

Development of a Novel Technique for the Automatic Generation of Dynamic Atmospheric Models

Shubhabrata Roy¹, Ryan Heule¹, Molly Schmidt¹, Lesli Joseph², David Courard-Hauri³
Drake University, Des Moines, IA 50311

¹Undergraduate Student, Computer Science Department;

²Undergraduate Student, Environmental Science and Policy Program

³Assistant Professor and PI, Environmental Science and Policy Program

e-mail: david.courard-hauri@drake.edu

515.271.3812

Abstract: The automatic generation of dynamic models from time series data could significantly improve understanding of many systems, because it would allow for the elucidation of certain types of nonlinear connections which are not amenable to study using current techniques. We have begun to develop a method of this sort based upon global optimization algorithms (Simulated Annealing and Genetic Algorithms). In this work, we converted much of our Fortran and C code into the C++ programming language in order to ease future undergraduate work on the project, and to allow for the dual-level technique that we have designed, but for which the original Adaptive Simulated Annealer was not well suited. Here we demonstrate the applicability of our technique to a simple class of small, first-order, chemical equations. We show in an example that the objective function tends to slope toward the optimal result, but that even for simple problems it is not monotonic, indicating that more efficient “downhill” optimizers are unlikely to succeed in solving this type of problem. While we have not yet sufficiently parameterized our algorithms to allow for the efficient determination of connectivity in models with more than fifteen optimization dimensions, our initial success with smaller models indicates that this is largely a problem of limited computing speed and algorithm optimization, and is not a significant barrier.

Introduction and Background

Over the past two decades, few environmental issues have captured international attention like anthropogenic climate change. Extreme heat in the summer of 1987, though hardly proof of greenhouse warming, brought the issue to the consciousness of average Americans in a dramatic way. Since then, an increasing number of studies have indicated that the global climate is warming (Grabherr *et al.*, 1994; Karl *et al.*, 1993; Schneider, 1994; IPCC, 2001a), and a consensus has begun to emerge in the climate community that a doubling in atmospheric CO₂-equivalent stocks (expected by the middle of this century) will most likely lead to an increase in global mean surface temperature of roughly 2.5°C, with an uncertainty range of about 1.5 to 4.5°C (IPCC, 1996; IPCC 2001a).

Most current models indicate that climate change is likely to be roughly proportional to the change in atmospheric greenhouse gasses (GHGs). Stephen Schneider suggests that as models become more complex, the linearity in their response to forcing by GHGs has become more pronounced, and nonlinear climatic "surprises" (called "singularities" in the 2001 IPCC report) seem less likely (Schneider, 1998, personal communication). Although climatologists acknowledge the possibility of anthropogenic emissions leading to dramatic, nonlinear changes in climate variables, and some researchers consider the possibility to be significant (Broecker, 1998; Woodwell, 1998; IPCC 1998, NAS 2001), in general the probability of such occurrences is deemed to be low (IPCC, 2001b, Section 19.5). There are two important reasons for this confidence: first, current global circulation models (GCMs) do not generally demonstrate significant nonlinear behavior, and second, credible mechanisms which have been suggested and which might lead to such behavior (for example a shutdown of the thermohaline circulation) do not appear likely to be of significant concern for a doubling of CO₂ (Wang *et al.*, 1999a, b; Stouffer and Manabe, 1999; Park, 1999; Tziperman, 2000; Oppenheimer, 1998; but see also Schmittner and Stocker, 1999; Jayne and Marotzke, 1999).

Paleoclimatological studies, however, do not present a picture of climate responding linearly to changes in forcing. Milankovic (1941) was the first to link cycles between glacial and interglacial periods to changes in orbital parameters which translated into regional changes in solar forcing, and later work has supported the hypothesis (Broecker *et al.*, 1968; Veeh and Chappell,

1970). But ice-cores and other evidence indicate that the transition between cold and warm periods is often relatively abrupt when compared to changes in solar forcing, and is, at times, surprisingly strong given the relatively weak change in insolation (Hare, 1979; Martinson *et al.*, 1987; Dansgaard *et al.*, 1993; Jouzel *et al.*, 1993; Zhao *et al.*, 1995; Zachos *et al.*, 2001). Late Pleistocene climate exhibits oscillations and dynamical behavior at various temporal and geographical scales (Jouzel, 1994; Frontval *et al.*, 1998; Raymo *et al.*, 1998), which are less easily correlated with solar forcing. Dansgaard/Oeschger (DO) cycles and Heinrich events, for example, are more likely related to internal climatic dynamics deriving from ice-ocean interaction in the North Atlantic (Dansgaard, *et al.*, 1993; Grootes, *et al.*, 1993; Taylor, *et al.*, 1993; Broecker, 1994), though the effects are seen globally (see, for example, Bender *et al.*, 1994; Lowell *et al.*, 1995; Porter and An, 1995; Roy *et al.*, 1996; Behl and Kennett, 1996). In many cases, the climate system appears to respond slowly to changes in forcing until a threshold is reached, at which point significant changes in variables such as temperature and precipitation occur rapidly on either a local or global scale. This point is made well in a recent publication by the National Academy of Sciences titled "Abrupt Climate Change: Inevitable Surprises" (NAS, 2001):

Abrupt climate changes were especially common when the climate system was being forced to change most rapidly. Thus, greenhouse warming and other human alterations of the earth system may increase the possibility of large, abrupt, and unwelcome regional or global climatic events. The abrupt changes of the past are not fully explained yet, and *climate models typically underestimate the size, speed, and extent of those changes.* (emphasis added)

This behavior is consistent with a multistable system, or perhaps, in the case of DO cycles, one which has crossed a Hopf bifurcation. Some authors have even cited evidence which suggests that at least regional climate systems may be considered to lie on a dynamical "strange attractor" with low dimensionality in state space (Abarbanel *et al.*, 1996). The climate system involves numerous subsystems which provide either positive or negative feedback. Ice albedo generally increases in a cooling world and decreases in a warming world, providing a positive feedback (Grosiman *et al.*, 1994; Nicolis and Prigogine, 1989, Section 1.8). Due to its longwave absorptive properties, water vapor provides another positive feedback (Moeller, 1963; Cess *et al.*, 1989), though the feedback through clouds is ambiguous (IPCC, 2001a; Washington, 1992). Biotic feedbacks are also likely to be extremely important, although they generally are not included in

most current models. Atmospheric CO₂ levels correlate strongly with temperature changes in the paleoclimate record (Jouzel *et al.*, 1993). Given the very large carbon fluxes into and out of the biosphere (Houghton, 1997, p. 23), it is not surprising that steady-state levels of atmospheric CO₂ are affected during biotic rearrangement. Methane is another greenhouse gas which some have suggested might provide feedbacks through both biota (Woodwell *et al.*, 1998) and methane hydrates (Dickens *et al.*, 1995).

These observations indicate that attempts at the construction of predictive models could be advantageously informed by a more general consideration of the properties of dynamical systems, as has indeed been suggested by Palmer (1993) and others (*e.g.*, Semenov and Porter, 1995). Particularly relevant here is an observation which is well-known throughout the modeling community, but which is, in practice, often not fully taken to heart when the local predictive power of one's model becomes apparent: *even models which are extremely well validated by observations in nearby regions of state space do not necessarily have predictive power regarding transitions, for example, to alternate attractive regions.*

Research on this subject is highly evolved in the field of nonlinear dynamics. Bruce Clarke (1980, 1992, 1993) has developed a technique for the analysis of available dynamical states in chemical models called Stoichiometric Network Analysis (SNA). This technique involves the mathematical reduction of a chemical mechanism to a series of *essential extreme currents*. Different extreme currents play a role in different attractive regions, and the analysis of these extreme currents gives insight into the behavior of the system across bifurcation points. A system can be quite faithfully modeled in one region of state space even if some set of extreme currents is entirely left out, while this left-out set may turn out to be the dominant current in another region.

With respect to climate models, we know that we are leaving out significant parts of the climate system in even our most complex models, and we know that models do not faithfully reproduce past climatic dynamics, or glacial-interglacial transitions, when parameterized to late Pleistocene conditions (Charles *et al.*, 1994; Broecker, 1995; Trenberth, 1997; Ganopolski *et al.* 1998), possibly because the system was in a different attractive region in which alternative dominant extreme current analogs were significant. The field of paleoclimate modeling is currently quite active, partially due to this very problem of poor confidence in models only locally parameterized and tested.

We are interested in the question of medium-term (decadal- to multicentury-scale) paleo and modern climate dynamics with the goal of determining whether climatic analogs to extreme currents exist, and whether these may be fundamentally different in various climate regimes. These studies will be useful in future model development, in improving our understanding of the differences in glacial and interglacial periods, and in assessing the robustness of current paleoclimate models in predicting the likelihood of certain types of dynamical mode-switching.

The use of adaptive techniques such as neural networks is well established in climate and weather modeling (Hsieh, 2001; Calvo *et al.*, 2000; Grieger and Latif, 1994). Similarly, there are numerous examples of the use of time-series data to develop predictive, low-dimensional models based upon the construction of a minimal set of equations of motion (Crutchfield and McNamara, 1987), mutual information analysis (Fraser and Swinney, 1986), principal interaction patterns, (Kwasniok, 1996, 1997a,b), and other variational methods (Jirsa and Haken, 1995). However, these techniques are generally used to develop a zero-dimensional predictive model, generally with little physical basis. Recently, John Ross of Stanford University and Adam Arkin of UC-Berkeley have attempted to develop methods for model construction based upon analysis of empirical time series in which reactive chemical or biological species are known, but interactions are not (Arkin and Ross, 1995; Gilman and Ross, 1995; Arkin *et al.*, 1997; Ross and Vlad, 1999; Tsuchiya and Ross, 2001; Arkin, personal communication, 2001).

In order to bring some of the power of these tools to bear upon the climate modeling problem, we will treat interacting global regions as individual reactive units, and use a variant of the above techniques to develop a minimal, plausible model for energy transfer between regions, based upon regional time-series data. Essentially, we intend to develop an empirical box model of the Earth as a series of interacting cells, each of which can transfer energy (or, for example, water vapor, though the goal will be to minimize the number of variables involved), according to a set of dynamical transfer coefficients. The data analyzed by the system will be regional paleoclimatic temperature proxies (this might also be expanded to include other measurable local properties if it becomes necessary), and these will be used to calculate transfer coefficients for this minimal system in a manner similar to the calculation of chemical rate coefficients in the above techniques. The resultant model would not be physically meaningful in the sense that it would not include mechanisms for energy transfer, but it will shed light upon important physical interactions between regions, which could then be translated into a greater understanding of climate dynamics for

incorporation into more realistic models, and it will be a unique minimal model demonstrating an analog to the very useful extreme currents in chemical reaction dynamics. The model formulation would also be analogous to many valuable abstract models currently being used (*e.g.*, de Verdiere and Huck, 2000; Lorentz, 1990).

To construct a mechanism using these techniques, a system is forced by varying external inputs and the response is followed in concentrations of the species that can be measured. In our case these are local temperature proxies (absolute temperature is less important than relative changes, which makes this technique nicely suited for use with paleoclimate data). An important condition for this type of analysis is an understanding of the main inputs to the system, although it is not necessary to include all of the relevant subsystems within the reactive mechanism itself (Ross and Vlad, 1999). In the case of climate, we will assume that the climate system exhibits internal dynamics, with continual or periodic external forcings. Along these lines, the most important external forcing is solar input at the top of the atmosphere in each interacting region. Reasonable solar forcing values can be calculated into the late Pleistocene (Imbrie and Imbrie, 1979; Imbrie *et al.*, 1993; Zachos *et al.*, 2001). Surface insolation can then either be approximated with a rough model, or allowed to vary within a range and determined along with other model variables. Actual solar intensity values are more problematic, though the resultant forcing ought not to be significant for our purposes and the characteristic time of the solar cycle may well be short enough for solar intensity to be treated as an average quantity. More detail here and elsewhere will be added as data become available. Volcanism is an additional significant forcing external to the system under consideration (Bradley and Jones, 1995; Santer *et al.*, 2001). In some cases event intensity and location can be estimated, while in others a clear volcanic signal is lacking. When data are available, for example in the form of sulfate spikes in ice cores (Hammer, 1977; Zielinski *et al.*, 1996; Hammer *et al.*, 1997; Palmer *et al.*, 2001), we will include volcanism as an external forcing signal, while in some cases it will need to be treated as noise within the system along with other, less well understood signals, such as the passage of the solar system through clouds of cosmic dust.

It is important to realize that this work differs from previous studies in that it will treat insolation of numerous interacting regions covering the entire planet, rather than focus upon one region or hemisphere at a time as in studies discussed above, although these localized applications of the technique are likely as well.

Results

A difficult problem in this type of model construction, and the main focus of this seed grant, regards correct attribution in mechanisms involving significant amounts of feedback and nonlinearities. Gilman and Ross (1995) have had some success along these lines using genetic algorithms to evolve multiple candidate models. We have begun to expand upon this effort. Using a new two-level numerical optimization technique developed by our laboratory, we have had success reconstructing simple mass-balance reaction models of about eight species and interactions. Our technique currently uses simulated annealing as a robust, global optimizer for both discrete and continuous optimizations (Aarts and Lenstra, 1997), and attempts to reconstruct the dynamical equations of the model with no information other than reaction order, species present, and measured concentrations. This is accomplished through a unique two-level mechanism, whereby an upper-level annealer samples connectivity space, and a lower-level annealer optimizes transfer coefficient space during each pass.

As an example, consider a simple four-box model, involving only first-order transfers from one box to the next, as shown in Figure 1. In addition, all of the transfer coefficients are symmetric and equal to 0.5 inverse time units. We can assign values of one unit to the reservoirs 2 and 4, and then run the model for twenty time steps and follow the redistribution of material between the boxes. Next, we can choose an arbitrary connectivity between boxes, and assign random transfer coefficients. For example, we may choose the set-up shown in Figure 2a, where all of the material flux is between box 3 and 1. If we choose arbitrary starting values for the transfer coefficients for all of the arrows (we use values of 1 to initialize), we can then run the model and compare the output with the results for the model run that we are attempting to replicate (that in Figure 1). The objective function we use is simply a sum of the squares of the differences at each time point chosen:

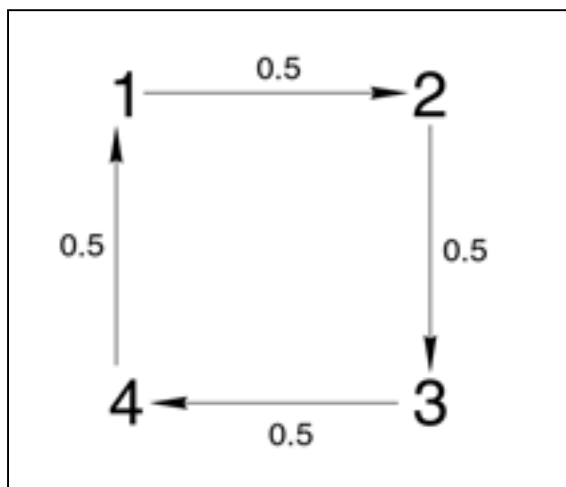


Figure 1. Schematic of simple example system. Material flows between reservoirs (large numbers) in the directions indicated by the arrows. In this case, the system is entirely symmetric, and there are no feedbacks to produce complex dynamics.

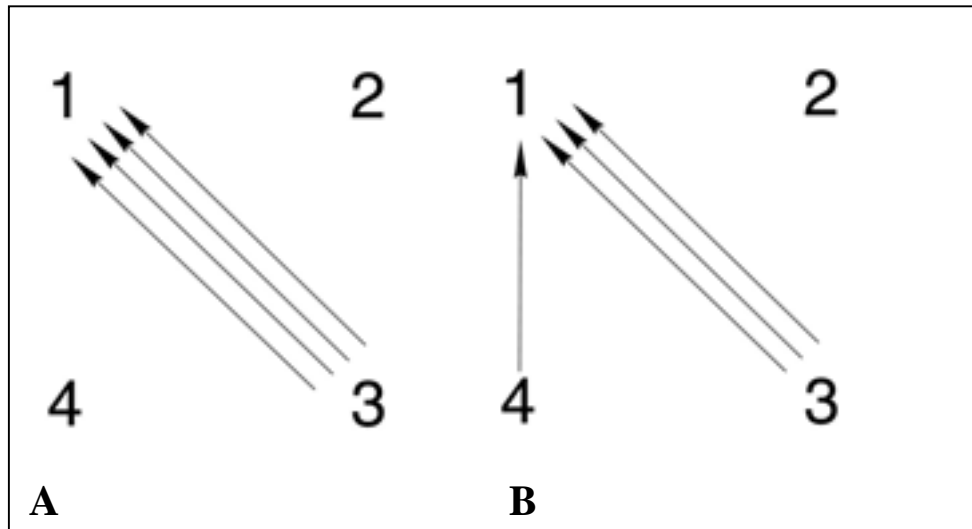


Figure 2. Schematics of early processes in the optimization technique. In A, all flux is from region 3 to 1, no flux is possible between other regions, or from 1 back to 3. In B, all targets remain on 1, but the source of one flux arrow has

$$O = \sum [y_{i,t}(test) - y_{i,t}(base)]^2$$

where O is the objective function we are trying to minimize, and $y_{i,t}$ is the value in the i th box (concentration, population, energy, *etc.*) at time t , measured in time units since the beginning of the run. Once we obtain a value for that run, we allow the values of the transfer coefficients to change, where the magnitude of the change is a function of the fraction of previously accepted to rejected steps (see Aarts and Lenstra, 1993, for a discussion of adaptive stepsize techniques), and the direction is a pseudo-random value. This allows us to construct a new model with the same connectivity, but different transfer coefficients. This new model system is then run, and the results compared with the base case to give a new value for O . If the new O is smaller than the value obtained in the previous run, then it is always accepted. If it is larger, then it is accepted according to the Metropolis criteria of Simulated Annealing (SA). In this way, an optimal solution is eventually obtained, which we take to be the closest possible match between results for the connectivity given. This is taken as the value of the objective function for the given connectivity. Connectivity is then changed slightly. Boxes from which arrows emerge or to which they point can be changed. There is a high likelihood that only a single arrow will change, and that it will only change either its origin or its target, but not both. Depending upon the “temperature” however, there is a fixed probability that more than one will be switched. In our example, the new connectivity might look like that in Figure 2b. The process of transfer coefficient optimization is then repeated, with the optimal configuration resulting in the value for the objective function for that connectivity. The acceptance criteria for the change in connectivity are similar to those for the change in transfer coefficient values. Ultimately, the system settles into a minimum value from which it cannot

improve. For systems to which this method of global optimization is suited, this final configuration is identical to the base case connectivity.

In order to determine the potential for SA in this type of problem, we took the system described above, and calculated the objective function for all possible connectivities. The first criterion for SA to be useful is that there must be some information contained in the overall slope of the objective function in state-space. This slope need not be monotonic (if it were, then local optimizers would be much better choices), and it need not obey many other constraints, but if the objective function is entirely random in state space then SA will do no better than a fully stochastic search (the same is true for all methods of global optimization). If we define “distance” as the

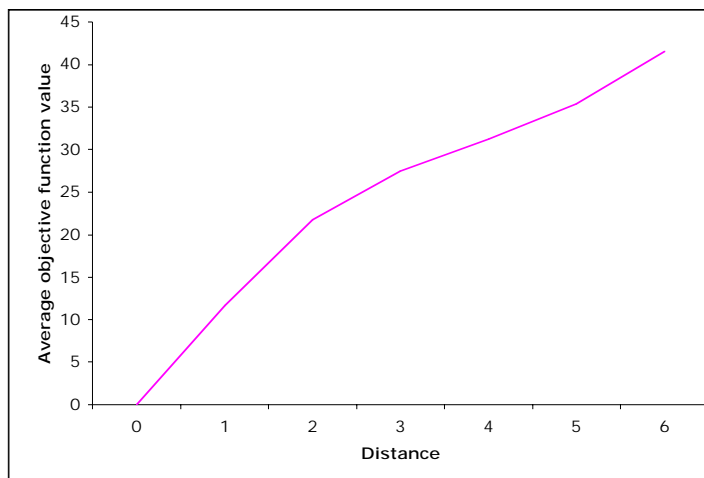


Figure 3. Average value of the objective function for given distances from the actual model (where distance is defined as the minimum number of changes in target or source for all arrows required to reproduce the correct connectivity). The steadily rising curve indicates that there is likely to be sufficient information in the surface for global optimization techniques to be applicable.

number of connections which must be changed in order to obtain the desired solution, we see in Figure 3 that this system conforms quite nicely to our criterion. As distance increases, the mean value for the objective function increases, indicating that there is plenty of information to guide a search of this type.

Next, we want to see if a simple downhill search would be sufficient, since significant computational resources could be saved if we were able to utilize such a method. Because we have been able to map out all of state space for this simple system, we can look at the surface to see if there are direct, monotonically decreasing paths to the final result. We find that there are not. Although some paths do lead directly to the desired result, and the desired result does have the lowest value for the objective function of all runs performed, in most cases if we always select the change which results in the lowest value of O , we encounter local minima that must be overcome to make progress, and also many loops where the “optimal” path leads back to local (but not global)

minima which the system has already sampled. That such a simple system results in a complex landscape for the objective function indicates that simple downhill searches will not be suitable for optimization, especially in more realistic scenarios.

We also looked into the suitability of genetic algorithms (GAs), another non-differentiation-based global optimizer. This technique is well-adapted to optimization in cases where the objective function lies on a complex landscape and where derivatives are difficult to calculate (Mongeau *et al.*, 2001). Unlike SA, GAs perform a search by randomly selecting a large starting population of possible solutions to the problem and then randomly combining features of various successful models (individuals) in a way that mimics genetic combination in breeding. One significant advantage of GAs is that their distributed solution strategy allows for easy parallelization, leading to the possibility of very fast, but relatively inexpensive computation in a cluster of fairly slow machines. Determining the suitability of GAs was an area where we focused a fair amount of our time, and had initial success in reproducing complex connectivities. However, it was later determined that the method used for choosing the initial population set was not as random as had been assumed, and so these results need to be reanalyzed.

As the next step, we intend to increase the complexity of the modeled system, but use distance-matrix techniques to gain information on likely linear interactions, thus decreasing the number of reactions which must be left undetermined for the optimizer. With this technique, we hope to decrease combinatorial complexity, but still allow for the elucidation of multidimensional nonlinear systems.

Conclusions

This seed grant has allowed us to demonstrate the applicability of our technique to a simple class of small, first-order, chemical equations. We have shown that the solution tends to slope toward the correct solution, but that even for simple problems it is not monotonic, indicating that more efficient “downhill” optimizers are unlikely to succeed in solving this type of problem. While we have not yet sufficiently parameterized our algorithms to allow for the efficient determination of connectivity in models with more than fifteen optimization dimensions, our initial success with smaller models indicates that this is more a problem of computing speed (so far our models have been run on a standard, 800 MHz Intel Pentium 3 system running Linux) and algorithm optimization than it is a significant barrier.

References

- Aarts, E.H.L., Lenstra, J.K. (1997) Local search in combinatorial optimization. (Wiley: New York), 522 pp.
- Abarbanel, H.D.I., Lall, U., Moon, Y-I., Mann, M.E., and Sangoyomi, T. (1996) Nonlinear dynamics and the Great Salt lake: a predictable indicator of regional climate. *Energy*, **21**, 655-665.
- Arkin, A., Shen, P., and Ross, J. (1997) A test case of correlation metric construction of a reaction pathway from measurements. *Science*, **277**, 1275-1279.
- Arkin, A., and Ross, J. (1995) Statistical construction of chemical reaction mechanisms from measured time-series. *J. Phys. Chem.*, **99**, 970-979.
- Behl, R.J., and Kennett, J.P. (1996) Brief interstadial events in the Santa Barbara Basin, NE Pacific, during the past 60 kyr. *Nature*, **379**, 243-246.
- Bender, M., Sowers, T., Dickson, M-L., Orchardo, J., Grootes, P., Mayewski, P.A., Meese, D.A. (1994) Climate correlations between Greenland and Antarctica during the past 100,000 years. *Nature*, **372**, 663-666.
- Bradley, R.S. (1999) *Paleoclimatology: Reconstructing Climates of the Quaternary*, 2nd ed. (Harcourt Academic Press: New York) 613 pp.
- Bradley, R.S., and Jones, P.D. (1995) *Climate Since A.D. 1500*. (Revised edition) London: Routledge.
- Broecker, W.S., Thurber, D.L., Goddard, J., Ku, T-L., Matthews, R.K., and Mesolella, K.J. (1968) Milankovich hypothesis supported by precise dating of coral reefs and deep-sea sediments. *Science*, **159**, 297-300.
- Broecker, W.S. (1994) Massive iceberg discharges as triggers for global climate change. *Nature*, **372**, 421-444
- Broecker, W.S. (1995) *The glacial world according to Wally*, 2nd ed., Palisades, NY: Eldigo Press.
- Broecker, W.S. (1998) The end of the present interglacial: how and when? *Quaternary Science Reviews*, **17**, 689-694.
- Calvo, R.A., Navone, H.D., Ceccatto, H.A. (2000) Neural network analysis of time series: applications to climatic data. In: *Southern Hemisphere paleo- and neoclimates* (Smolka, P., and Volkheimer, W., ed.). New York: Springer, 7-16.
- Campbell, I., Campbell, C., Apps, M., Rutter, N., Bush, A. (1998) Late Holocene ~1500 yr climate periodicities and the implications. *Geology*, **26**, 471-473.
- Charles, C.D., Rind, D., Jouzel, J., Koster, R.D., and Fairbanks, R.G. (1994) Glacial-interglacial changes in moisture sources for Greenland: influences on the ice core record of climate. *Science*, **263**, 508-511.
- Cess, R.D., Potter, G.L., Blanchet, J.P., Boer, G.J., Ghan, S.J., Keihl, J.T., Le Treut, H., Li, Z.-X., Liang, X.-Z., Mitchell, J.F.B., Morcrette, J.-J., Randall, D.A., Riches, R.R., Roeckner, E., Schlese, U., Slingo, A., Taylor, K.E., Washington, W.M., Wetherald, R.T., Yagai, I. (1989) Interpretation of cloud-climate feedback as produced by 14 atmospheric general circulation models. *Science*, **245**, 513-516.
- Clarke, B. (1980) Stability of complex reaction networks. *Advances in Chemical Physics*, **43**, 1-216.
- Clarke, B. (1992) General method for simplifying chemical networks while preserving overall stoichiometry in reduced mechanisms. *Journal of Chemical Physics*, **97**, 4066-4071.
- Clarke, B., and Jiang, W. (1993) Method for deriving Hopf and saddle-node bifurcation hypersurfaces and application to a model of the Belousov-Zhabotinskii system. *Journal of Chemical Physics*, **99**, 4464-4478.

- Courard-Hauri, D (2003) Multi-level optimization as a new technique for automatic model generation. *In preparation*.
- Crutchfield, J.P., McNamara, B.S. (1987) Equations of motion from a data series. *Complex Systems*, **1**, 417-452.
- Dansgaard, W., Johnsen, S.J., Clausen, H.B., Dahl-Jensen, D., Gundestrup, N.S., Hammer, C.U., Hvidberg, C.S., Steffensen, J.P., Sveinbjornsdottir, A.E., Jouzel, J., and Bond, G. (1993) Evidence for general instability of past climate from a 250-kyr ice-core record. *Nature*, **364**, 218-220.
- de Verdiere, A.C., Huck, T. (2000) A 2-degree of freedom dynamical system for interdecadal oscillations of the ocean-atmosphere. *J. Climate*, **13**, 2801-2817.
- Dickens, G.R., Castillo, M.M., Walker, J.C.G. (1995) Blast of gas in the latest Paleocene: simulating first-order effects of massive dissociation of oceanic methane hydrate. *Geology*, **25**, 259-262.
- Fraser, A.M., Swinney, H.L. (1986) Independent coordinates for strange attractors from mutual information. *Physical Review A*, **33**, 1134-1140.
- Frontval, T., Janse, E., Haflidason, H., Sejrup, H.P. (1998) Variability in surface and deep water conditions in the nordic seas during the last interglacial period. *Quat. Sci. Rev.*, **17**, 963-985.
- Ganopolski, A., Rahmstorf, S., Petoukhov, V., Claussen, M. (1998) Simulation of modern and glacial climates with a coupled global model of intermediate complexity. *Nature*, **391**, 351-356.
- Gilman, A., Ross, J (1995) Genetic-algorithm selection of a regulatory structure that directs flux in a simple metabolic model. *Biophysical Journal*, **69**, 1321-1333.
- Grabherr, G., Gottfreid, M., Pauli, H. (1994) Climate effects on mountain plants. *Nature*, **369**, 448.
- Grieger, B., Latif, M. (1994) Reconstruction of the El Nino attractor with neural networks. *Climate Dynamics*, **10**, 267-276.
- Grootes, P.M., Stuiver, M., White, J.W.C., Johnsen, S., Jouzel, J. (1993) Comparison of oxygen isotope records from the GISP2 and GRIP Greenland ice cores. *Nature*, **366**, 552-554.
- Grosiman, P.Ya., Karl, T.R., Wright, R.W. (1994) Observed impact of snow cover on the heat balance and the rise of continental spring temperatures. *Science*, **263**, 198-200.
- Hammer, C.U. (1977) Past volcanism revealed by Greenland ice sheet impurities. *Nature*, **270**, 482-486.
- Hammer, C.U., Clausen, H.B., Langway, Jr., C.C. (1997) 50,000 years of recorded global volcanism and its climatic impact. *Nature*, **288**, 230-255.
- Hansen, N.F., Ross, J. (1998) Relative stability of multiple stationary states related to fluctuations. *J. Phys. Chem.*, **102**, 7123-7126.
- Hare, F.K. (1979) Climatic variation and variability: empirical evidence from meteorological and other sources. In: *Proc. World Climate Conference*. Publication No. 537, World Meteorological Organization, Geneva, 51-87.
- Hargreaves, J.C., and Annan, J.D. (2002) Assimilation of paleo-data in a simple Earth System model. *Climate Dynamics*, **19**, 371-381.
- Houghton, J. (1997) *Global Warming: the Complete Briefing*, 2nd ed (Cambridge University Press: Cambridge, UK) 251 pp.

- Hsieh, W.W. (2001) Nonlinear canonical correlation analysis of the tropical pacific climate variability using a neural-network approach. *J. Climate*, **14**, 2528-2539.
- Imbrie, J., and Imbrie, K.P. (1979) *Ice ages: solving the mystery*. London: Macmillan.
- Imbrie, J., Mix, A.C., Martinson, D.G. (1993) Milankovic theory viewed from Devil's Hole. *Nature*, **363**, 531-533.
- IPCC (1998) *IPCC Workshop on rapid non-linear climate change*. IPCC Workshop Report, Noordwijkerhout, The Netherlands.
- IPCC (2001a) *Climate Change 2001: The Scientific Basis*. Cambridge: Cambridge University Press, 944 pp.
- IPCC (2001b) *Climate Change 2001: Impacts, Adaptation, and Vulnerability*. Cambridge: Cambridge University Press, 1000 pp.
- Jayne, S.R., Marotzke, J. (1999) A destabilizing thermohaline circulation-atmosphere-sea ice feedback. *J. Climate*, **12**, 642-651.
- Jirsa, V.K., Haken, F.H. (1995) Reconstruction of the spatio-temporal dynamics of a human magnetoencephalogram. *Physica D*, **89**, 100-122.
- Jones, P.D., Osborn, T.J., Briffa, K.R. (2001) The evolution of climate over the last millennium. *Science*, **292**, 662-667.
- Jouzel, J. (1994) Ice cores north and south. *Nature*, **372**, 612-613.
- Karl, T.R., Johes, P.D., Knight, R.W., Kukla, G., Plummer, N., Razuvayev, V., Gallo, K.P., Linseay, J., Charlson, R.S., Peterson, T.C. (1993) Asymmetric trends of daily maximum and minimum temperature. *Bull. Am. Met. Soc.*, **74**, 1007-1023.
- Jouzel, J., Barkov, J.I., Barnola, J.M., Bender, M., Chappellaz, J., Genthon, C., Kotlyakov, V.M., Lipenkov, V., Lorius, C., Petit, J.R., Raynaud, D., Raibeck, G., Ritz, C., Sowers, T., Stievenard, M., Yiou, F., and Yiou, P. (1993) Extending the Vostok ice-core record of paleoclimate to the penultimate glacial period. *Nature*, **364**, 407-412.
- Kwasniok, F. (1996) The reduction of complex dynamical systems using principal interaction patterns. *Physica D*, **92**, 28-60.
- Kwasniok, F. (1997a) Low-dimensional models of complex systems using principal interaction patterns. *Nonlinear Analysis, theory, Methods, & Applications*, **30**, 489-494.
- Kwasniok, F. (1997b) Optimal Galerkin approximations of partial differential equations using principal interaction patterns. *Physical Review E*, **55**, 5365-5375.
- Lorenz, E.N. (1990) Can chaos and intransitivity lead to interannual variability? *Tellus*, **42A**, 378-389.
- Lowell, T.V., Heusser, C.J., Andersen, B.G., Moreno, P.I., Hauser, A., Heusser, L.E., Schluchter, C., Marchant, D.R., Denton, G.H. (1995) Interhemispheric correlation of late Pleistocene glacial events. *Science*, **269**, 1541-1549.
- Mahootian, F., Hauri, D., and Earley, J.E. (1992) New region of oscillations in the chlorite-bromate-iodide system of internally coupled chemical oscillators. *Journal of Physical Chemistry*, **96**, 1014-1015.
- Marotzke, J. and Willebrand, J. (1991) Multiple equilibria of the global thermohaline circulation. *Journal of Physical Oceanography*, **21**, 1713-1728.
- Marotzke, J. (2000) Abrupt climate change and thermohaline circulation: Mechanisms and predictability, *Proceedings of the National Academy of Sciences*, **97**, 1347-1350.

- Martinson, D.G., Pisias, N.G., Hays, J.D., Imbrie, J., Moore, T.C., and Shackleton, N.J. (1987) Age dating and the orbital theory of the ice ages: development of a high resolution 0 to 300,000-year chronostratigraphy. *Quaternary Res.*, **27**, 1-29.
- Milankovic, M.M. (1941) *Cannon of insolation and the ice-age problem*. Beograd: Koniglich Serbische Akademie. [English translation by the Israel Program for Scientific Translations, published for the US Department of Commerce, and the National Science Foundation, Washington, DC (1969)].
- Moeller, F. (1963) On the influence of changes in the CO₂ concentration in air on the radiation balance of the Earth's surface and on the climate. *J. Geophys. Res.*, **68**, 3877-3886.
- Mongeau, M., Karsenty, H., Rouze, V., Hiriart-Urruty, J.-B. (2001) Comparison of public-domain software for black box global optimization. *Optimization Methods & Software*, accepted.
- NAS (2001) *Abrupt Climate Change: Inevitable Surprises* Prepublication Copy (National Academy Press: Washington, DC), 193 pp.
- National Research Council (1999) *Global Environmental Change: Research Pathways for the Next Decade* (National Academy Press: Washington, DC), 595 pp.
- Nicolis, G., and Prigogine, I. (1989) *Exploring Complexity* (W.H. Freeman & Co.: New York) 313 pp.
- Oppenheimer, M. (1998) Global warming and the stability of the West Antarctic Ice Sheet. *Nature*, **393**, 325-332.
- Palmer, T.N. (1993) A nonlinear dynamical perspective on climate change. *Weather*, **48**, 314-325.
- Palmer, A.S., van Ommen, T.D., Curran, M.A.J., Morgan, V., Souney, J.M., Mayewski, P.A. (2001) High-precision dating of volcanic events (A.D. 1301-1995) using ice cores from Law Dome, Antarctica. *J. Geophys. Res.*, **106**, 28,089-28,096.
- Park, Y.-G. (1999) The stability of thermohaline circulation in a two-box model. *J. Phys. Geog.*, **29**, 3101-3110.
- Porter, S.C., and An, Z. (1995). Correlation between climate events in the North Atlantic and China during the last glaciation. *Nature*, **375**, 305-308.
- Raymo, M.E., Ganley, K., Carter, S., Oppo, D.W., McManus, J. (1998) Millennial-scale climate instability during the early Pleistocene epoch. *Nature*, **392**, 699-702.
- Ross, J., Vlad M.O. (1999) Nonlinear kinetics and new approaches to complex reaction mechanisms. *Annual Review of Physical Chemistry*, **50**, 51-78.
- Roy, K., Valentine, J.W., Jablonski, D., Kidwell, S.M. (1996) Scales of climatic variability and time averaging in Pleistocene biotas: implications for ecology and evolution. *Trends in Ecology and Evolution*, **11**, 458-463.
- Santer, B.D., Wigley, T.M.L., Doutriaux, C., Boyle, J.S., Hansen, J.E., Jones, P.D., Meehl, G.A., Roeckner, E., Sengupta, S., Taylor, K.E. (2001) Accounting for the effects of volcanoes and ENSO in comparisons of modeled and observed temperature trends. *J. Geophys Res.* **106**, 28,033-28,060.
- Schmittner, A., Stocker, T. (1999) The stability of the thermohaline circulation in global warming experiments. *J. Climate*, **12**, 1117-1113.
- Schneider, S.H. (1994) Detecting climatic change signals: are there any "fingerprints"? *Science*, **263**, 341-347.
- Semenov, M.A., Porter, J.R. (1995) Non-linearity in climate change impact assessments. *J. Biogeog.*, **22**, 597-600.

- Stouffer, R.J., Manabe, S. (1999) Response of a coupled ocean-atmosphere model to increasing atmospheric carbon dioxide: sensitivity to the rate of increase. *J. Climate*, **12**, 2224-2237.
- Taylor, K.C., Hammer, C.U., Alley, R.B., Clausen, H.B., Dahl-Jensen, D., Gow, A.J., Gunderstrup, N.S., Kipfstuhl, J., Moore, J.C., Waddington, E.D. (1993) Electrical conductivity measurements from the GISP and GRIP Greenland ice cores. *Nature*, **366**, 549-552.
- Trenberth, K.E. (1997) The use and abuse of climate models. *Nature*, **386**, 131-133.
- Tsuchiya, M., Ross, J. (2001) Application of genetic algorithms to chemical kinetics: determination of reaction mechanism and rate coefficients for a complex reaction network. *J. Phys. Chem.*, **105**, 4052-4058.
- Tziperman, E. (2000) Proximity of the present-day Thermohaline Circulation to an instability threshold. *J. Phys. Geog.*, **30**, 90-104.
- Veeh, H.H. and Chappell, J.M.A. (1970) Astronomical theory of climatic change: support from New Guinea. *Science*, **167**, 862-865.
- Wang, X, Stone, P.H., Marotzke, J. (1999a) Global Thermohaline Circulation. Part I: sensitivity to atmospheric moisture transport. *J. Climate*, **12**, 71-82.
- Wang, X, Stone, P.H., Marotzke, J. (1999b) Global Thermohaline Circulation. Part II: sensitivity to interactive atmospheric transports. *J. Climate*, **12**, 83-91.
- Washington, W.M. (1992) Climate-model responses to increased CO₂ and other greenhouse gasses. In *Climate System Modeling*, Kevin E. Trenberth, ed. (Cambridge University Press: Cambridge, UK) 643-668.
- Wolff, A., Ross, J. (1992) Slowing down near the critical point in optically bistable ZnSe. *J. Chem. Phys.*, **96**, 1602-1606.
- Woodwell, G., Mackenzie, F., Houghton, R., Apps, M., Gorham, E., Davidson, E. (1998) Biotic feedbacks in the warming of the earth. *Climate Change*, **38**, 495-518.
- Zachos, J., Pagani, M., Sloan, L., Thomas, E., Billups, K. (2001) Trends, rhythms, and aberrations in global climate 65 Ma to present. *Science*, **292**, 686-693.
- Zhao, M., Beveridge, N.A.S., Shackleton, N.J., Sarnthein, M., Eglinton, G. (1995) Molecular stratigraphy of cores off northwest Africa: sea surface temperature history over the last 80 ka. *Paleoceanography*, **10**, 661-675.
- Zielinski, G., Mayewski, P.A., Meeker, L.D., Whitlow, S., Twickler, M.S. (1996) A 110,000-yr record of explosive volcanism from the GISP2 (Greenland) ice core. *Quaternary Research*, **45**, 109-118.