

Introduction to
Polyphemus

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and
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Resources

Next...

Introduction to Polyphemus

First SAEMC-IAI, STIC-AmSud Workshop

Meryem Ahmed de Biasi, Irène Korsakissok, Vivien
Mallet and Lin Wu

5 June 2007

Outline

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- 4 Data Assimilation
- 5 Resources
- 6 Next...

Polyphemus Images

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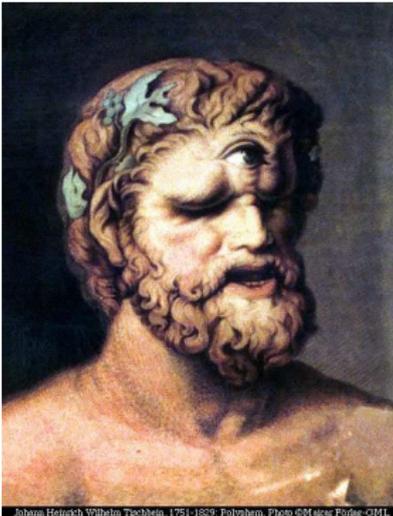
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Greek Mythology

- Polyphemus, cyclops in
Odyssey

Why this name ?

- “Poly” : **multiple**
- “phemus” : speech



Multiple Goals

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Next...

Multiple Models

- Scales : from local scale to continental scale
- Formulations : Gaussian, Eulerian, . . .

Multiple Pollutants

- Passive, radionuclides
- Photochemistry
- Aerosols
- Persistent organic pollutants, heavy metals, . . .

Multiple Inputs

- From meteorological models : MM5, ECMWF
- Ground data : GLCF, USGS

Multiple Methods

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Data Assimilation

- Sequential
- Variational
- Inverse modeling (parameter estimation)

Ensemble Forecast

- Multimodels
- Monte Carlo
- Models combinations (“superensembles”, ...)

Models Coupling

- Feedbacks
- Impact

Constraints

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Perennial Code

- System maintenance
- Scalable, integration of new developments

Open

- Availability, distribution
- Development or contributions from other teams

Field Context

- From research to operational use

Overall structure

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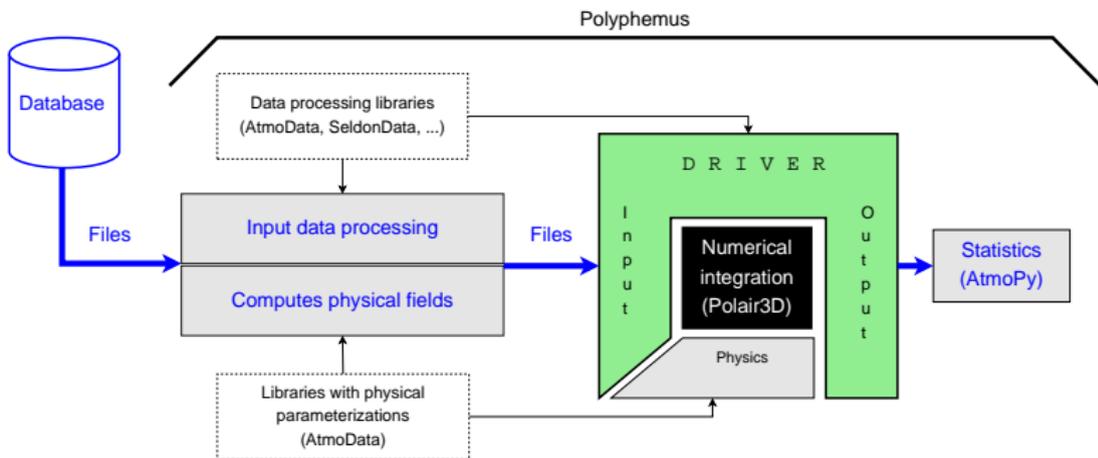
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Libraries

- Talos : operations on configuration files and management of dates
- SeldonData : input-output operations
- AtmoData : extension of SeldonData to atmospheric sciences, physical parameters
- AtmoPy : postprocessing

Preprocessing

- Meteorological fields from ECMWF or MM5
- Ground data : Land Use Cover, Emission, Deposition
- Boundary conditions from Mozart 2 or Inca for gaseous species and Gocart for aerosols
- Gaussian models.

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Models

- Gaussian Models
 - Stationary Gaussian model and puff Gaussian model
 - Gas and aerosols
 - Several parameterizations to compute the dispersion
- Eulerian Models
 - Castor (clone of the **gas** version of Chimere)
 - Polair3D (passive, chemical, aerosol and adjoint [for gas] versions)
 - Modules for transport, chemistry and aerosols

Postprocessing

- Comparison to observations
- Water diagnosis in a plume
- Visualization

Programming Choices

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Main language : C++

- Efficient for scientific computing
- Advanced object design
 - Inheritance, genericity
 - Management of complex objects
 - Exceptions
- Widely used and perennial

Programming Choices

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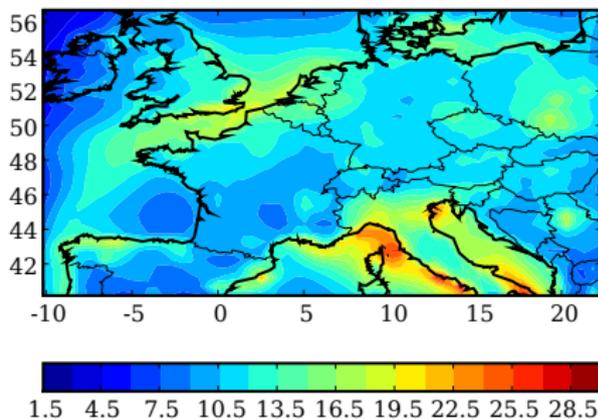
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Next...

Complementary Language : Python

- Dynamic, interactive
- Visualization
- Scripts
- Increasingly used in scientific computing



Programming Choices

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Historical Language : Fortran 77

- Automatic differentiation
- Continuity
- Calls from C++

Policy

- To avoid dealing with too many languages
- To use primarily languages with strong potential and productivity

Application and References

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Main Reference

Main article for Polyphemus :

"Technical Note : The air quality modeling system Polyphemus", V. Mallet, D. Quélo, B. Sportisse, M. Ahmed de Biasi, É. Debry, I. Korsakissok, L. Wu, Y. Roustan, K. Sartelet, M. Tombette and H. Foudhil, Atmos. Chem. Phys. Discuss., 7 (3), 2007

Partners

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Main Organizations

- 1 ENPC
- 2 EDF
- 3 INRIA

Impact studies of thermal power plants

data assimilation

French partners

- 1 IRSN (Nuclear safety)
- 2 INERIS (industrial risks)
- 3 CETE (urban equipment)
- 4 DGA (Defense)

Radionuclides

Local scale, ozone forecasting, liquid water content diagnosis

Evaluation of Urban mobility plan

Local scale, network evaluation

International collaborations

- 1 CRIEPI in Japan
- 2 EDF Polska
- 3 IER Stuttgart, European projects
- 4 CMM in Chile, STIC-AMSUD project

Sensitivity studies over Europe, Paris and Tokyo

Impact studies, air quality modeling

Health impact evaluation

Air quality forecasting, data

assimilation

Some Applications

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Aerosols at Regional and Continental Scales

- Polair3D hosts an aerosol model (SIREAM).
 - Validations over Europe and Asia, and over Paris, Marseille and Lille.
 - Sensitivity studies over Europe, Paris and Tokyo.
-
- M. Tombette and B. Sportisse. Aerosol modeling at regional scale : Model-to-data comparison and sensitivity analysis over Greater Paris. *Atmos. Env.*, 2007. In press
 - K. Sartelet, E. Debry, K. Fahey, M. Tombette, Y. Roustan, and B. Sportisse. Simulation of aerosols and gas phase species over Europe with the POLYPHEMUS system. Part I : model-to-data comparison for year 2001. *Atmos. Env.*, 2007. doi :10.1016/j.atmosenv.2007.04.024
 - K. Sartelet, H. Hayami, and B. Sportisse. Dominant aerosol processes during high-pollution episodes over Greater Tokyo. *J. Geophys. Res.*, 2007. Accepted for publication

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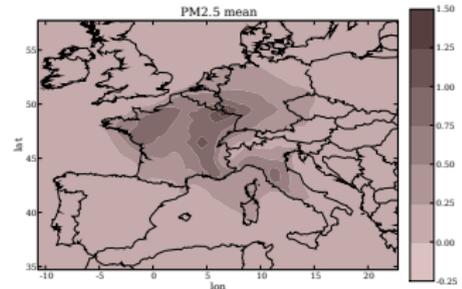
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Next...

Impact Studies at Continental Scale

- Sensitivity study of ozone concentrations with respect to emissions
- Evaluation of air quality in Polska
- Evaluation of the emissions from French thermal power plants for the year 2005



- Vivien Mallet and Bruno Sportisse. A comprehensive study of ozone sensitivity with respect to emissions over Europe with a chemistry-transport model. *J. Geophys. Res.*, 110(D22), 2005

Some Applications

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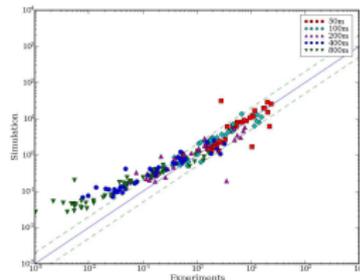
Next...

Local scale models

- Comparison of sigma parameterizations
- Network design for defense applications

Plume in Grid model

- Better modeling of major point source emissions
- Application to passive tracers (ETEX, Chernobyl)



- Irène Korsakissok. Performance evaluation of Polyphemus Gaussian models with Prairie Grass experiment. Technical Report 2007-15, CEREAs, 2007

Some Applications

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Air Quality Modeling over Lille

- Assessment of health impact of the Urban Mobility Plan (CETE)
- Coupling with emission and traffic model, and indicators of health impact
- Inverse modeling of emissions with 4D-var and second-order sensitivity

- Denis Quélo, Vivien Mallet, and Bruno Sportisse. Inverse modeling of NO_x emissions at regional scale over Northern France. Preliminary investigation of the second-order sensitivity. *J. Geophys. Res.*, 110(D24310), 2005
- D. Quélo, R. Lagache, and B. Sportisse. Etude de l'impact qualité de l'air des scénarios PDU sur Lille à l'aide du modèle de Chimie-Transport Polair3D. Technical Report 2004-28, CEREAs, 2004. Rapport PREDIT
- R. Lagache, C. Declercq, D. Quélo, B. Sportisse, P. Palmier, B. Quetelard, and F. Haziak. Evaluation du PDU de Lille-Métropole sur le trafic, les concentrations de polluants atmosphériques et la mortalité. In *Actes de la 15ième conférence sur les transports et la pollution de l'air*, 2006

Some Applications

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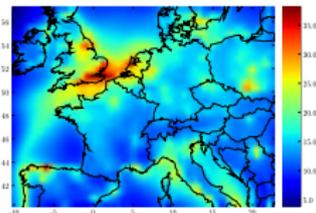
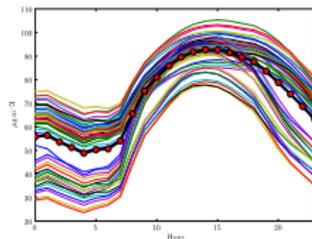
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Next...

Air Quality Ensemble Forecast

- Estimation of the uncertainties in the output
- Model sequential aggregation with weights learned over the past
- Ozone forecasting over Europe (Prév'air operational platform).



- Vivien Mallet and Bruno Sportisse. Ensemble-based air quality forecasts : a multi-model approach applied to ozone. *J. Geophys. Res.*, 111(D18) :18302, 2006
- Vivien Mallet and Bruno Sportisse. Uncertainty in a chemistry-transport model due to physical parameterizations and numerical approximations : an ensemble approach applied to ozone modeling. *J. Geophys. Res.*, 111(D01302), 2006

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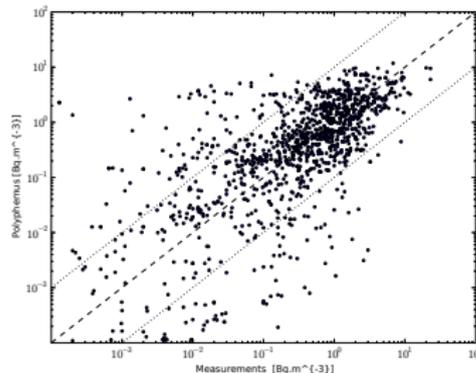
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Dispersion of Radionuclides

- Polyphemus is the support of the new operational forecast system at the Emergency Center of IRSN
- Simulation of the Chernobyl accident, sensitivity studies
- Inverse modeling applied to simulations of the ETEX exercise and Algeciras accident.



Some Applications

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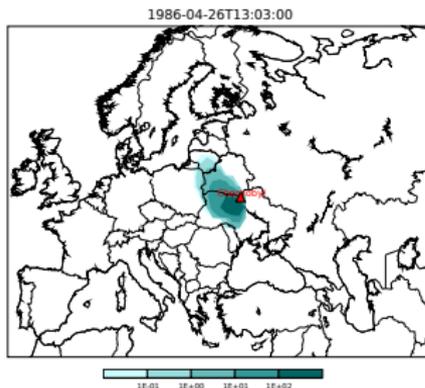
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Next...

Chernobyl Accidental Release, 25 April-5 May 1986

Polyphemus run, Forecast Emergency Center IRSN/CEREA



- D. Quélo, M. Krysta, M. Bocquet, O. Isnard, Y. Minier, and B. Sportisse. Validation of the POLYPHEMUS system : the ETEX, Chernobyl and Algeciras cases. *Atmos. Env.*, 2007.
doi :10.1016/j.atmosenv.2007.02.035
- B. Sportisse. A review of parameterizations for modeling dry deposition and scavenging of radionuclides. *Atmos. Env.*, (41) :2683–2698, 2007

Data Assimilation

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Why ?

To improve the results (*analysis*) using several sources of information (model, observations).

How ?

Data assimilation involves three component :

- A model (currently only possible with Polair3D model and gaseous species)
- Observations
- An assimilation algorithm which combines both (implemented as a driver in Polyphemus)

Notations

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- \mathbf{x} : model state vector.
- \mathbf{x}^t : true state.
- \mathbf{x}^b : background estimates.
- \mathbf{x}^a : analysis.
- \mathbf{y} : observation vector.
- ϵ^b : $\mathbf{x}^b - \mathbf{x}^t$ background errors.
- ϵ^a : $\mathbf{x}^a - \mathbf{x}^t$ analysis errors.
- H : Observation operator
- \mathbf{B} (also noted \mathbf{P}^b) : $\frac{(\epsilon^b - \bar{\epsilon}^b)(\epsilon^b - \bar{\epsilon}^b)^T}{(\epsilon^b - \bar{\epsilon}^b)(\epsilon^b - \bar{\epsilon}^b)^T}$ background error covariance matrix.
- \mathbf{A} (also noted \mathbf{P}^a) : $\frac{(\epsilon^a - \bar{\epsilon}^a)(\epsilon^a - \bar{\epsilon}^a)^T}{(\epsilon^a - \bar{\epsilon}^a)(\epsilon^a - \bar{\epsilon}^a)^T}$ analysis error covariance matrix.
- ϵ^o : $\mathbf{y} - H(\mathbf{x}_t)$ observation errors.
- \mathbf{R} : $\frac{(\epsilon^o - \bar{\epsilon}^o)(\epsilon^o - \bar{\epsilon}^o)^T}{(\epsilon^o - \bar{\epsilon}^o)(\epsilon^o - \bar{\epsilon}^o)^T}$ observation error covariance matrix.

Optimal Interpolation

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Principle

Combination of background
and background departure.

Formulae

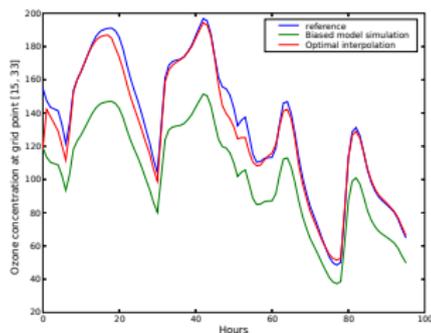
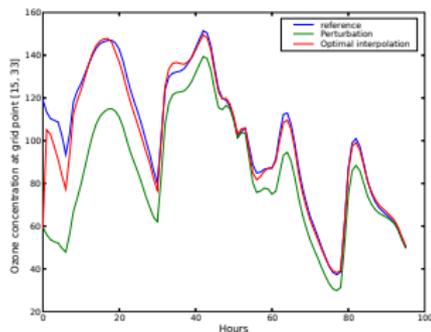
$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{K}(\mathbf{y} - H(\mathbf{x}^b)),$$
$$\mathbf{K} = \mathbf{B}\mathbf{H}^T(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R})^{-1}.$$

Study

B : using Balgovind
correlation function.

$$f(r) = \left(1 + \frac{r}{L}\right) \exp\left(-\frac{r}{L}\right) v^b$$

- Perturbs ICs (upper).
- Biased model (lower).



Ensemble Kalman filter (EnKF)

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Principle

Time-dependent error covariance matrices. Ensemble statistics are used to approximate \mathbf{P}^f and \mathbf{P}^a at each time.

Formulae

- Initialization : given initial pdf $p(\mathbf{x}_0^t)$, an ensemble of r members are generated randomly,

$$\{\mathbf{x}_0^{a,i}, \quad i = 1, \dots, r\}$$

$$\bar{\mathbf{x}}_0^a = \frac{1}{r} \sum_{i=1}^r \mathbf{x}_0^{a,i}$$

$$\tilde{\mathbf{P}}_0^a = \frac{1}{r-1} \sum_{i=1}^r \left(\mathbf{x}_0^{a,i} - \bar{\mathbf{x}}_0^a \right) \left(\mathbf{x}_0^{a,i} - \bar{\mathbf{x}}_0^a \right)^T$$

Formulae

- Forecast formula :

$$\mathbf{x}_k^{f,i} = M_{k-1}[\mathbf{x}_{k-1}^{a,i}] + \eta_{k-1}^i$$

$$\tilde{\mathbf{P}}_k^f = \frac{1}{r-1} \sum_{i=1}^r \left(\mathbf{x}_k^{f,i} - \bar{\mathbf{x}}_k^f \right) \left(\mathbf{x}_k^{f,i} - \bar{\mathbf{x}}_k^f \right)^T$$

where $\bar{\mathbf{x}}_k^f$ is the mean of ensemble $\{\mathbf{x}_k^{f,i}, i = 1, \dots, r\}$

- Analysis formula :

$$\mathbf{x}_k^{a,i} = \mathbf{x}_k^{f,i} + \tilde{\mathbf{K}}_k \left(\mathbf{y}_k^i - H_k[\mathbf{x}_k^{f,i}] \right)$$

$$\mathbf{x}_k^a = \frac{1}{r} \sum_{i=1}^r \mathbf{x}_k^{a,i}$$

$$\tilde{\mathbf{P}}_k^a = \frac{1}{r-1} \sum_{i=1}^r \left(\mathbf{x}_k^{a,i} - \mathbf{x}_k^a \right) \left(\mathbf{x}_k^{a,i} - \mathbf{x}_k^a \right)^T$$

Reduced rank square root Kalman filter : RRSQRT

Heemink et al. 2001

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Principle

Also approximate error covariance matrices, but using a low-rank representation $\mathbf{L}\mathbf{L}^T$.

\mathbf{L} is the *Mode Matrix* whose q columns represent the dominant directions of the forecast.

In addition, square root of \mathbf{Q} (the error model) is approximated using ensemble statistics.

Formulae

- Initialization : $\mathbf{x}_0^a, \mathbf{L}_0^a = [\mathbf{l}_0^{a,1}, \dots, \mathbf{l}_0^{a,q}]$

Formulae

- Forecast formula :

$$\mathbf{x}_k^f = M_{k-1 \rightarrow k}(\mathbf{x}_{k-1}^a)$$

$$\mathbf{l}_k^{f,i} = \frac{1}{\epsilon} \{ M_{k-1 \rightarrow k}(\mathbf{x}_{k-1}^a + \epsilon \mathbf{l}_{k-1}^{a,i}) - M_{k-1 \rightarrow k}(\mathbf{x}_{k-1}^a) \}, \quad \epsilon = 1$$

$$\tilde{\mathbf{L}}_k^f = [\mathbf{l}_k^{f,1}, \dots, \mathbf{l}_k^{f,q}, \mathbf{Q}_{k-1}^{\frac{1}{2}}], \quad \mathbf{L}_k^f = \Pi_k^f \tilde{\mathbf{L}}_k^f$$

- Analysis formula :

$$\mathbf{P}_k^f = \mathbf{L}_k^f \mathbf{L}_k^{f,T}$$

$$\mathbf{K}_k = \mathbf{P}_k^f \mathbf{H}_k^T (\mathbf{H}_k \mathbf{P}_k^f \mathbf{H}_k^T + \mathbf{R}_k)^{-1},$$

$$\mathbf{x}_k^a = \mathbf{x}_k^f + \mathbf{K}_k (\mathbf{y}_k - H(\mathbf{x}_k^f)),$$

$$\tilde{\mathbf{L}}_k^a = [(\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \mathbf{L}_k^f, \mathbf{K}_k \mathbf{R}_k^{\frac{1}{2}}], \quad \mathbf{L}_k^a = \Pi_k^a \tilde{\mathbf{L}}_k^a$$

Four-Dimensional Variational Assimilation : 4D-Var

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A cost function $J(\mathbf{x})$ that deals with a set of observations :

$$\underbrace{\frac{1}{2}(\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}^b)}_{J_b} + \underbrace{\frac{1}{2} \sum_{k=0}^N \overbrace{(\mathbf{y}_k - H_k(\mathbf{x}_k))^T \mathbf{R}_k^{-1}(\mathbf{y}_k - H_k(\mathbf{x}_k))}^{J_{oi}}}_{J_o}$$

where the assimilation window is $0 - N$,

$\mathbf{x}_k = M_{0 \rightarrow k}(\mathbf{x}) = M_k M_{k-1} \dots M_1 \mathbf{x}$ The gradient is calculated
by the backward integration of adjoint model

- $\tilde{\mathbf{x}}_N = 0$
- For $k = N, \dots, 1$, calculates $\tilde{\mathbf{x}}_{k-1} = \mathbf{M}_k^T (\tilde{\mathbf{x}}_k - \mathbf{H}_k^T d_k)$,
where $d_k = \mathbf{R}_k^{-1} (\mathbf{y}_k - H_k(\mathbf{x}_k))$
- $\tilde{\mathbf{x}}_0 := \tilde{\mathbf{x}}_0 - \mathbf{H}_0^T(d_0)$ gives the gradient of J_o with respect
to \mathbf{x}

Results

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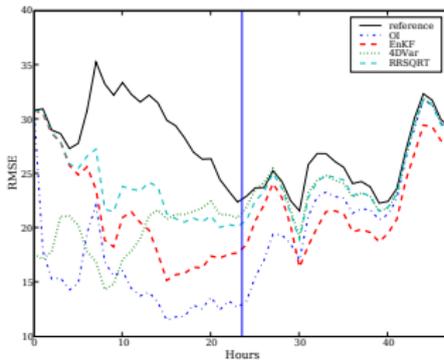
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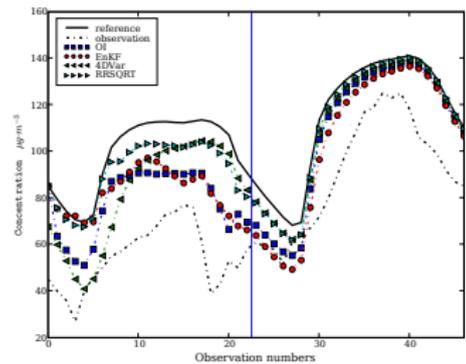
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Root mean square errors.



Results at Montandon station.

Resources

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Current Developers

- | | | |
|----|-------------------------------|----------------------|
| 1 | Meryem Ahmed de Biasi (INRIA) | diffusion |
| 2 | Édouard Debry (ENPC) | aerosols |
| 3 | Karine Kata-Sartelet (ENPC) | aerosols |
| 4 | Irène Korsakissok (ENPC) | local, plume-in-grid |
| 5 | Vivien Mallet (ENPC) | ensemble |
| 6 | Denis Quélo (IRSN) | passive |
| 7 | Yelva Roustan (ENPC) | impact |
| 8 | Bruno Sportisse (ENPC) | aerosols |
| 9 | Marilyne Tombette (ENPC) | aerosols |
| 10 | Lin Wu (INRIA) | assimilation |

Resources

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Next...

Documentations for users

- User's guide (150 pages)
- Scientific documentation for AtmoData
- Reference documentation for AtmoPy

Documentations for developers

- Guide and reference documentation for SeldonData
- Reference documentation for AtmoData
- Guide and reference documentation for Talos

Examples

- Test cases (Eulerian and Gaussian)
- Practical sessions (primarily for courses at ENSTA and ENPC)

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A Graphical User Interface

The screenshot shows the Polyphemus graphical user interface. The window title is "polyphemus_display.py". The menu bar includes "File", "Edit", and "Help". The path to the Polyphemus installation is displayed as "/u/cergrene/a/ahmed-dm/Polyphemus-1.1/".

The "Date shown:" field is set to "2004-08-09_16-00-00". The main display area shows a map of a region with a color scale ranging from 27.0 (blue) to 37.5 (red). The map axes are labeled with values: x-axis from -10 to 20, and y-axis from 42 to 58.

Configuration parameters on the right side include:

- x_min = -10, Delta x = 0.5, Nx = 65
- y_min = 40.5, Delta y = 0.5, Ny = 33
- Nz = 5, Levels: /configuration/levels.dat
- MM5 file: /TestCase-1.1-Eulerian/raw_data/MM5/MM5-2004-08-09
- From: 2004-08-09_01-00-00 To: 2004-08-12_00-00-00
- Species: Tracer, Source: /point-emission.dat
- Initial quantity: 30
- Kz parameterization: Troen and Mahrt

At the bottom, there are fields for "Visualization for time step:" (15) and "Visualization for level:" (0), along with navigation buttons "<<" and ">>". The status bar at the bottom left says "Displaying results". At the bottom right, there are buttons for "Preprocessing", "Simulation", "Clear", and "Quit".

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<http://cerea.enpc.fr/polyphemus/>

The screenshot shows a web browser window titled "Polyphemus - Konqueror". The address bar displays "http://cerea.enpc.fr/polyphemus/applications.html". The page header features the "POLYPHEMUS Air Quality Modeling System" logo and navigation menus: "Document", "Édition", "Affichage", "Aller", "Signets", "Outils", "Configuration", "Fenêtre", and "Aide".

The main content area is titled "Applications" in green. Underneath, the section "Dispersion of Radionuclides" is highlighted in red. The text below this section reads: "The objective of this work is to investigate the validity of Polyphemus for the dispersion of radionuclides. Model-to-data comparisons have been performed for three cases: the ETEX campaign, the Chernobyl accident (see film) and the Algeciras release. The results are similar to those usually given in the literature by state-of-the-art models. Some preliminary sensitivity analysis indicate the main sources for uncertainties. This study is the first step before the operational use of the Polyphemus system for the future emergency system for long-range dispersion of radionuclides at IRSN (Institute of Radiation Protection and Nuclear Safety). Click on the image to launch the film:"

Below the text is a map of Europe with a red triangle and the label "Chernobyl" indicating the location of the Chernobyl nuclear power plant. Above the map, the timestamp "1986-04-26T00:43:00" is displayed.

The left sidebar contains several menu items: "About Polyphemus" (Introduction, News, Applications, People and Contacts, Positions and Internships), "Resources" (Download, Eulerian Test Case, Gaussian Test Case, Training Sessions, Graphical User Interface), "Polyphemus Modules" (AtmoData, AtmoPy, Aerosol Modules), and a "Contact" link.

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Models (mostly implemented, but not yet included in Polyphemus)

- Secondary organic aerosols
- Modal aerosol module (MAM)
- Heavy metals, mercury
- Persistent organic pollutants (POP)
- Passive hemisphere model

Next Steps

- Parallelization
- Lagrangian particle model
- Drivers for assimilation and coupling