

Association of parameter, software, and hardware variation with large-scale behavior across 57,000 climate models

Christopher G. Knight^{*}, Sylvia H. E. Knight^{†‡}, Neil Massey^{†§}, Tolu Aina[†], Carl Christensen[†], Dave J. Frame[†], Jamie A. Kettleborough^{¶||}, Andrew Martin[§], Stephen Pascoe^{||}, Ben Sanderson[†], David A. Stainforth[†], and Myles R. Allen[†]

^{*}Manchester Interdisciplinary Biocentre, University of Manchester, 131 Princess Street, Manchester M1 7DN, United Kingdom; [†]Atmospheric, Oceanic, and Planetary Physics, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, United Kingdom; [§]Oxford University Computing Laboratory, Wolfson Building, Parks Road, Oxford OX1 3QD, United Kingdom; [¶]The Met Office, FitzRoy Road, Exeter, Devon EX1 3PB, United Kingdom; and ^{||}Science and Technology Facilities Council, Rutherford Appleton Laboratory, Didcot, Oxon OX11 0QX, United Kingdom

Edited by Stephen H. Schneider, Stanford University, Stanford, CA, and approved May 21, 2007 (received for review September 15, 2006)

In complex spatial models, as used to predict the climate response to greenhouse gas emissions, parameter variation within plausible bounds has major effects on model behavior of interest. Here, we present an unprecedentedly large ensemble of >57,000 climate model runs in which 10 parameters, initial conditions, hardware, and software used to run the model all have been varied. We relate information about the model runs to large-scale model behavior (equilibrium sensitivity of global mean temperature to a doubling of carbon dioxide). We demonstrate that effects of parameter, hardware, and software variation are detectable, complex, and interacting. However, we find most of the effects of parameter variation are caused by a small subset of parameters. Notably, the entrainment coefficient in clouds is associated with 30% of the variation seen in climate sensitivity, although both low and high values can give high climate sensitivity. We demonstrate that the effect of hardware and software is small relative to the effect of parameter variation and, over the wide range of systems tested, may be treated as equivalent to that caused by changes in initial conditions. We discuss the significance of these results in relation to the design and interpretation of climate modeling experiments and large-scale modeling more generally.

classification and regression trees | climate change | distributed computing | general circulation models | sensitivity analysis

Simulation with complex mechanistic spatial models is central to science from the level of molecules (1) via biological systems (2, 3) to global climate (4). The objective typically is a mechanistically based prediction of system-level behavior. However, both through incomplete knowledge of the system simulated and the approximations required to make such models tractable, the “true” or “optimal” values of some model parameters necessarily will be uncertain. A limiting factor in such simulations is the availability of computational resources. Thus, combinations of plausible parameter values rarely are tested, leaving the dependence of conclusions on the particular parameters chosen unknown.

Observations of the modeled system are vital for model verification and analysis, e.g., turning model output into probabilistic predictions of real-world system behavior (5–7). However, typically, few observations are available relative to the complexity of the model. There also may be little true replicate data available. For instance, there can be only one observational time series for global climate. Thus, if the same observations are used to fit parameter values, there is a severe risk of overfitting, gaining limited verisimilitude at the cost of the mechanistic insight and predictive ability for which the model originally was designed.

To avoid fitting problems, parameter estimates must be refined directly. In some biological systems, direct and simultaneous measurement of large numbers of system parameters (e.g., protein binding or catalytic constants) soon may be possible. In other systems such as climate models, this approach is not an option.

Thus, it is vital to focus efforts in parameter refinement. Deciding how to do this refinement presents challenges: (i) to determine whether there is dependence of model behavior of interest on parameter variation within plausible bounds, (ii) to determine whether dependence applies to all uncertain parameters or only a more tractable subset, and (iii) to quantify the nature of parameter dependence. Because parameters interact in complex and unknown ways, meeting these challenges entails considering a very large parameter space.

In this article we address all three challenges for a state-of-the-art general circulation model (GCM) of global climate. Without fitting to observations, we analyze an ensemble of over 57,000 model runs in which 10 parameters and initial conditions were systematically varied. Although large studies traditionally have been carried out on supercomputers, it currently only is possible to perform this many simulations via a distributed computing approach. Before this project, the largest published comparable ensemble was of 53 model runs (8, 9). We have achieved such a large data set via the *climateprediction.net* project (www.climateprediction.net) by using idle processing capacity on personal computers volunteered by members of the public. This approach entails variation in hardware and software used to run the model, and serious concerns have been raised that results might depend only on this variation. Processes of rounding that vary between systems and lead to small differences in simple calculations are a well known issue highlighted in projects working with a similar distributed computing architecture (10). Given the enormous numbers of such calculations in a GCM, such minuscule effects of hardware/software may multiply to influence overall model behavior. Because the GCM is highly nonlinear, even small quantitative differences in model behavior of this sort in principle could produce qualitatively different results. We address this issue directly, treating hardware/software variation equivalently to parameter variation.

Considering plausible values of six parameters and a smaller number of model runs, Stainforth *et al.* (4) demonstrated that, although accepted predictions of 2–5 K global warming in response to a doubling in carbon dioxide (11) indeed were representative of model results, equally plausible parameter values gave global

Author contributions: C.G.K., S.H.E.K., N.M., T.A., C.C., D.J.F., J.A.K., A.M., S.P., D.A.S., and M.R.A. designed research; C.G.K. and N.M. performed research; C.G.K. contributed new reagents/analytic tools; C.G.K., N.M., and B.S. analyzed data; and C.G.K. wrote the paper.

The authors declare no conflict of interest.

This article is a PNAS Direct Submission.

Abbreviations: CS, climate sensitivity to a doubling of carbon dioxide; GCM, general circulation model; CV, coefficient of variation (standard deviation as a percentage of the mean).

[†]To whom correspondence should be addressed. E-mail: sknight@atm.ox.ac.uk.

This article contains supporting information online at www.pnas.org/cgi/content/full/0608144104/DC1.

© 2007 by The National Academy of Sciences of the USA

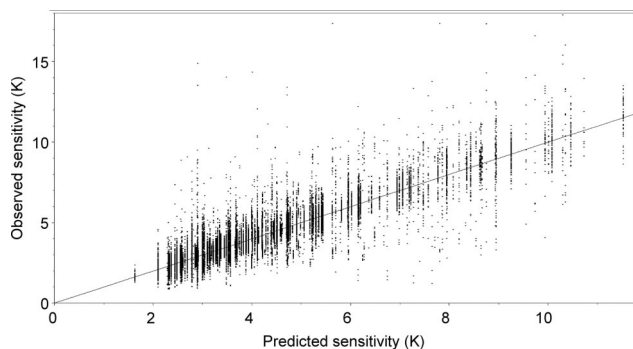


Fig. 3. Observed climate sensitivities for all 43,710 model runs where it was calculable plotted against those predicted by the optimal regression tree on the basis of their parameter, hardware, and software values (Fig. 2 and SI Table 3).

values behaving in unexpected ways or particular hardware/software giving spurious results. We used a similar tree-based approach fitting success or failure to the same explanatory variables as before (Table 1).

Unsurprisingly, the proportion of variation in fitting failure that can be explained is much less than the proportion of variation explicable for CS itself. Nonetheless, 33% of total variation in the data can be explained by an optimal tree (SI Fig. 8 and SI Table 4). Although RAM size and the processor used to run the model do

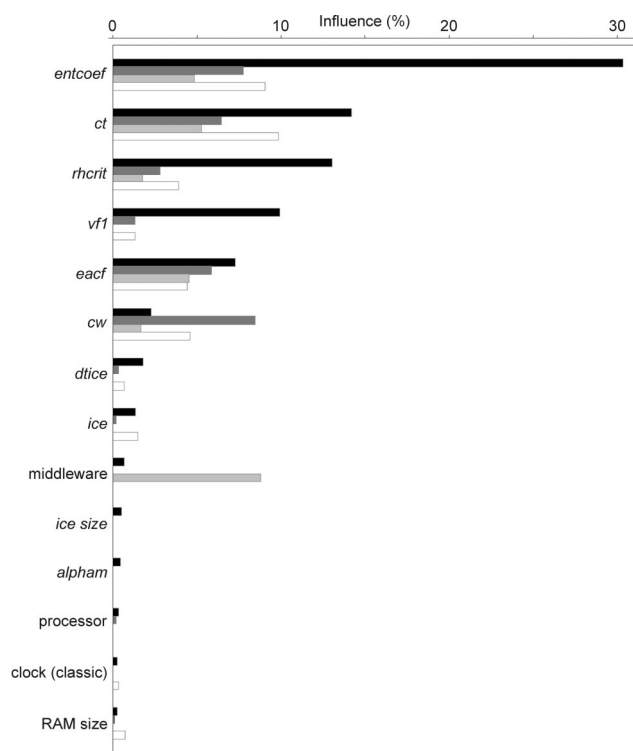


Fig. 4. Influence of variables in the trees. Each bar measures the percentage of the total variation explained by all splits based on that variable in one of the optimal trees. For each variable, there are four bars: 1, black, tree of the magnitude of CS (Fig. 2); 2, dark gray, tree of failure to fit an adequate CS (SI Fig. 8); 3, light gray, tree of variation attributable to hardware/software among otherwise identical runs (Fig. 6); and 4, white, tree of variation among runs with identical parameters but different initial conditions (SI Fig. 10). Residual variation (unexplained by any of the parameters) is not shown but, estimated by cross-validation, is 18%, 67%, 73%, and 66%, respectively. Only parameters with at least 0.1% influence in at least one tree are shown.

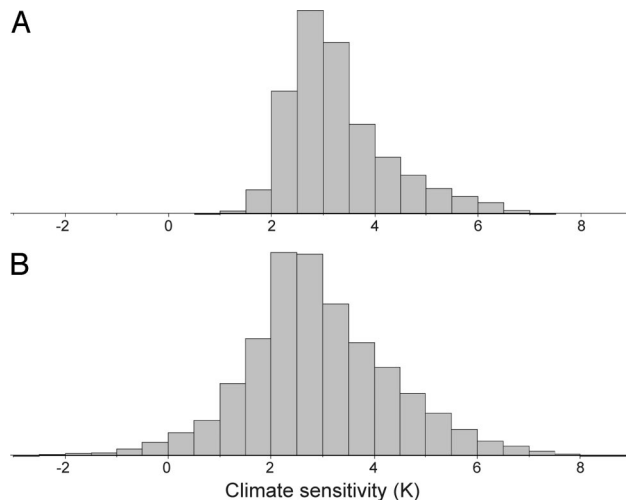


Fig. 5. Frequency distributions for CS as calculated by taking the difference of average global mean temperature for the latter half of the control and doubled CO_2 phases. (A) For the 43,677 model runs where a fitted CS as used for all other analyses was obtained. The relationship of these sensitivities to the fitted sensitivities is shown in SI Fig. 9. (B) For the 13,313 model runs where an adequate fitted sensitivity could not be obtained (26 outliers in B fall outside the range graphed).

have an effect on failure to produce a fit, the most important factors, as for CS itself, are model parameters (Fig. 4).

Because there is a systematic element that depends on the parameter set in our failure to fit a CS, there also may be systematic loss of particular values of sensitivity. To test for systematic loss of particular CS values, we considered an alternative estimate of CS, the average temperature difference between control and doubled CO_2 phases for the last 8 of the 15 years considered. This measure seriously underestimates high CS, as compared with nonlinear fitting, but is a reasonable approximation at low values (SI Fig. 9). We compared the frequency distribution of this measure for those runs where we obtained a CS by nonlinear fitting with those where we did not (Fig. 5). The distributions are very similar in shape for sensitivities of ≈ 2.5 K and above with only a slight overrepresentation of high sensitivities in those not fitted. However, there is a tail of sensitivities ≤ 1 K that is missed almost entirely by the fitting procedure. Overall, 985 runs (1.7%) show such a low sensitivity by the difference measure, but only 6 of these (0.6%) have fitted CS (compare with the fact that 78% have fits in the rest of the data set). One example of a time series where no curve could be fit, but showing a 1-K sensitivity by the alternative measure, is shown in Fig. 1. These “missing” low-sensitivity runs show a larger than expected proportion (87% rather than 11%, $P < 10^{-15}$, χ^2 test) of strong CO_2 phase cooling in the Eastern tropical Pacific characteristic of a known artifactual effect of mixed layer oceans (4). These missing runs also drift more than expected in the control phase (85% rather than 46%, $P < 10^{-15}$, χ^2 test), which also may indicate unphysical behavior. Almost all low-sensitivity runs that are missed by the fitting procedure (93.5% of them) have at least one of these issues, either drift or Eastern tropical Pacific cooling.

Role of Hardware and Software. A subset of the runs analyzed above contained identical parameters and initial conditions. The number of combinations of parameters and initial conditions that had at least two and up to six runs giving a CS was 4,762. Although many such “duplicate” sets (1,062 of them) gave identical results, most did not. For each parameter combination, we calculated the CV of the CS. We then fit a regression tree for this quantity in a similar way to earlier trees. An optimal tree (Fig. 6 and SI Table 5) explained

Simulation output is inevitably detailed and highly multivariate. To make it useful requires simplification and assumptions to derive humanly interpretable measures of interest. We have calculated CS as a quantity of interest by using a nonlinear fitting approach. This fitting assumes that there is an equilibrium difference in global mean temperature to be fit, and it is approached via an arbitrarily good approximation to an assumed form of curve. For the large majority of runs these assumptions hold. However, we find those runs where they do not hold are a nonrandom subset with respect to CS. Specifically, a small tail of runs with low sensitivity cannot be assigned a CS (Fig. 5). In these cases, e.g., as shown in Fig. 1 where temperatures in the control and doubled carbon dioxide phases diverge very little, the signal-to-noise ratio is high, making adequate fits less likely (an effect that might be ameliorated by a longer run). If there is no divergence at all or a linear divergence, one of the two parameters in the fit is undefined, so there will be no fit (an effect that would not be altered by longer runs). Here, by using more than one estimate of CS, we have demonstrated the effects of our assumptions. The “lost” low-sensitivity runs are not likely to affect estimates of real-world CS, both because they tend to agree poorly with observations (6, 7) and because we find most display known nonphysical effects. However, these findings highlight the care needed in parameter scanning modeling studies such as this to ensure important results from plausible parameter sets are not misinterpreted or excluded simply through their failure to fit prior assumptions.

Despite increases in supercomputing power, distributed and grid approaches are increasingly necessary to tackle ever more complex modeling studies. One result is a variety of hardware and even software being used to run the model. Such differences have systematic effects on calculations, a recognized issue (10) sometimes tackled as a subset of sabotage, that also poses risks here (14). Here, we have quantified these effects on a model result of interest relative to the effects of parameter variation. Sometimes the CS predicted by the model did vary with whether the model was run on an Intel Pentium 4 or an AMD Athlon processor. However, there is no clear association, for example, that Intel chips give higher CS. Similarly, RAM size has an effect, but different model versions respond differently, in four of the six cases of splits based on RAM size, the smaller RAM size gives the higher sensitivity, but in two cases the reverse is true. It may be that RAM size is acting as a surrogate for other differing aspects of hardware. We have not covered all possible hardware and software variants, notably we have not used a 64-bit architecture. However, in the large variety of permutations that are covered in this data set, systematic hardware/software effects are reassuringly small relative to the effects of model parameters. Of the seven splits based on particular processors, at most 564 runs are affected (1.3% of the total), and together all 7 splits only account for 0.3% of the variation, whereas even the fifth most explanatory model parameter (*eacf*) gives 28 splits affecting up to $\approx 14,000$ runs (33% of the total) each and accounting for >20 times as much variation as the processors (SI Table 4).

Important effects of hardware/software, however, may be less systematic. We identified a single software effect as important here. Runs with identical parameters and starting conditions average a CV in CS of only 1.6% when run exclusively under the original (classic) *climateprediction.net* client middleware. However, when run under a mixture of middlewares, or the more widely used BOINC client middleware (<http://boinc.berkeley.edu>), that average can rise to 40% depending on parameter values. The causes of this difference are unclear. We speculate that it may be caused by different “controller” code that appeared more sensitive to small computational errors in the classic middleware. This sensitivity resulted in more crashes and thus failure to submit results for the classic middleware. BOINC was more likely to let the model run to completion despite computational problems. There also was a change of compiler for the underlying code between the two middlewares that could have had an effect. Whatever the cause, it

is clear client middleware is much more important than other hardware/software and, unlike other hardware/software, can be controlled by the experimenter.

The computing power of distributed systems offers an approach to explore large tracts of plausible parameter space for a complex model. Alternative and potentially complementary approaches for climate models have focused on speeding up models by simplifications (reduced temporal or spatial resolution, dimensionality, physics, or dynamics) relative to state-of-the-art GCMs such as that used here. For instance, FAMOUS is based on a similar model (HadCM3) but with reduced temporal and spatial resolution so it runs ≈ 10 times quicker. This speed made it possible to tune parameter values by using a conventional supercomputer (13). However, the challenge of uncertain or undefined parameters remains great. Even in this study, we only have been able to investigate 10 model parameters. Expert choice decided the parameters to investigate and the range of levels they should take. With models as complex as these, such reliance on human skill may miss parameters that affect the results through nonobvious mechanisms. Even for parameters we considered, the number of levels used may be insufficient to define adequately their complex influences (e.g., the variety of high and low climate sensitivities associated with particular levels of *entcoef* discussed above). Both of these observations suggest that investigating more parameters in more detail would be desirable and perhaps necessary to tune the model adequately. However, the vast numbers of model runs involved in comprehensively scanning combinations of parameters would exceed the resources of any distributed computing setup or speeded up model on a conventional system. To add to the challenge, recent work suggests it is unreasonable to hope for a generally optimized climate model, the model parameters need tuning to the specific question being asked (5). Ultimately such questions undoubtedly extend beyond the timescale of decades used here to computationally extensive questions involving paleoclimate. It also will be important to compare different models. Findings for one model may not be transferable to another, or even to different versions of the same model, for example, with altered resolution. If these modeling challenges are to be met computationally, it will require not only improvements in model speed and access to computing power but also improved methods of exploring the complex parameter space. The latter requires a carefully designed experimental (15) and computing (16) strategy. It also may entail adaptive techniques, adjusting the model versions run in response to results received, which poses particular challenges in a distributed computing context where it is uncertain when or whether any particular run will be returned. Adaptive techniques include evolutionary computation and refined combinations of approaches, including recursive splitting of parameter space as used in this study (17). Similar methods have been applied successfully in many fields, including identification of optimal model versions given uncertain parameters in computationally simpler, but nonetheless nonlinear and complex, economic climate models (18).

In conclusion, by considering an unprecedentedly large ensemble of climate model runs, we have a series of findings relevant not only to the implementation, interpretation, and improvement of models predicting climate change but also to studies using large and complex models more generally. Our findings reinforce the fact that variation of parameters within plausible bounds may have a substantial systematic effect on large-scale model behavior. However, we find only a small subset of parameters to be associated with most of the variation in a specific behavior (CS). Those associations are complex and interacting but the small number of parameters involved provides a focus for future model refinement. In addition, we have identified how the very process of making model results interpretable affects the findings. The effect of the precise hardware/software implementation of the model typically was small and indistinguishable from perturbations introduced by different initial conditions.

Methods

Model and Distributed Computing. The *climateprediction.net* project is the first multithousand member ensemble of climate simulations using a state-of-the-art GCM. Members of the public worldwide download an executable version of the Met Office Unified Model. This model comprises the HadAM3 atmosphere (19) at standard resolution (3.75° longitude by 2.5° latitude, 19 vertical levels) with increased numerical stability, coupled to a mixed-layer ocean with heat transport prescribed by using a heat-flux convergence field varying with position and season but not with year.

Participants are allocated a particular set of parameter perturbations and initial conditions enabling them to run one 45-year simulation. For each simulation, the heat-flux convergence field is calculated in the first 15 years simulated, where sea surface temperatures (SSTs) are fixed. In the subsequent 30 years simulated, the SSTs vary according to the atmosphere-ocean heat flux. In the middle 15 years, the control phase, CO₂ is held constant at preindustrial levels (282 ppm). It is doubled for the last 15-year period.

Data Set. The first 57,067 simulations returned to *climateprediction.net* servers were considered. Each simulation was classified according to parameter set, initial conditions, hardware, and software used to run the model. These 18 explanatory variables are listed in Table 1 and SI Table 2.

Analysis. Simulated CS is taken as the predicted equilibrium difference between global mean temperature in the doubled CO₂ and control phases. This quantity was calculated via a self-starting nonlinear regression fit using a Gauss–Newton algorithm, to the difference in the annual global mean temperatures between the doubled CO₂ and control phases. The curve fit had the form $\Delta T = S(1 - \exp(-Ft/SC))$ derived from an energy balance model where ΔT is difference in global mean temperature, S is CS, t is time, C is the effective heat capacity of the model, and F is the radiative forcing caused by a doubling of CO₂, taken to be 3.74 W·m⁻². Fits that failed to converge after many iterations (1,000), gave a residual SE >0.2 K, or failed to reach half their predicted equilibrium temperature in the period of the fit were rejected. Runs with a full set of data were deemed to have failed only on the basis of our failure to produce an adequate fit by these criteria, not on the bases of either temperature drift in the control phase or the relationship to observations, constraints that have been used in previous studies using similar data (4, 5).

For analyses of CS variation (Fig. 6 and SI Fig. 10), we created explanatory variables capturing variation in the hardware and software for each set of duplicate runs: for contin-

uous variables (RAM size and clock measures) we used CV; for discrete variables (processor, operating system, and middleware) we created a discrete variable detailing whether the duplicate runs had a particular level or a mix of levels. We used these quantities as explanatory variables in these trees alongside the parameters used (see SI Table 2).

To determine the association of explanatory variables with model response, we used classification and regression trees (20). These techniques recursively split data to minimize variation (measured as deviance for continuous variables and entropy for categorical variables) for the two resulting subsets of data. Splitting, in principle, can continue as long as there are multiple observations to be split and different levels of explanatory variables within subsets. However, although the fit of the resulting tree to the data used to create it will only improve by further splitting, the ability of the tree to predict data not used to create it will not. We used a standard approach of creating large trees (considering splits down to those reducing the lack of fit by a factor 1×10^{-4}) and then pruning them to an optimal size. This size was determined by 100-fold cross-validation, i.e., splitting the data randomly into 100 equally sized subsets, with the 99th as a training set and the 100th as a test set. From the test set results, we calculated the error in prediction (cross-validation error) averaged over the 100 possible training and test sets. The optimal tree was chosen as the smallest where the cross-validation error lay within 1 SE of the minimum cross-validation error.

To identify unphysical cooling in the tropical East Pacific (4), surface temperature differences between the final year of the doubled CO₂ and calibration phases were taken for the 78.75 W, 2.5 N box and corrected for overall change by subtracting the figure for 48.75 W, 2.5 N in 13,983 BOINC runs. This quantity is distributed with the principal mode at 0 K and a secondary mode around -27.5 K; values less than -15 K was deemed to show strong evidence for this cooling.

Software. Statistical analyses used R 2.0.1 (21) and JMPIN 5.1 (22). Within R, classification and regression trees were fitted by using the rpart v.3.1–23 package.

We thank all *climateprediction.net* participants, Tessella Support Services plc, Research Systems Inc., Numerical Algorithms Group Ltd., the CMIP II modeling groups, Joshua Knowles, Ed Tredger, and Philippa Knight. This work was supported by the Natural Environment Research Council's Coupled Ocean Atmosphere Processes and European Climate, e-Science, and fellowship programs; Department of Trade and Industry; and Department for Environment, Food and Rural Affairs Grant PECD/7/12/37.

- Karplus M, McCammon JA (2002) *Nat Struct Biol* 9:646–652.
- Noble D (2002) *Science* 295:1678–1682.
- Snoep JL (2005) *Curr Opin Biotechnol* 16:336–343.
- Stainforth DA, Aina T, Christensen C, Collins M, Faull N, Frame DJ, Kettleborough JA, Knight S, Martin A, Murphy JM, et al. (2005) *Nature* 433:403–406.
- Frame DJ, Booth BBB, Kettleborough JA, Stainforth DA, Gregory JM, Collins M, Allen MR (2005) *Geophys Res Lett* 32:L09702.
- Knutti R, Meehl GA, Allen MR, Stainforth DA (2006) *J Climate* 19:4224–4233.
- Piani C, Frame DJ, Stainforth DA, Allen MR (2005) *Geophys Res Lett* 32:L23825.
- Murphy JM, Sexton DM, Barnett DN, Jones GS, Webb MJ, Collins M, Stainforth DA (2004) *Nature* 430:768–772.
- Barnett DN, Brown SJ, Murphy JM, Sexton DMH, Webb MJ (2006) *Clim Dyn* 26:489–511.
- He Y, Ding CHQ (2001) *J Supercomput* 18:259–277.
- Houghton JT, ed (2001) *Contribution of Working Group 1 to the Third Assessment Report of the Intergovernmental Panel on Climate Change* (Cambridge Univ Press, Cambridge, UK).
- Anderson DP (2004) in *Fifth IEEE/ACM International Workshop on Grid Computing (GRID '04)* (IEEE, Pittsburgh), pp 4–10.
- Jones C, Gregory J, Thorpe R, Cox P, Murphy J, Sexton D, Valdes P (2005) *Clim Dyn* 25:189–204.
- Germain-Renaud C, Playez N (2003) in *Proceedings of the 17th Annual International Conference on Supercomputing* (ACM Press, New York), pp 226–233.
- Sacks J, Welch WJ, Mitchell TJ, Wynn HP (1989) *Statistical Sci* 4:409–435.
- Casanova H, Zagorodnov D, Berman F, Legrand A (2000) in *Proceedings of the Ninth Heterogeneous Computing Workshop* (IEEE Computer Society, Washington, DC), pp 349–363.
- Gramacy RB, Lee HKH, Macready WG (2004) in *Proceedings of the 21st International Conference on Machine Learning* (ACM Press, New York), Vol 69, pp 45–52.
- Moles CG, Banga JR, Keller K (2004) *Appl Soft Comput* 5:35–44.
- Pope VD, Gallani ML, Rowntree PR, Stratton RA (2000) *Clim Dyn* 16:123–146.
- Breiman L, Friedman JH, Olshen RA, Stone CJ (1984) *Classification and Regression Trees* (Wadsworth International, Monterey, CA).
- R Development Core Team (2004) *R: A Language and Environment for Statistical Computing* (R Foundation for Statistical Computing, Vienna).
- Sall J, Creighton L, Lehman A (2005) *JMP Start Statistics* (Thomson Learning, Belmont, CA).