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Chemical weather forecasting and assessment: SILAM

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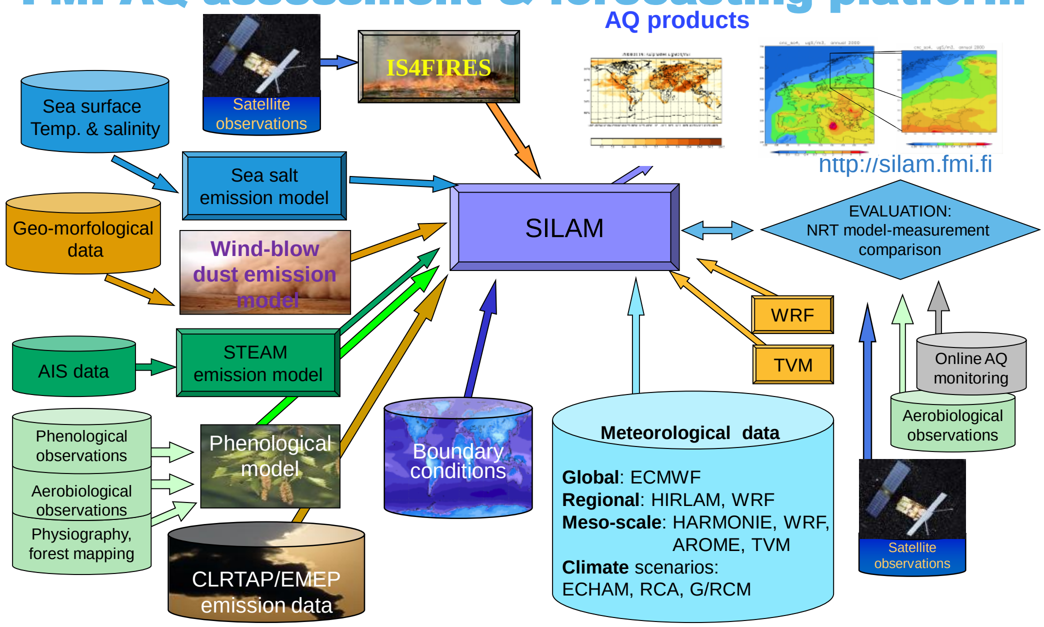
FMI AQ assessment & forecasting platform



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SILAM application types & scales

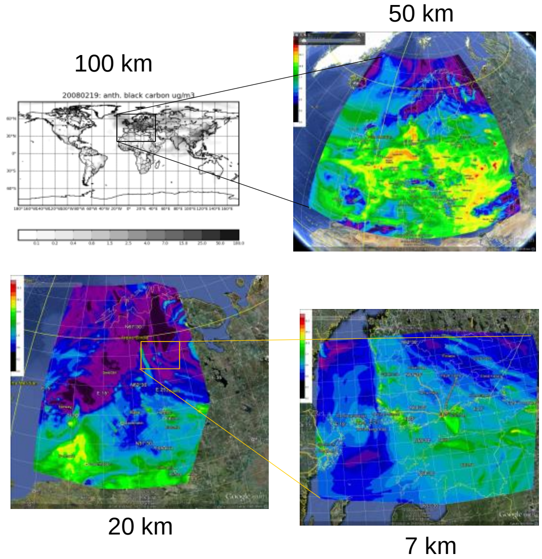
Short-term forecasting and re-analysis
- atmospheric chemical composition
- allergenic air pollution
- plumes of wild-land fires

Emergency preparedness
- nuclear
- volcanic

Source apportionment studies
- anthropogenic sources
- natural sources: allergenic pollen, volcanoes, fires

Risk assessment
- chemical
- nuclear

Climate change forcing and impact



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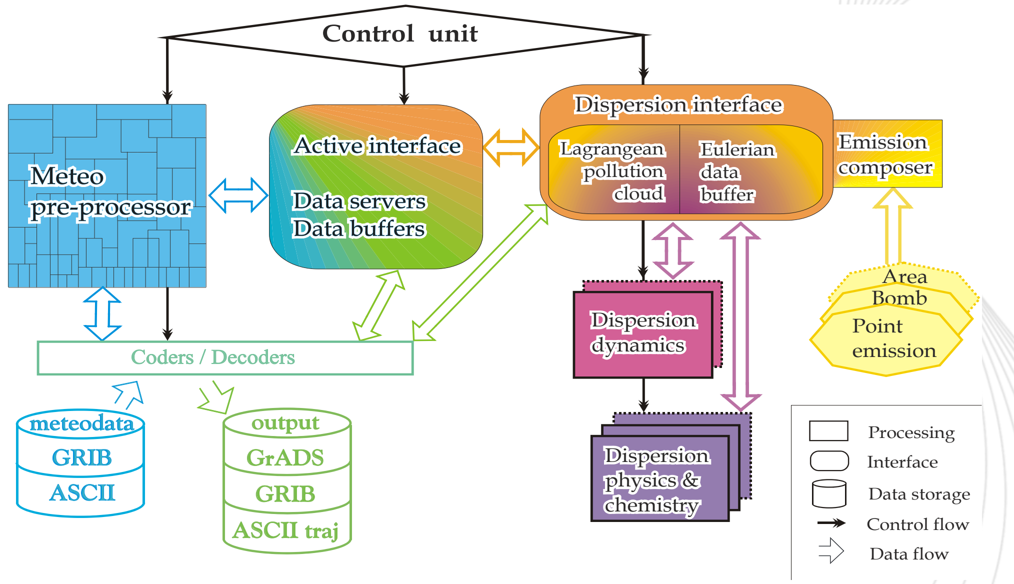
SILAM modelling system



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SILAM v.5.5

Atmospheric dispersion simulation

1) Forward problem: to estimate concentrations

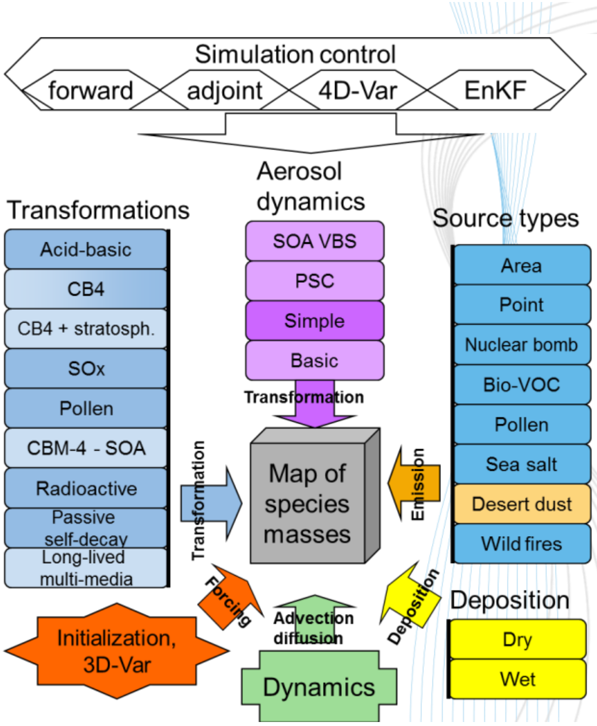
$$L=\frac{\partial}{\partial t}+\frac{\partial}{\partial x_i}(u_i)-\frac{\partial}{\partial x_i}\mu_{ii}\frac{\partial}{\partial x_i}+\sigma;\quad L\varphi=f;\ M=(p,\varphi)$$

2) Adjoint problem: source apportionment

$$L^*=-\frac{\partial}{\partial t}-\frac{\partial}{\partial x_i}(u_i)-\frac{\partial}{\partial x_i}\mu_{ii}\frac{\partial}{\partial x_i}+\sigma,\quad L^*\varphi^*=p;\ M=(f,\varphi^*)$$

Modules

- 9 chemical and physical transformation modules (7 open for operational use),
- 8 source terms (all open),
- 4 aerosol dynamics (1 open)
- 3D-,4D- Var, EnKF



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Dynamics

Eulerian and Lagrangian schemes

- **Euler**
  - split the domain in grid cells
  - track the mass budget of each cell
  - turbulent mixing described as diffusion
  - SILAM v4, v5
- **Lagrange**
  - track the motion of the pollutant represented by finite number of model particles
  - count model particle density to obtain concentration (mass/volume)
  - turbulent mixing described as a random process
  - SILAM v4, v5.x
- **Lagrange attractive especially for point sources, but**
  - handling diffuse emission sources is expensive
  - handling nonlinear chemistry is very difficult

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Dynamics

Eulerian advection schemes

- **Classical finite difference schemes rarely useful for advection**
  - Behave poorly with sharp gradients
  - Godunov's theorem: a linear, monotonous scheme is at most first order accurate
  - Stability requires a small Courant number $C = \frac{v\Delta t}{\Delta x}$
- **Practical advection schemes are nonlinear**
- **One approach: borrow elements from Lagrangian schemes**
  - no strict stability constraints
  - Example: the Galperin scheme, as used in SILAM

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Dynamics

Comments on the Galperin scheme

- **Very low numerical diffusion**
- **Mass conservative**
- **Positively definite, but not monotonous**
- **Stable at any Courant number**
  - but accuracy suffers at high *C*!
- **Good computational performance, but requires 3 additional tracers for each chemical species (first moment of mass in 3 dimensions)**
- **In SILAM:**
  - V2 advection: first order time integration
  - V3 advection: second order implicit time integration
  - V3 slower than V2, but better performance for long-lived species (especially in complex terrain)

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Dynamics

Vertical discretization in Eulerian models

- **Model vertical layers may be defined in terms of pressure, height from ground, altitude, etc.**
  - constant height
  - hybrid terrain influenced
- **SILAM:**
  - “standard” setup – levels defined by height
  - “hybrid levels” as option since v5.1
- **Vertical advection:**
  - slower than horizontal, but not negligible!
  - Galperin’s scheme

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Dynamics

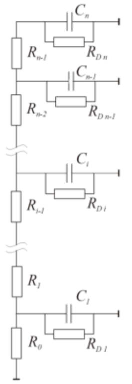
Vertical diffusion

Vertical diffusion is based on extended resistive analogy of Sofiev (2002), Figure 3). The scheme realises the adaptive vertical structure with fixed layer thicknesses but varying position of the centre of masses in the layer (the capacities C_i are fixed while resistances R_i are dynamic). The latter directly links the diffusion and vertical advection as they both utilise the advection-controlled sub-grid variable – the first moment of the mass located in the grid cell.

Parameterization of the diffusion coefficient for resistances is based on K-theory after Genikhovich *et al.* (2004).

Diffusion is evaluated species-wise and the scheme incorporates the substance-specific “regular” velocities, such as gravitational sedimentation.

Dry deposition and re-evaporation are embedded into the diffusion algorithm as a boundary condition at the surface.



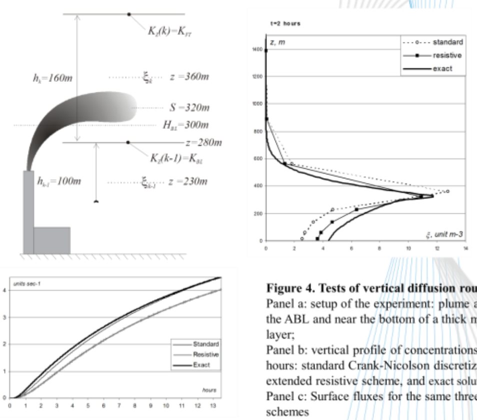


Figure 4. Tests of vertical diffusion routine.
Panel a: setup of the experiment: plume above the ABL and near the bottom of a thick model layer;
Panel b: vertical profile of concentrations after 2 hours: standard Crank-Nicolson discretization, extended resistive scheme, and exact solution
Panel c: Surface fluxes for the same three schemes

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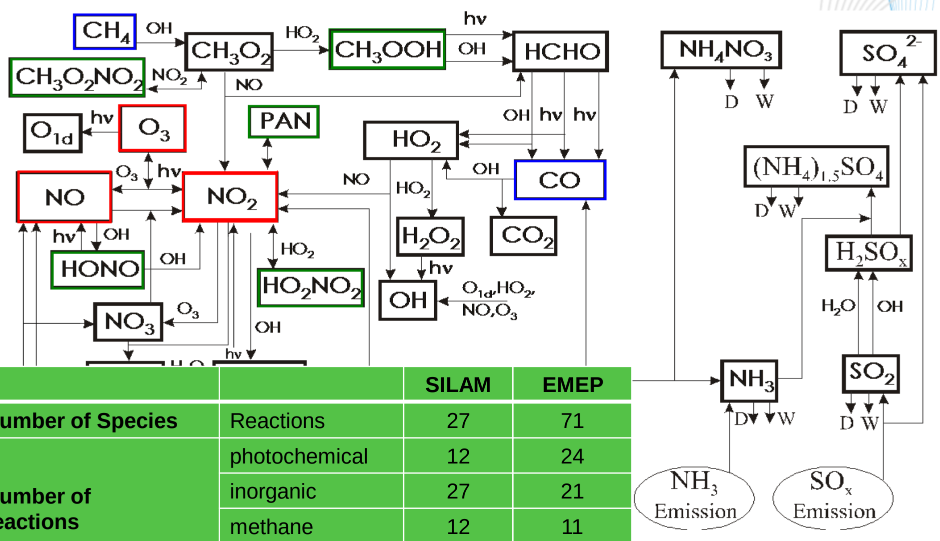
SILAM acid-basic chemistry



		SILAM	EMEP
Number of Species	Reactions	27	71
Number of reactions	photochemical	12	24
	inorganic	27	21
	methane	12	11
	ethane	2	15

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Apart from reactions

- Partition of NOx
- OH & HO2 analytical solution for fast dynamics is computed (equilibria)
- O3 & CO: Initialisation and boundary conditions
- Split between nighttime and daytime reactions
- Sequential computation of reactions (fastest first) analytical solutions for equilibria and near-equilibria
- In most cases, chemistry timestep = model timestep (10-15 min)

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SILAM CB4 chemistry+ addition

- New species: 22
  - Terpenes
  - VBS
    - Anthropogenic 1 NVOC, 4 SVOC (gas + aerosol), 3 IVOC
    - Biogenic 1 NVOC, 4 SVOC (gas + aerosol)
- New reactions: 31
  - Terpene oxydation: 4
  - SOA formation: 20
    - XYL, TOL, ISOP, TERP; lo and hi NOx
  - SOA aging 11
- Gas – aerosol partitioning: 8

- CB4 - possibly not good enough
  - 32 species, 81 reactions
- Large uncertainties emissions
  - IVOC - Primary OC emission * 2.5
  - Composition of anthropogenic NMVOC
  - Biogenic emissions of isoprene, monoterpenes ec

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Aerosols in SILAM

- Chemically active and inert species
- Emitted from anthropogenic and natural sources
- Size distribution: bin and modal descriptions
- Microphysics: all basic processes, under testing
- Effect on radiation and visibility
- Specific non-anthropogenic aerosols:
  - **Sea-salt**: wide spectrum, wind driven emission, dependent on water features
  - **Pollen**: biogenic, phenology driven emission, controlled by long-term and actual meteorology
  - **Fire-induced PM**: smoke, vegetation and fire-type dependent