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Studying Atmospheric Transport Through Lagrangian Models

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Lagrangian models (LMs) track the movement of fluid parcels in their moving frame of reference. As such, scientists using LMs are forced, in a way, to imagine themselves moving with the parcel and experiencing the effects of advection, turbulence, and changes in the parcel's environment.

LMs have advanced in sophistication over recent decades, allowing them to be used increasingly for both scientific and societal purposes. For example, it is common practice now for researchers around the world to apply LMs to examine a wide spectrum of geophysical phenomena. Atmospheric chemists can track intercontinental transport of pollution plumes [*Stohl et al.,* 2002] or airborne radioactivity [*Wotawa et al.,* 2006]. By running LMs backward in time [*Flesch et al.,* 1995; *Lin et al.,* 2003], instrumentalists can establish the source regions of observed atmospheric species with high computational efficiency [*Ryall et al.,* 2001]. Therefore, LMs are being used increasingly to quantify sources and sinks of greenhouse gases by combining simulations with observations in an inverse modeling framework [*Trusilova et al.,* 2010]. Such "top-down" emissions estimation is receiving growing acceptance as an independent tool to test the veracity of emissions inventories and to verify adherence to treaties.

A recent indication of the tremendous societal importance of LMs was their role in predicting the spread of volcanic ash from the eruption of Eyjafjallajökull volcano in Iceland. Figure 1 demonstrates the power of LMs to accurately track the multiday dispersion of a plume as it eventually transforms into a complicated filamentary structure. The example further demonstrates the great potential of applying LMs in combination with data assimilation and inverse modeling to improve source estimates and the simulation of hazardous plumes.

As Lagrangian modeling increases in complexity and popularity, it is imperative to reexamine the physical foundations and implementation aspects of LMs used today. From this, scientists can build a road map of further steps needed to move Lagrangian modeling forward and to ensure its successful application in the future.

Physical and Technical Constraints

As opposed to Eulerian models (which use grid cells that are fixed in place), LMs are known to create minimal numerical diffusion and thus are capable of preserving gradients in tracer concentration. Additionally, Lagrangian integration is numerically stable, meaning that models can take bigger time steps. Furthermore, the Lagrangian framework is a natural way to model turbulence, as it is a closer physical analog to the pathways traced by eddies.

These advantages served as the inspiration from which Lagrangian particle dispersion models (LPDMs) have evolved, in which air parcels are modeled as infinitesimally small particles that are transported with random velocities representing turbulence. LPDMs often track many thousands to millions of particles in three dimensions and are more sophisticated than simple trajectory or puff models. With the availability of computational resources, full three-dimensional LPDM simulations that were expensive to run just a decade ago are now routinely carried out.

A key guiding principle for the development of LPDMs has been the "well-mixed criterion" (WMC), a consequence of the second law of thermodynamics [*Thomson,* 1987]. The WMC states that particles that are distributed according to atmospheric density (i.e., that are "well mixed") must remain so in the LPDM simulation. LPDMs can violate the WMC due to physical inconsistencies in meteorological fields or model parameterizations. One way to reveal such inconsistencies is by comparing forward- versus backward-time simulations that, in the ideal case, should yield the same results [*Lin et al.,* 2003]. However, imposing the WMC does not determine a unique model formulation except in simple cases [*Wilson and Flesch,* 1993].

Lagrangian simulations are usually driven with observed meteorological data sets or full meteorological fields outputted from general circulation models (GCMs) or numerical weather prediction (NWP) models. Because of limited computational resources, variables may be omitted or resolution may be degraded in the output. This can lead to violation of basic conservation principles (mass, energy, momentum) with adverse effects on the quality of the simulations [*Nehrkorn et al.,* 2010].

Parameterizing subgrid-scale processes is probably the least advanced aspect of Lagrangian modeling today. For example, parameterizing the planetary boundary layer (PBL) height is crucial, since transport of trace gases is strongly dependent on it; yet methods to diagnose PBL height from NWP-outputted meteorological fields are still unsatisfactory [*Seibert et al.,* 2000]. Another example is parameterization of moist convection. The role of convection in redistributing atmospheric tracers necessitates a description of updrafts/downdrafts that are consistent with the parent models (GCM or NWP). While the corresponding mass fluxes can be used to describe the convective motion of Lagrangian particles [*Forster et al.,* 2007], departures from WMC can result if such mass fluxes are not properly constructed [*Nehrkorn et al.,* 2010].

Moving forward, it will be important for LPDM developers to maintain close linkages with parent gridded models as well as to improve parameterizations of subgrid-scale processes.

Quantifying Uncertainties

LMs are widely used in applications requiring uncertainty estimates, such as determining greenhouse gas emissions and preparing for emergencies associated with toxic releases (as witnessed in the recent nuclear disaster at Japan's Fukushima I power plant). Because of this, it is important to construct methods that enable errors in LMs to be propagated into the resulting predictions, e.g., tracer concentrations or air parcel positions given with quantifiable uncertainties. Errors in LMs have roughly five origins: interpolation in space and time, numerical truncation, ill-defined starting position, wind fields, and model formulation (see the review paper by *Stohl* [1998] for exposition on each of these error sources).

Several methods have been proposed to deal with such uncertainties. Ensemble

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methods originally developed for NWP applications and governed by the idea that a series of different models or model runs can be used to represent uncertainty have inspired similar approaches in LPDMs [*Galmarini et al.*, 2004]. Another approach is to calculate "error trajectories" [*Kahl and Samson,* 1988] that incorporate uncertainties within the motions of the Lagrangian air parcels. This can be implemented by simply increasing the diffusivity [*Maryon and Best,* 1995] or by modifying the trajectory traced by the air parcel with an error velocity that reflects quantified uncertainties in wind fields [*Lin and Gerbig,* 2005].

LMs ultimately need to be tested against observations. Such comparisons can reveal the aggregate impact of errors from all five sources, helping to constrain model parameters. Laboratory experiments of dispersion in different media have served as good tests for LMs under idealized conditions. But for tests in the real atmosphere over regional scales, tracer release experiments have served as the "gold standard" for evaluating models. In these experiments, known tracer amounts are released at known locations into the atmosphere and measured at downwind locations. Despite their value, more than 15 years have elapsed since the last major tracer release experiment was carried out. Furthermore, with a few notable exceptions (e.g., Across North America Tracer Experiment (ANATEX) over 3 months [*Draxler and Heffter,* 1989]), such experiments have been limited in temporal scope. More comprehensive tracer release experiments will be required in the future.

Looking Ahead

The development and application of Lagrangian modeling have experienced explosive growth over the past decade. The rise in computing power enables the development of newer, more sophisticated LMs by different research groups around the world. Some new developments include coupling of large-eddy simulations with LMs [*Weil et al.,* 2004], sophisticated atmospheric chemistry models that predict concentration fluctuations in turbulent flow [*Sawford,* 2006], and the use of Lagrangian air parcels themselves to solve the atmospheric dynamical equations [*Alam and Lin,* 2008].

As the use of LMs continues to increase, several issues must be considered in their future development. For example, how can fundamental physical principles be satisfied by LMs as they increase in complexity and sophistication? How can parameterizations of atmospheric processes in LMs be improved? How can uncertainties in Lagrangian simulations be quantitatively assessed? How can LMs be properly coupled to Eulerian NWP/GCM models? What observations are available to test and validate LMs?

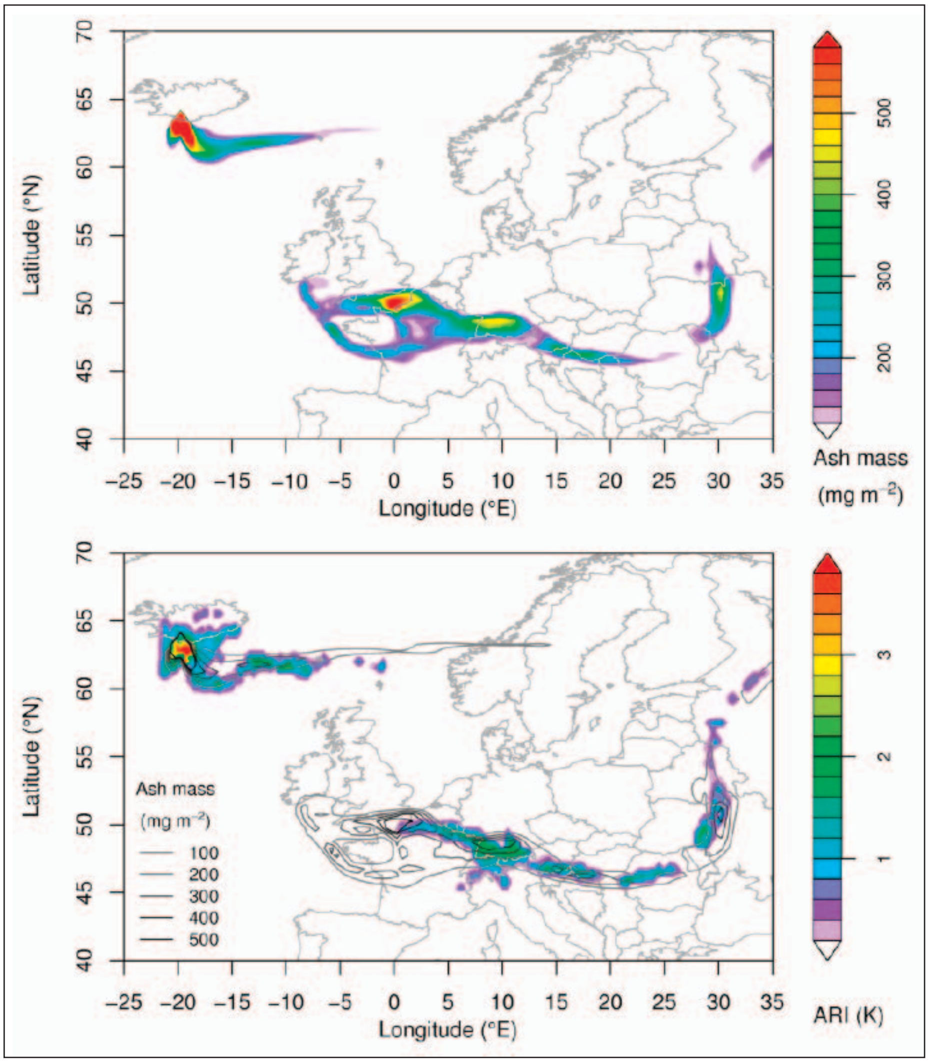

Fig. 1. Comparison of a dispersion simulation of the Eyjafjallajökull volcanic ash plume against satellite observations on 17 April 2010 at 1000 UTC, about 2 days after the main eruption. (top) Simulated ash columns (courtesy of Stephan Henne) based on the Lagrangian particle dispersion model (LPDM) FLEXPART that includes several million particles released proportional to emission strengths estimated through inverse analysis by Stohl et al. *[2011]. (bottom) Satellite-derived ash radiance index (ARI), which represents the brightness temperature difference (in kelvins) between infrared channels at 8.12 and 8.62 microns (courtesy of Lieven Clarisse). ARI data are from the Infrared Atmospheric Sounder Interferometer (IASI) and are approximately proportional to ash column mass* [Clarisse et al., *2010]. For ease of comparison, contours of FLEXPART-simulated ash column mass are also shown. Note the good similarity between simulation and observation, demonstrating how LPDMs can be used to anticipate the effects of events that have geologic and societal importance.*

Because Lagrangian simulations are becoming commonplace, familiarity can breed contempt, and the danger is that LMs will be taken for granted. Lest LMs be improperly developed or used, certain issues need to be kept in mind. These include the need for

- attention to physical principles such as the well-mixed criterion and conservation properties;
- large-scale tracer release experiments that take place over a long period of time and cover regional scales;
- communication between NWP centers and users of the meteorological fields in LMs to ensure seamless information transfer; and
- quantification of uncertainties and development of error propagation methods into the variables of interest.

With these issues in mind, LMs can continue to evolve into an even more robust method for studying atmospheric processes in the future.

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References

Alam, J. M., and J. C. Lin (2008), Toward a fully Lagrangian atmospheric modeling system, *Mon. Weather Rev., 136*(12), 4653–4667, doi:10.1175/2008MWR2515.1.

Clarisse, L., F. Prata, J.-L. Lacour, D. Hurtmans, C. Clerbaux, and P.-F. Coheur (2010), A correlation method for volcanic ash detection using hyperspectral infrared measurements, *Geophys. Res. Lett., 37,* L19806, doi:10.1029/2010GL044828.

Draxler, R. R., and J. L. Heffter (Eds.) (1989), *Across North America Tracer Experiment (ANATEX),* vol. I, *Description, Ground-Level Sampling at Primary sites, and Meteorology, NOAA Tech. Memo., ERL ARL-167,* 83 pp.

Flesch, T. K., J. D. Wilson, and E. Yee (1995), Backward-time Lagrangian stochastic dispersion models and their application to estimate gaseous emissions, *J. Appl. Meteorol., 34*(6), 1320–1332, doi:10.1175/1520-0450(1995)034<1320:BTLSDM>2.0.CO;2.

Forster, C., A. Stohl, and P. Seibert (2007), Parameterization of convective transport in a Lagrangian particle dispersion model and its evaluation, *J. Appl. Meteorol. Climatol., 46*(4), 403–422, doi:10.1175/JAM2470.1.

Galmarini, S., et al. (2004), Ensemble dispersion forecasting—Part I: Concept, approach and indicators, *Atmos. Environ., 38*(28), 4607–4617, doi:10.1016/j.atmosenv.2004.05.030.

Kahl, J. D., and P. J. Samson (1988), Uncertainty in estimating boundary-layer transport during highly convective conditions, *J. Appl. Meteorol., 27*(9), 1024–1035, doi:10.1175/1520-0450(1988)027<1024:UIEBLT>2.0.CO;2.

Lin, J. C., and C. Gerbig (2005), Accounting for the effect of transport errors on tracer inversions, *Geophys. Res. Lett., 32,* L01802, doi:10.1029/2004GL021127.

Lin, J. C., C. Gerbig, S. C. Wofsy, A. E. Andrews, B. C. Daube, K. J. Davis, and C. A. Grainger (2003), A near-field tool for simulating the upstream influence of atmospheric observations: The Stochastic Time-Inverted Lagrangian Transport (STILT) model, *J. Geophys. Res., 108*(D16), 4493, doi:10.1029/2002JD003161.

Maryon, R. H., and M. J. Best (1995), Estimating the emissions from a nuclear accident using observations of radioactivity with dispersion model products, *Atmos. Environ., 29*(15), 1853–1869, doi:10.1016/1352-2310(95)00042-W.

Nehrkorn, T., J. Eluszkiewicz, S. C. Wofsy, J. C. Lin, C. Gerbig, M. Longo, and S. Freitas (2010), Coupled weather research and forecasting—Stochastic Time-Inverted Lagrangian Transport (WRF-STILT) model, *Meteorol. Atmos. Phys., 107*(1), 51–64, doi:10.1007/s00703-010-0068-x.

Ryall, D. B., R. G. Derwent, A. J. Manning, P. G. Simmonds, and S. O'Doherty (2001), Estimating source regions of European emissions of trace gases from observations at Mace Head, *Atmos. Environ., 35*(14), 2507–2523, doi:10.1016/S1352-2310(00)00433-7.

Sawford, B. L. (2006), Lagrangian stochastic modelling of chemical reaction in a scalar mixing layer, *Boundary Layer Meteorol., 118*(1), 1–23, doi:10.1007/s10546-005-4737-0.

Seibert, P., F. Beyrich, S.-E. Gryning, S. Joffre, A. Rasmussen, and P. Tercier (2000), Review and intercomparison of operational methods for the determination of the mixing height, *Atmos. Environ., 34,* 1001–1027.

Stohl, A. (1998), Computation, accuracy and applications of trajectories—A review and bibliography, *Atmos. Environ., 32*(6), 947–966, doi:10.1016/S1352-2310(97)00457-3.

Stohl, A., S. Eckhardt, C. Forster, P. James, and N. Spichtinger (2002), On the pathways and timescales of intercontinental air pollution transport, *J. Geophys. Res., 107*(D23), 4684, doi:10.1029/2001JD001396.

Stohl, A., et al. (2011), Determination of time- and height-resolved volcanic ash emissions for quantitative ash dispersion modeling: The 2010 Eyjafjallajökull eruption, *Atmos. Chem. Phys. Discuss., 11,* 5541–5588, doi:10.5194/acpd-11-5541-2011.

Thomson, D. J. (1987), Criteria for the selection of stochastic models of particle trajectories in turbulent flows, *J. Fluid Mech., 180,* 529–556, doi:10.1017/S0022112087001940.

Trusilova, K., C. Rödenbeck, C. Gerbig, and M. Heimann (2010), Technical note: A new coupled system for global-to-regional downscaling of CO$_2$ concentration estimation, *Atmos. Chem. Phys., 10*(7), 3205–3213, doi:10.5194/acp-10-3205-2010.

Weil, J. C., P. P. Sullivan, and C.-H. Moeng (2004), The use of large-eddy simulations in Lagrangian particle dispersion models, *J. Atmos. Sci., 61*(23), 2877–2887, doi:10.1175/JAS-3302-1.

Wilson, J. D., and T. K. Flesch (1993), Flow boundaries in random-flight dispersion models: Enforcing the well-mixed condition, *J. Appl. Meteorol., 32*(11), 1695–1707, doi:10.1175/1520-0450(1993)032<1695:FBIRFD>2.0.CO;2.

Wotawa, G., L.-E. De Geer, A. Becker, R. D'Amours, M. Jean, R. Servranckx, and K. Ungar (2006), Inter- and intra-continental transport of radioactive cesium released by boreal forest fires, *Geophys. Res. Lett., 33,* L12806, doi:10.1029/2006GL026206.av

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