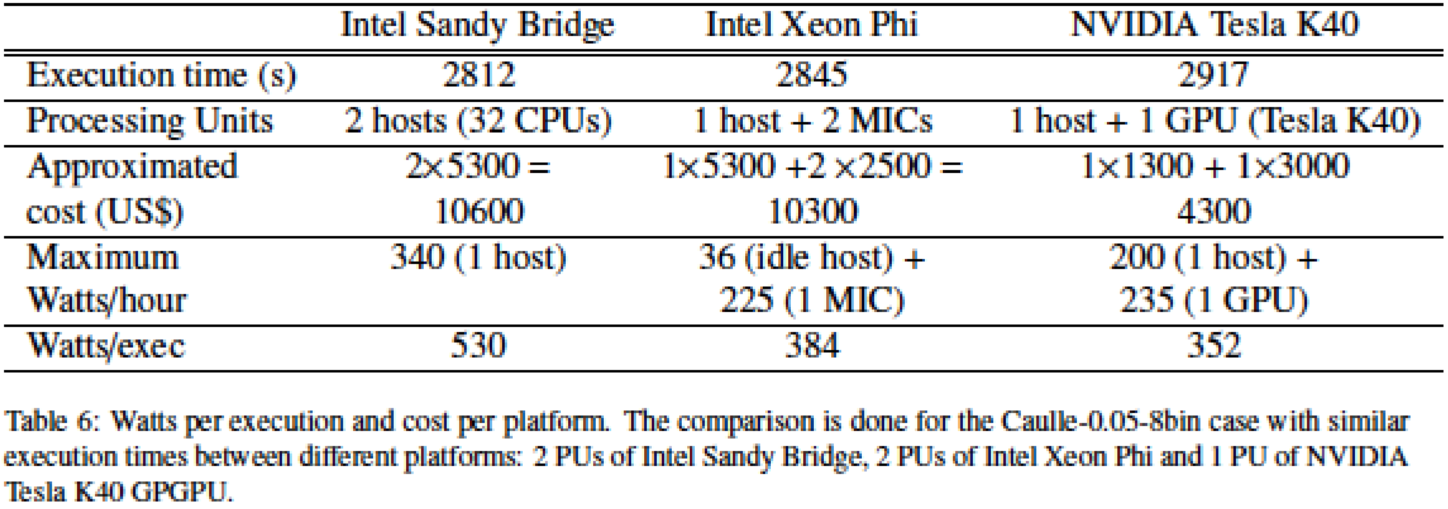
- Intel Xeon Phi 5110P (Many Integrated Core architecture - MIC).
- NVIDIA Tesla K40 GPUs (Graphic Processing Unit).

3. Code optimization and porting



	Processing Units	Intel Sandy Bridge Pure MPI (naive)	Intel Sandy Bridge MPI+OMP (optimized)	Intel Xeon Phi (MIC)	NVIDIA GPUs (Tesla K40)
16 CPU →	1	7.3	9.6	9.1	17.6
	2	8.3	14.6	14.6	25.3
	4	12.7	23.3	-	44.3
	8	16.9	41.0	-	-
256 CPU →	16	16.0	55.2	-	-

Table 5: Speed-up time factor with respect to the FALL3D original implementation for the Caulle-0.05-8bin case considering 3 days of simulation and hourly I/O.



	Intel Sandy Bridge	Intel Xeon Phi	NVIDIA Tesla K40
Execution time (s)	2812	2845	2917
Processing Units	2 hosts (32 CPUs)	1 host + 2 MICs	1 host + 1 GPU (Tesla K40)
Approximated cost (US$)	2×5300 = 10600	1×5300 +2 ×2500 = 10300	1×1300 + 1×3000 4300
Maximum Watts/hour	340 (1 host)	36 (idle host) + 225 (1 MIC)	200 (1 host) + 235 (1 GPU)
Watts/exec	530	384	352

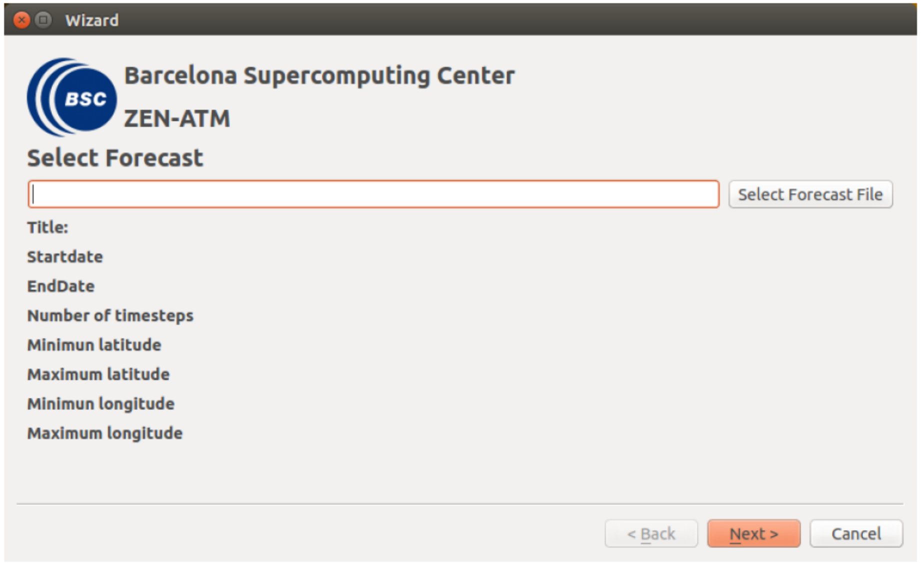
Table 6: Watts per execution and cost per platform. The comparison is done for the Caulle-0.05-8bin case with similar execution times between different platforms: 2 PUs of Intel Sandy Bridge, 2 PUs of Intel Xeon Phi and 1 PU of NVIDIA Tesla K40 GPGPU.

Conclusion: optimization is a must for operational ensemble forecast !

4. Air traffic impact evaluation tool

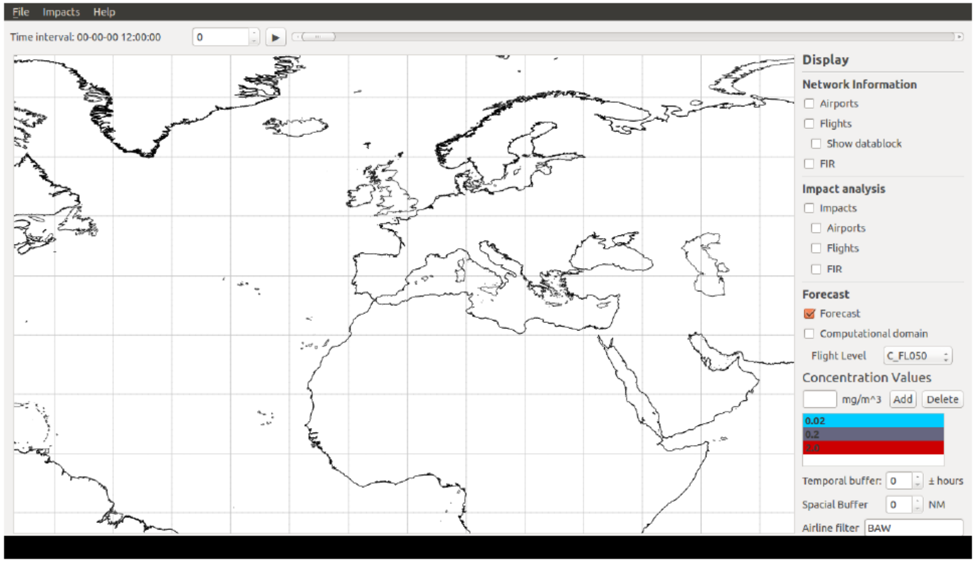
ZEN-ATM:

- A tool to evaluate **the impact of volcanic ash and mineral dust on civil aviation**.
- The prototype works with FALL3D (for ash) and WMO Sand and Dust Storm Warning Advisory and Assessment System (SDS-WAS) for dust.
- ZEN-ATM merges model forecasts and ATM databases (airports, routes, FIRs and flights) to evaluate impacts based on user-defined criteria (*e.g.* concentration threshold, maximum dose, visibility at surface).
- Filtering by airlines, countries, FIRs or airports is possible.



Barcelona Supercomputing Center
ZEN-ATM
Select Forecast

Title:
Startdate
EndDate
Number of timesteps
Minimun latitude
Maximum latitude
Minimun longitude
Maximum longitude

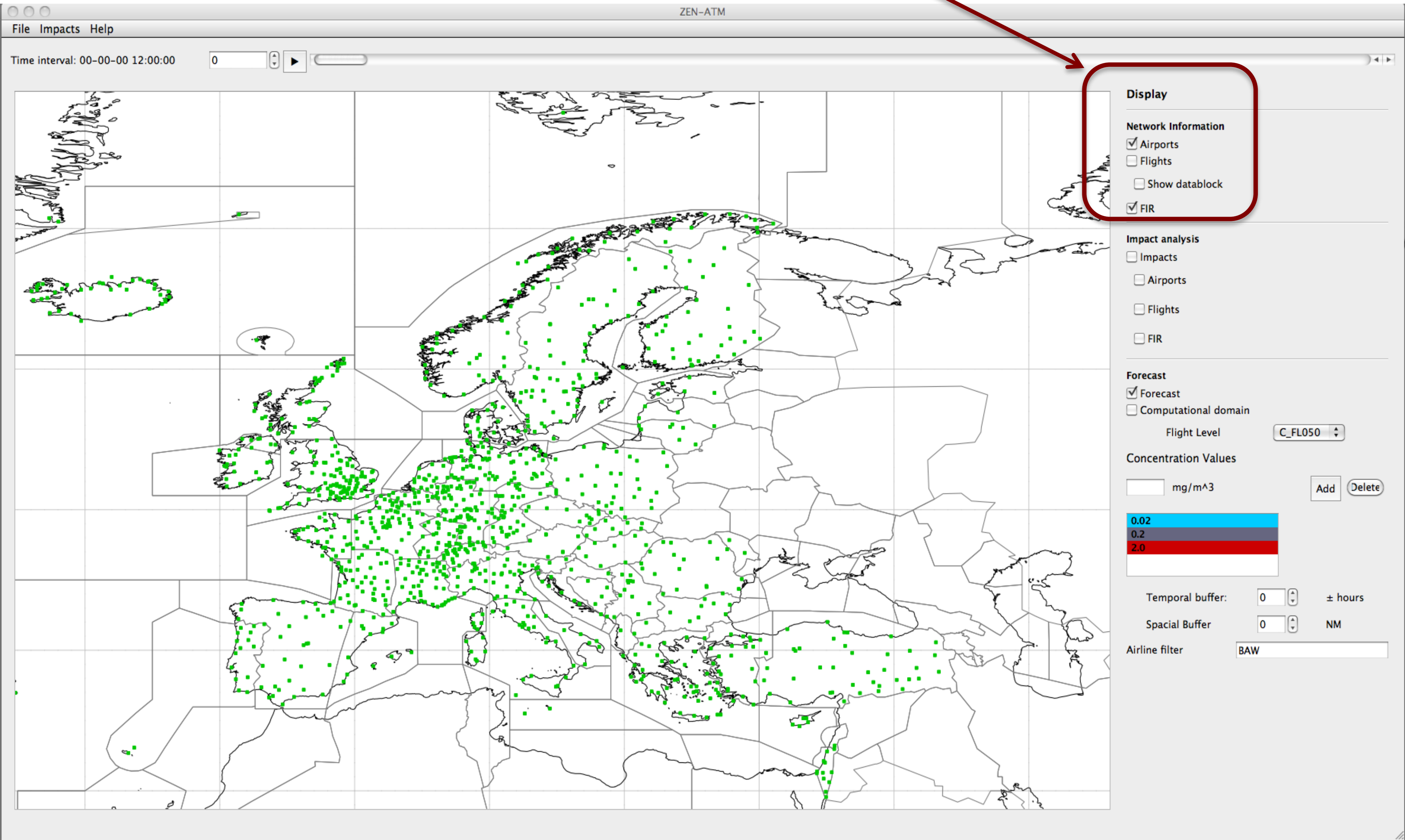


Time interval: 00-00-00 12:00:00 | 0

☐ Airports
☐ Flights
☐ Show datablock
☐ FIR
☐ Impacts
☐ Airports
☐ Flights
☐ FIR
☑ Forecast
☐ Computational domain
Flight Level: C_FL050
mg/m^3
0.02
0.2
2.0
Temporal buffer: 0 ± hours
Spacial Buffer: 0 NM
Airline filter: BAW

4. Air traffic impact evaluation tool

Display network information



Time interval: 00-00-00 12:00:00 0

Display

Network Information
☑ Airports
☐ Flights
☐ Show datablock
☑ FIR

Impact analysis
☐ Impacts
☐ Airports
☐ Flights
☐ FIR

Forecast
☑ Forecast
☐ Computational domain
Flight Level C_FL050

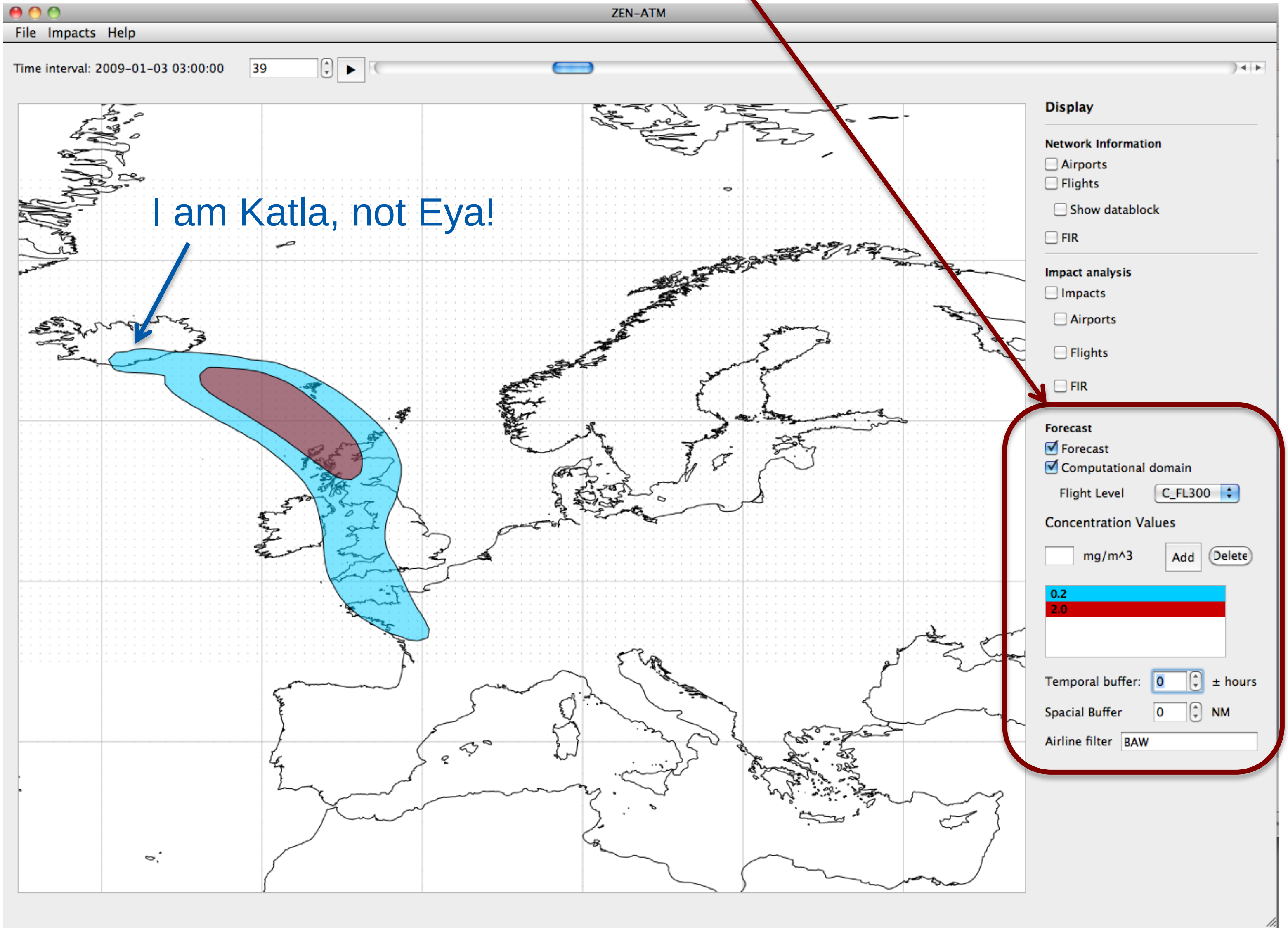
Concentration Values
mg/m^3

0.02
0.2
2.0

Temporal buffer: 0 ± hours
Spacial Buffer 0 NM
Airline filter BAW

4. Air traffic impact evaluation tool

Display forecast



I am Katla, not Eya!

Time interval: 2009-01-03 03:00:00 39

Display

Network Information

- ☐ Airports
- ☐ Flights
  - ☐ Show datablock
- ☐ FIR

Impact analysis

- ☐ Impacts
  - ☐ Airports
  - ☐ Flights
  - ☐ FIR

Forecast

- ☑ Forecast
- ☑ Computational domain

Flight Level C_FL300

Concentration Values

mg/m^3

0.2

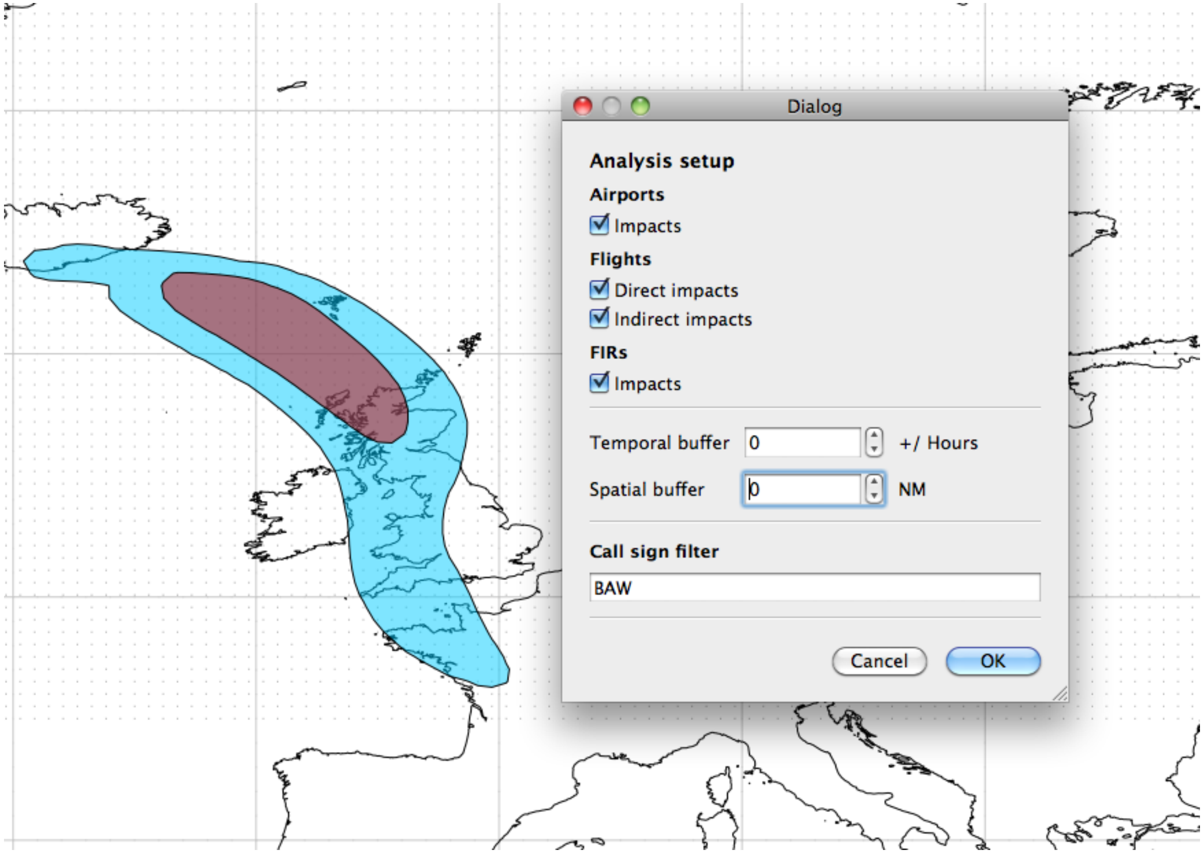
2.0

Temporal buffer: 0 ± hours

Spacial Buffer 0 NM

Airline filter BAW

4. Air traffic impact evaluation tool



Analysis setup

Airports

☑ Impacts

Flights

☑ Direct impacts

☑ Indirect impacts

FIRs

☑ Impacts

Temporal buffer 0 +/ Hours

Spatial buffer 0 NM

Call sign filter

BAW

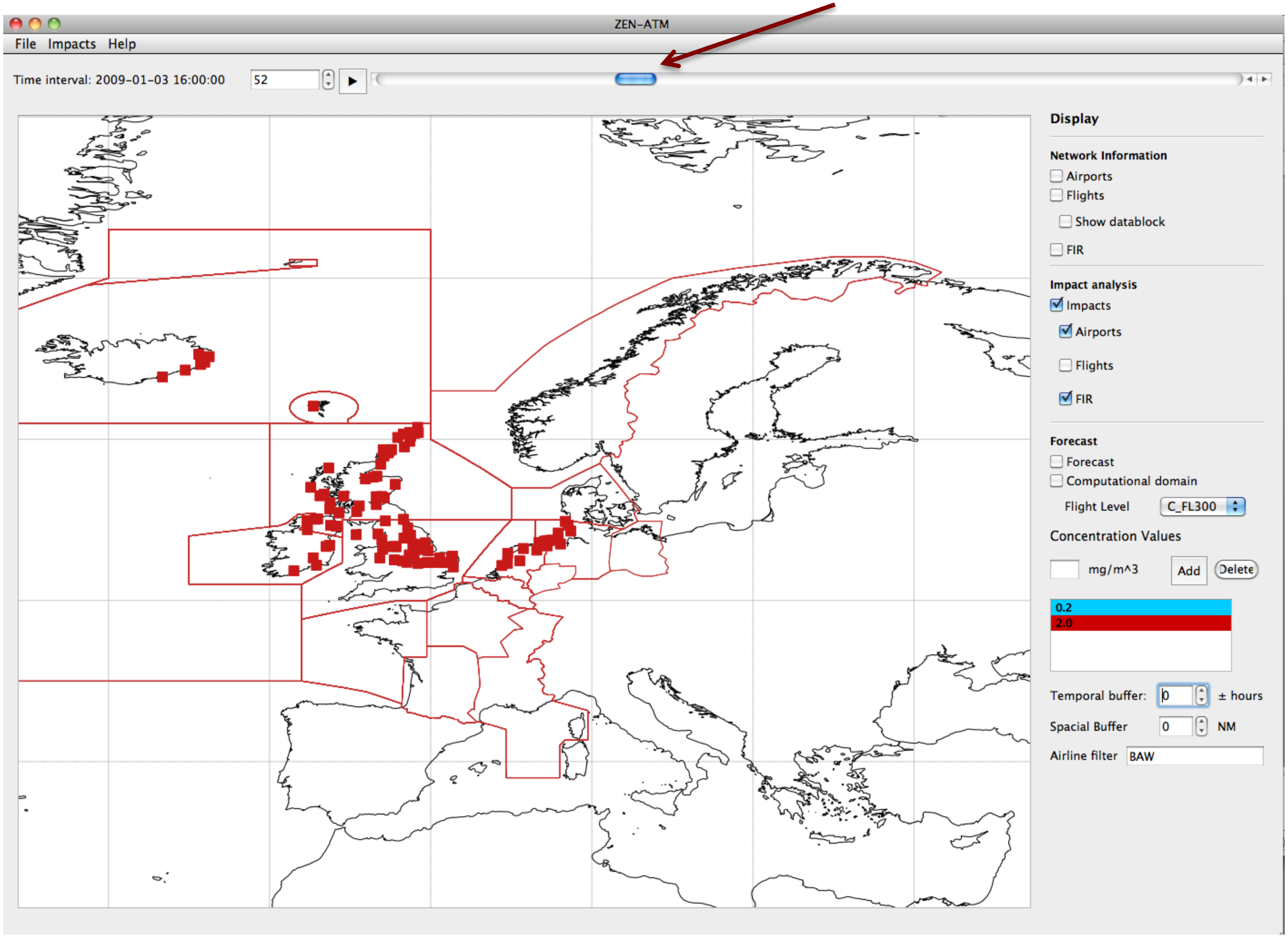
Perform the impact analysis on

1. Airports (FL050)
2. Flights
    - Direct
    - Indirect
3. FIRs

Define buffers depending un confidence

4. Air traffic impact evaluation tool

Show impacts on airports and FIRs (time dependent)



Time interval: 2009-01-03 16:00:00 52

Display

Network Information
☐ Airports
☐ Flights
☐ Show datablock
☐ FIR

Impact analysis
☑ Impacts
☑ Airports
☐ Flights
☑ FIR

Forecast
☐ Forecast
☐ Computational domain

Flight Level: C_FL300

Concentration Values

mg/m^3

0.2
2.0

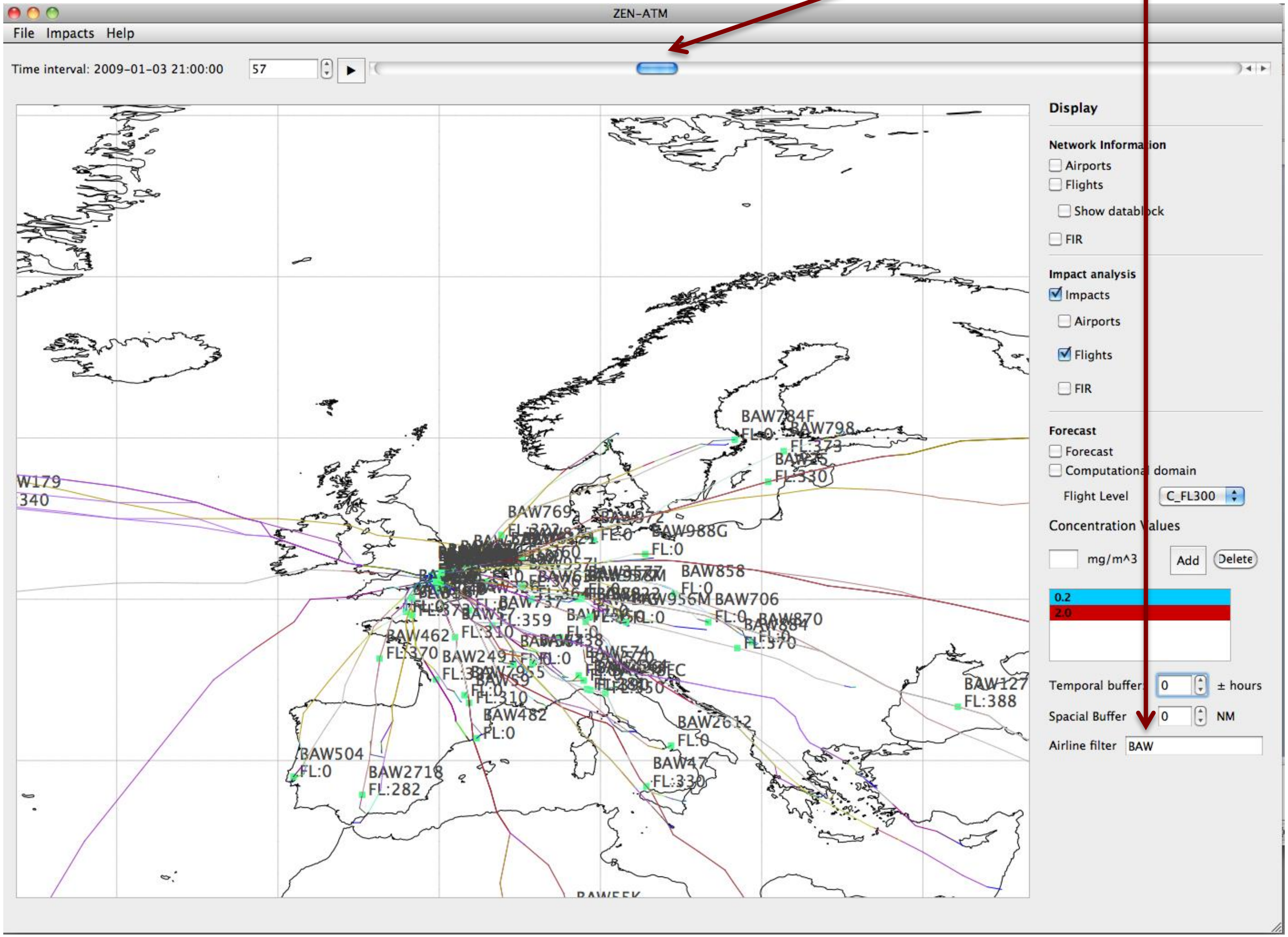
Temporal buffer: 0 ± hours

Spacial Buffer: 0 NM

Airline filter: BAW

4. Air traffic impact evaluation tool

Shows impacts on flights (time dependent, filtered by airline)



Time interval: 2009-01-03 21:00:00 57

Display

Network Information

- ☐ Airports
- ☐ Flights
  - ☐ Show datablock
- ☐ FIR

Impact analysis

- ☑ Impacts
  - ☐ Airports
  - ☑ Flights
  - ☐ FIR

Forecast

- ☐ Forecast
- ☐ Computational domain

Flight Level C_FL300

Concentration Values

mg/m^3

0.2
2.0

Temporal buffer 0 ± hours

Spacial Buffer 0 NM

Airline filter BAW

Conclusion

Several innovations at a scientific level are mature enough for transfer into operations (after further validation)

THANK YOU!

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