Pragmatic aspects of uncertainty propagation: A conceptual review

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Abstract

When quantifying the uncertainty of the response of a computationally costly oceanographic or meteorological model stemming from the uncertainty of its inputs, practicality demands getting the most information using the fewest simulations. It is widely recognized that, by interpolating the results of a small number of simulations, results of additional simulations can be inexpensively approximated to provide a useful estimate of the variability of the response. Even so, as computing the simulations to be interpolated remains the biggest expense, the choice of these simulations deserves attention. When making this choice, two requirements should be considered: (i) the nature of the interpolation and (ii) the available information about input uncertainty. Examples comparing polynomial interpolation and Gaussian process interpolation are presented for three different views of input uncertainty.

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1. Introduction

Numerical models are important tools for understanding the behavior of the ocean and atmosphere. In particular, they can be used to make quantitative predictions of future conditions. For the value of such predictions to be assessed, they should be accompanied by quantitative information about their reliability.

While the model’s formulation — the physical processes and how they are treated — has a major impact on its prediction, the impact of alternative formulations is not discussed here¹. Instead, the model is regarded as a reliable black box and the focus is on assessing the uncertainties of the numbers it produces (its *outputs* or *responses*), which result from the uncertainties of the numbers it is given (its *inputs*). When making planning decisions, only a few of a model’s many outputs are generally of interest, so estimates of accuracy can be restricted to those few outputs. Computational resources limit the number of uncertain inputs that can be treated simultaneously to a manageable few, so most of the inputs must be treated as known even though their values are by no means certain. What we discuss here should be regarded as *conditional uncertainties* — uncertainties conditioned on the values assumed to be known and on the model’s formulation. We are interested in how the model transforms information about the uncertainty of selected inputs into

¹Webster and Sokolov (2000) discuss the role of model formulation when quantifying uncertainty of climate projections.

21 information about key outputs.

22 Suppose uncertainties of the inputs are quantified as a probability density
23 centered on their most likely values, and suppose that a large ensemble of
24 possible inputs are sampled according to this density. Then, assuming suffi-
25 cient computational resources are available, for each set of inputs from this
26 ensemble the model can be run to provide corresponding responses, and a
27 histogram of these responses can approximate the probability density quanti-
28 fying the uncertainty of the model’s response stemming from the uncertainty
29 of its inputs. In order to carry out this Monte Carlo agenda, two practical
30 issues must be addressed: (1) how to proceed when the model’s computa-
31 tional requirements limit the number of runs that can be made and (2) how
32 to proceed when there is limited information about the uncertainties of the
33 models inputs².

34 Before computers were available propagating uncertainty had already
35 been recognized as being important. Wiener (1938) addressed the problem
36 within the context of a single uncertain input and a single response. Rather
37 than addressing issue (2), he assumed the input density to be a known Gaus-
38 sian. His approach was to approximate the response as a polynomial function
39 of the input expressed as a truncated expansion in Hermite polynomials³,
40 and solving for the expansion coefficients became the major computational

²Webster and Sokolov (2000) discuss the issue of uncertainty about input uncertainty.

³His use of Hermite polynomials was tied to his use of a Gaussian probability density, since Hermite polynomials are orthogonal when weighted by a Gaussian density. If he had expanded in Legendre polynomials, the method requires a uniform input density, and Laguerre polynomials require an exponential density. See, for example, Eldred et al. (2008) or Xiu (2009).

task.⁴ Because of the orthogonality of Hermite polynomials when weighted by the Gaussian density⁵, statistics such as the mean and variance of the response could be expressed as simple functions of the expansion coefficients, so there was no need to sample from the input density. Wiener’s approach has spawned a great deal of recent activity and is referred to as *polynomial chaos* in the engineering literature⁶.

Although Wiener (1938) did not appear to recognize it, the most important aspect of his approach was approximating a nonlinear response using an inexpensively evaluated polynomial function, which could serve as an *emulator* or *surrogate* for the original model. Because running the emulator is much less expensive than running the original model, Monte Carlo sampling becomes affordable. This reduces issue (1) to the more manageable concern of how using emulated responses impacts our view of response uncertainty. Moreover, it also provides an answer to issue (2) — how to deal with *uncertainty about input uncertainty*: simply consider several alternative descriptions of the input uncertainty and construct histograms of the response for each. Comparing the histograms to assess the impacts of the the alternative views of input uncertainty clearly must reflect how they alter practical decisions.

Running the emulator is simple. The bulk of the computation effort is in building it, as the model must be run repeatedly to generate enough responses to interpolate. A major point of this paper is that it is best to organize

⁴See Appendix A for a brief discussion of how the coefficients might be computed.

⁵Recall its use in the context of the meridional structure of equatorial Rossby waves.

⁶The reviews of Najm (2009) and Xiu (2009) provide brief introductions to polynomial chaos and references to much of its literature.

63 computational effort in such a way that allows alternative input densities to
64 be explored in a flexible and cost-effective manner. For each input density,
65 sampling should reflect its more likely values, so that the response is most
66 accurate where it is most important. When using quadrature to compute
67 the expansion coefficients, the polynomial chaos formulation that links the
68 input density to the orthogonality of the polynomials guarantees this sort
69 of sampling as long as the input density is correct, but changing the input
70 density requires redoing the sampling⁷. Our point is that it is important to
71 be able to interpolate more flexibly so that sampling and interpolating can
72 be incremental, so that as the view of input uncertainty changes existing
73 samples need only be supplemented by a few more to improve accuracy for
74 input values previously considered unlikely. Solving an algebraic system for
75 the expansion coefficients, rather than using quadrature, provides this needed
76 flexibility⁸.

77 An emulator need not be restricted to polynomial interpolation. Gaus-
78 sian process interpolation has also been used for this purpose⁹. Rather than
79 treating the response as a sum of specified functions of the random inputs,
80 the response function itself is regarded as a *random function*. More specifi-
81 cally, for each input, the output has a specified mean and variance, and for
82 each pair of inputs there is a specified covariance. It is easy to recognize

⁷See Appendix B.

⁸See Appendix C.

⁹Rougier et al. (2009) have used Gaussian processes for characterizing responses of climate models. See also the articles by Sacks et al. (1989) and by Kennedy and O’Hagan (2000) and the excellent book by Rasmussen and Williams (2006). Appendix D provides a brief discussion of Gaussian process interpolation. A reviewer recommended the following articles as potentially inspiring: French (2003); Ratto et al. (2009); Yang (2011); Borgonovo et al. (2012); Castaings et al. (2012).

83 this as a novel application of optimal interpolation, as it corrects a prior
84 description of the response surface using an assumed covariance function to
85 interpolate the information provided by model simulations. Using Gaussian
86 processes shifts the focus from determining coefficients of a polynomial ap-
87 proximation to choosing appropriate mean and covariance functions. Once
88 these choices have been made and the responses of the exploratory ensemble
89 have been assimilated, the updated mean function serves as the approximate
90 response function and the updated variance function provides a measure of
91 its accuracy.

92 We use a single input and a single output for illustrating these ideas, as
93 that allows the underlying issues to be discussed more clearly. To illustrate
94 our points, we use a model that simulates the fate of oil droplets emerging
95 from a deep underwater source and rising due to their buoyancy as they
96 are advected by a prescribed velocity field. This model was chosen because
97 a database of its simulations was available and new simulations could be
98 avoided. Uncertainty in droplet size is the single uncertain input of interest
99 and the single response is the surface concentration of oil in a region some
100 distance from the source. The details of this model are unimportant here.
101 What matters is that the response is a highly nonlinear function of the input.
102 In the examples discussed below, polynomials and Gaussian processes provide
103 alternative interpolations for the same sets of simulated responses and thus
104 a framework in which the separate roles of the choice of input density and
105 the choice of the interpolation method can be addressed.

106 These simulations had previously been used at an early stage of model
107 development to check how the uncertainty of surface oil concentration within

108 a restricted region depended on the uncertainty of droplet size at the spill
109 site. These simulations are from two different quadrature ensembles, one pro-
110 viding a 6th-degree polynomial approximation to the response function and
111 the other providing a 20th-degree polynomial approximation, which might
112 be regarded as being exact over the range of inputs considered. When com-
113 bined and then sub-sampled they provide the possibility of exploring different
114 approaches to interpolation and different views of input uncertainty.

115 This paper takes a step-by-step approach to illustrate the above ideas
116 incrementally. Section 2 describes the data from the database of quadrature
117 simulations and discusses the differences in the resulting 6th- and 20th-degree
118 polynomial approximations to the response curve, both of which indicate that
119 the response is a highly nonlinear function of droplet size. Section 3 discusses
120 the histograms characterizing the uncertainty in surface-concentration re-
121 sponse, which reflect the differences between these two views of the response
122 curve, under the assumption that the uniform probability density for droplet
123 size on which the quadrature ensembles were based is the correct density.
124 Section 4 illustrates how the existing 20th-degree polynomial approximation
125 to the response can be used to assess the uncertainty of the surface oil con-
126 centration when the initial assumption of uniform probability of droplet size
127 is replaced with alternate assumptions — *without the need of any new simu-*
128 *lations*. Section 5 illustrates how decoupling the polynomial approximation
129 from the input probability density can provide a more flexible choice of simu-
130 lations. And section 6 explores Gaussian process interpolation as an alterna-
131 tive to polynomial interpolation and illustrates its impact on the propagation
132 of uncertainty from droplet size to surface concentration. As the focus is on

133 practicality, methodological details are confined to appendices. The paper
134 ends with a few concluding remarks.

135 **2. Simulated data**

136 The context of this study is provided by a model being constructed for
137 simulating the effects of the Deepwater Horizon oil spill in the Gulf of Mexico.
138 While that model has many uncertain inputs and many responses worthy of
139 study, here we focus on one particular uncertain input and one particular
140 response, as they had been examined in the early stages of model construction
141 and those quadrature simulations offered a convenient context for this study.
142 The uncertain input is the size of the oil droplets at the trap height where
143 the droplets accumulate at the site of the spill¹⁰, and the uncertain output
144 is the concentration of oil at the sea surface in a region some distance from
145 the spill site.

146 For illustrating the separate roles of the approximate response function
147 and the assumed nature of the input's uncertainty, a detailed description of
148 the model that transforms droplet size to surface oil concentration is unnec-
149 essary. It is sufficient to know that the droplets are injected at depth and
150 are carried by spatially and temporally varying eddies and currents driven by
151 meteorological forcing as they rise to the surface due to their size-dependent
152 buoyancy. Thus, the response function for the region reflects the itinerary
153 taken by each droplet on its way to the surface of the study region at a

¹⁰In actuality, there is a distribution of droplet sizes and the parameters characterizing the shape of this distribution might be taken as uncertain inputs, but for simplicity all droplets were taken to have the same size and the uncertainty of the size provided a proxy for a size distribution.

Figure 1: Triangles indicate simulated data at quadrature points based on droplet size being uniformly likely between 200 and 500 m. Curves indicate corresponding polynomial approximations to the response curve. Magenta indicates data and approximation for 6th degree polynomial approximation; cyan, 20th-degree.

specific time after the start of the spill. As uncertainties of many processes ultimately contribute to the uncertainty of the surface concentration, by focusing on droplet size and excluding the rest, we are exploring the uncertainty conditioned on all other inputs, *e.g.* the advecting velocity field.

Two sets of simulations were available for this study: the first for droplet sizes corresponding to quadrature points for evaluating the coefficients of a series of Legendre polynomials¹¹ truncated after the first 7 terms and the second, truncated after the first 21 terms, which approximate the surface concentration of oil using polynomials of 6th-degree and 20th-degree, respec-

¹¹The Legendre polynomials are appropriate for a uniform probability density. Here droplets are assumed to range from 200 to 500 μm in size.

163 tively. For more details about using quadrature to evaluate coefficients of
164 polynomial expansions, see Appendix B.

165 Figure 1 illustrates both the quadrature data and the interpolating poly-
166 nomials. While both approximations have roughly the same shape¹², they
167 differ in details of the small scales. The magenta curve misses many of the
168 blue triangles, and the cyan curve, although passing through most of the
169 magenta triangles, slightly misses a few for the larger droplet sizes. So it is
170 clear that, even with 21 terms, the polynomial series has not yet converged.
171 This raises the question: how does lack of convergence impact our view of the
172 uncertainty of the surface concentration of the oil in the region of interest?
173 That question will be addressed in the next section.

174 The maximum near $225\text{ }\mu\text{m}$ and minimum near $275\text{ }\mu\text{m}$, which are clearly
175 seen in both approximations, indicate a highly nonlinear response and suggest
176 that droplets in different size ranges follow quite different paths from the
177 source to the surface of the target region. In fact, given their widely different
178 behavior, droplets from the three intervals separated by the extrema might be
179 regarded as separate populations and treated separately. Section 4 will show
180 how the existing response curves can be used to examine such possibilities.

181 **3. Uncertainty propagation via Legendre polynomial expansions.**

182 Figure 2 shows histograms of the surface oil concentration when droplet
183 size is assumed to be equally likely for all values between 200 and $500\text{ }\mu\text{m}$ and

¹²This particular output was chosen because of the presence of the relative extrema of its response curve, as that highly nonlinear shape provided a nice example for illustrating the interaction between the input probability density and the response curve in quantifying the uncertainty of the output.

Figure 2: Histograms of surface oil concentration based on 10,000 droplet sizes sampled uniformly from 200 to 500 μm have bin width of 0.02 kg/m^2 . Upper panel: 6th degree polynomial approximation of response function. Lower panel: 20th- degree approximation.

184 completely unlikely for values outside this range. Each histogram bin corre-
 185 sponds to an interval¹³ on the vertical axis of the plot in figure 1. Projecting
 186 that interval onto the response curve and then projecting those portions of
 187 the response curve onto the horizontal axis reveals the values of droplet size
 188 that contribute to that bin. As the droplet size is uniformly distributed, the
 189 height of the histogram for that bin is simply proportional to the sum of the
 190 lengths of these projections¹⁴. For example, consider the bins with the cyan
 191 and blue bars near 0.7 kg/m^2 : because the 6th-degree polynomial is consid-
 192 erably flatter in those interval, it has larger projections onto the horizontal
 193 axis and thus its histogram has a peak (upper panel) that is noticeably ab-
 194 sent when the 20th-degree polynomial is used (lower panel). Clearly, what
 195 appear to be relatively minor differences between the 6th-degree and 20th-
 196 degree approximations to the response curve induce noticeable differences in
 197 the probability density of the response.

198 The question remains as to the practical significance of these differences.
 199 Both histograms indicate a distribution that is far from Gaussian and even
 200 multi-modal, and both support the conclusion that the surface oil concen-
 201 tration is highly likely to be greater than 0.44 kg/m^2 but never greater than
 202 0.86 kg/m^2 . The greater accuracy of the 20th-degree approximation provided
 203 little additional *useful* information. Using a polynomial of even higher degree

¹³To emphasize the relationship between the response curves and the histograms, the horizontal grid lines were chosen to correspond to bin boundaries.

¹⁴If the response function were monotonic, the output density could be obtained from the input density via a change in scale where the resulting change in shape is associated with stretching or squeezing according to changes in slope for different droplet sizes. But the presence of relative extrema induce a folding in addition to the squeezing and stretching.

204 would not would not appear to be warranted.

205 It is important to recognize that this conclusion reflects the assumption
206 that the size of the droplet is confined to be between 200 and 500 μm with
207 no preference for one value over another within this range. This assumption
208 of uniformity was made for the convenience of computing the polynomial
209 response using Legendre polynomials. The range simply reflected a droplet
210 size that might be expected with no firm conviction that sizes outside this
211 range were impossible or that all allowed sizes were truly equally likely. Fur-
212 thermore, as the histogram bins between 0.42 and 0.52 kg/m^2 contain contri-
213 butions from three different segments of the response curve corresponding to
214 distinctly different paths to the target region, surface concentrations within
215 this range can be expected to be highly sensitive to changing the assumed
216 size distribution to exclude droplets from one or two of the three size ranges.
217 Clearly, the extent to which alternative characterizations of droplet size un-
218 certainty impact the uncertainty of the surface concentration of oil in the
219 target region is worth exploring.

220 4. Reconsidering the assumption of uniformity.

221 Once the response function has been approximated in a way that is easy
222 to evaluate, it is easy to explore the consequences of alternate character-
223 izations of the input uncertainty. Here we show the consequences of two
224 different distributions of possible droplet size when the surface concentration
225 is approximated by the 20th-degree polynomial discussed above.

226 Suppose that uncertainty of the droplet size is considerably less than that
227 characterized by the uniform density, which provided the rational for the

Figure 3: Data from the 20th degree polynomial approximation of response function shown in figure 1. Upper panel: 10,000 approximate response points sampled from a normally distributed droplet-size distribution with mean $250 \mu\text{m}$ and standard deviation $10 \mu\text{m}$ as indicated by the brown curve with unlabeled ordinate. Colors correspond to the histogram bins in the lower panel. Lower panel: Corresponding histogram of possible surface oil concentration in the target region.

228 quadrature simulations used to construct the initial approximate responses.
 229 For example, assume instead that the input probability density is a Gaussian
 230 centered at $250\ \mu\text{m}$ with standard deviation of $10\ \mu\text{m}$. The upper panel of
 231 figure 3 shows this density (scaled to an arbitrary height) and the approx-
 232 imate response for 10,000 droplet sizes randomly drawn from this density.
 233 The histogram in the lower panel, as before, reflects the number of samples
 234 between each pair of adjacent horizontal grid lines, which have been plot-
 235 ted in different colors so they can be identified more easily. But, as the
 236 probability density is no longer uniform, the histogram heights are no longer
 237 simple projections of intervals from the response axis onto segments of the
 238 response curve and then onto the input axis. Instead, the length of these
 239 projections must be multiplied by a factor accounting for the probability of
 240 the droplet size being there. Concentrations that project onto the tails of
 241 the density clearly contribute negligibly to the histogram. The result is a
 242 histogram that is more nearly Gaussian than its predecessor shown in lower
 243 panel of figure 2. If the response function were linear, then the probability
 244 density for the surface concentration would in fact be Gaussian. But as the
 245 response function has a maximum at about $225\ \mu\text{m}$ and a minimum at about
 246 $275\ \mu\text{m}$ — roughly 2.5 standard deviations on either side of the center — the
 247 histogram’s black and orange bars are a bit longer than would be expected
 248 for surface oil concentration described by a Gaussian density.

249 If this same $N(250, 10^2)$ probability density were propagated using the
 250 less accurate 6th-degree polynomial approximation of the response function
 251 shown in figure 1, the resulting histogram characterizing the surface concen-
 252 tration would be expected to be much the same, because the two approximate

Figure 4: Same as figure 3 except that the possible droplet size is normally distributed with mean 350 μm and standard deviation 30 μm .

253 response functions are quite similar for droplet sizes likely to be encountered.
254 For either response curve you could conclude that it would be highly unlikely
255 for the surface concentration to be outside the range of 0.44 to 0.54 kg/m²
256 and that the most likely values would be about 5.0 kg/m².

257 Figure 4 shows another example using the 20th-degree polynomial ap-
258 proximation of the response function, this one with droplet size thought to
259 be larger and less certain as described by a Gaussian density centered on
260 350 μm with a standard deviation of 30 μm . Because the response function
261 is clearly nonlinear over the range of likely values for droplet size, the resulting
262 histogram reflects a clearly non-Gaussian density. For example, its change
263 in slope near 350 μm causes the central orange, black, and magenta bars to
264 be longer than the blue, cyan, and magenta bars to their left. And the local
265 minimum for small values causes the black, magenta, and cyan bars between
266 0.44 and 0.50 kg/m² to be relatively long.

267 If this wider $N(350, 30^2)$ probability density were propagated using the less
268 accurate 6th-degree polynomial interpolation, its resulting histogram would
269 be different. In particular, the change in its slope near 380 μm should cause
270 surface concentrations greater than 0.68 kg/m² to be more likely and con-
271 centrations less than 0.68 kg/m² be less likely, in effect shifting expectations
272 towards higher surface concentrations. Nevertheless both curves would sup-
273 port the conclusion that surface oil concentrations are unlikely to be outside
274 the range of 0.44 to 0.74 kg/m² and more likely to be between 0.60 and
275 0.70 kg/m².

276 The most dramatic sort of revision allows for a significant chance of a
277 droplet being larger (or smaller) than the sizes supporting the presumed uni-

278 form density. For example, suppose that the previous density were centered
 279 at $450\text{ }\mu\text{m}$ rather than $350\text{ }\mu\text{m}$, so that a droplet size larger than $500\text{ }\mu\text{m}$
 280 must be considered. In such a case the polynomial approximation must be
 281 extrapolated beyond the data. Such an extrapolation is likely to provide
 282 nonsensical values. For example, figure 1 suggests that the 6th-degree and
 283 20th-degree polynomials would extrapolate rapidly in totally different di-
 284 rections — the former toward smaller concentrations and the latter toward
 285 larger concentrations. Obviously, a better approximation to the response
 286 function would be needed, which would require additional simulations for
 287 larger droplet sizes. Unfortunately, if the same polynomial chaos approach
 288 that had been used over the interval from 200 to $500\text{ }\mu\text{m}$ were to be used
 289 to approximate the response over the enlarged range of droplet size, a new
 290 ensemble of quadrature simulations would be needed.

291 A general conclusion to be drawn from these examples is that lack of
 292 knowledge of the probability density characterizing the uncertainty of the
 293 input can have an impact on the propagated uncertainty as large as or larger
 294 than that resulting from the imprecision of the approximation of the response
 295 function. This suggests that the strategy of approximating the response
 296 function using quadrature simulations, which are tied to an input density
 297 that is likely later to be revised, is an inefficient use of limited computational
 298 resources.

299 **5. Severing the coupling between polynomials and input density.**

300 The previous section has illustrated that there is no need to stick with the
 301 initial view of the relatively poorly known input density: once an approximate

302 response curve has been obtained, it can be used to quantify the uncertainty
 303 of the response resulting from some other input density. Here we address the
 304 possibility of obtaining more flexibility in the choice of simulations by cut-
 305 ting the tie of the polynomial approximation to the input probability density.
 306 This requires abandoning the integral expressions for coefficients needed to
 307 approximate the response for all possible inputs. Instead of exploiting or-
 308 thogonality, we can determine the coefficients of a polynomial approximating
 309 the response over the range of likely inputs by solving a system of coupled
 310 linear equations. Details are provided in Appendix C.

311 To test this more flexible approach, we combined the two sets of quadra-
 312 ture points, so that we could sample from these without having to compute
 313 new simulations. In this way we could explore how well low-degree polyno-
 314 mial approximations determined using likely values of droplet size can char-
 315 acterize the uncertainty of the resulting surface oil concentration. As we have
 316 already examined the uncertainties propagated from two different Gaussian
 317 input densities, it is instructive to revisit those cases. For each case, 7 simula-
 318 tions centered on the respective density were used to determine a 6th-degree
 319 polynomial approximation to a restricted part of the response function.

320 Figure 5 illustrates the results for the Gaussian density centered at $250\ \mu\text{m}$
 321 with standard deviation of $10\ \mu\text{m}$. The simulated responses are indicated by
 322 triangles, one for the droplet's most likely size, the three next larger sizes,
 323 and the three next smaller. Comparing their locations with the brown Gaus-
 324 sian curve reveals that the data span the most likely values. Within the span
 325 of the data the gray approximate response curve agrees quite well with the
 326 20th-degree polynomial discussed above, but when extrapolated beyond the

Figure 5: Upper panel: The wide gray curve is the 6th-degree polynomial determined from the data indicated by triangles and the superimposed colored dots indicate the approximate response for each of 10,000 randomly drawn samples from a Gaussian distribution with mean 250 μm and standard deviation 10 μm . The cyan curve is the 20th-degree polynomial from figure 1 and the brown curve indicates the Gaussian density. Lower panel: Corresponding histogram of the 10,000 approximate responses.

327 data, this 6th-degree polynomial quickly plunges to nonsensical negative sur-
 328 face concentrations. Because these nonsensical values correspond to droplet
 329 sizes that are highly unlikely, they have insignificant impact on the uncer-
 330 tainty of the surface oil concentration in the target region. Consequently,
 331 the histogram in the lower panel agrees quite well with its counterpart in
 332 figure 3.

333 Results for the Gaussian density centered at $350\text{ }\mu\text{m}$ with standard devi-
 334 ation of $30\text{ }\mu\text{m}$, which are shown in figure 6, illustrate what happens when
 335 the simulations don't quite span the reasonable values of the input. While its
 336 ability to interpolate the simulations is excellent, when extrapolating this 6th-
 337 degree polynomial suggests unbelievably large surface concentrations. The
 338 small fraction of the 10,000 random samples having responses that were ex-
 339 trapolated contribute to a very long tail in the output distribution¹⁵. But
 340 except for this tail of high surface concentration resulting from the extrap-
 341 olation, the histogram in the lower panel is quite similar to that shown in
 342 figure 4.

343 These examples support the conclusion that when simulations sample the
 344 likely values of uncertain inputs, a polynomial approximation of the response
 345 function can be sampled to give a good quantitative description of the un-
 346 certainty of the output.

¹⁵In fact the plot has been truncated to omit the 27 samples with response greater than 1 kg/m^2 , as they comprise a negligible 0.27% of all samples.

Figure 6: Same as figure 5 except that the possible droplet size is normally distributed with mean 350 μm and standard deviation 30 μm .

347 6. Reconsidering polynomials.

348 In this section we illustrate the use of Gaussian processes as an alternative
 349 to polynomials for interpolating simulated responses and we explore what
 350 consequences this might have on the quantification of the uncertainty of the
 351 response. The previous section showed that loosening the tight coupling of
 352 polynomials to the input probability density allowed for a more flexible choice
 353 of simulations. This flexibility extends to the use of Gaussian processes, as
 354 the input density plays no role in their formulation.

355 A Gaussian process is specified jointly by its mean function, which pro-
 356 vides the estimate of the response in the absence of data, and its covariance
 357 function, which governs how smoothly the response is expected to change
 358 with changing value of the input. Most often the covariance function is taken
 359 to be a function of the distance between pairs of values of the input, which
 360 returns a small covariance as the separation of the pair gets large. This study
 361 uses constant mean functions and squared-exponential covariance functions.
 362 For more details, see Appendix D.

363 Figure 7 shows the results obtained with a Gaussian process using the
 364 same seven data points as used for the locally determined 6th-degree poly-
 365 nomial shown in figure 5. The mean function was taken to be the mean of
 366 the seven data: a constant response of 0.49 kg/m^2 surface concentration for
 367 all possible values of droplet size. The value of Gaussian process variance
 368 parameter was set to $1 \text{ kg}^2/\text{m}^4$, even though this choice had no impact on the
 369 results that are shown¹⁶. And the length scale of the covariance function was

¹⁶In computing the mean posterior response, the value of the process variance parameter σ_p^2 cancels out. For details, see equation(D.5) in Appendix D. However, this choice would

Figure 7: Same as figure 5 except that the response is approximated using a Gaussian process with mean set to the mean of the data and with a covariance function that is a squared exponential with length scale of $10\mu\text{m}$, which is the same as the standard deviation characterizing the uncertainty of droplet size.

370 set at the standard deviation of the $N(250, 10^2)$ probability density account-
 371 ing for uncertainty in droplet size: $10 \mu\text{m}$. The close agreement between the
 372 gray and cyan curves indicates that this choice of length scale provides an
 373 excellent approximation to the response curve for any reasonably likely value
 374 of droplet size. Note that, when extrapolating beyond the data points, the
 375 Gaussian process regresses toward the prior mean, avoiding the unreasonable
 376 values that plague polynomial extrapolation¹⁷. As the Gaussian-process ap-
 377 proximation is almost identical to the 6th-degree polynomial approximation
 378 of figure 5 within the interval of all reasonably likely values for droplet size,
 379 differences being less than the thicknesses of the plotted lines, the histograms
 380 of figures 7 and 5 are essentially indistinguishable.

381 Figure 8 shows a similar comparison of approximate response curves and
 382 histograms of Gaussian process and polynomial interpolation using the same
 383 data as in figure 6 for the case where the uncertainty in droplet size is
 384 $N(350, 30^2)$. Following the pattern of the previous case, the mean function
 385 was taken to be the mean of the seven data points: 0.60 kg/m^2 ; the length
 386 scale of the covariance function was set at the standard deviation of the input

be reflected in the posterior covariance function for the Gaussian process and could have
 been illustrated as an envelope about the gray curve. If added, it would show the envelope
 decreasing to zero at the data points, increasing between them, and getting quite large
 as the response curve extrapolates beyond the data. As this choice of σ_p^2 was somewhat
 arbitrary and the plot already complicated, this extra information was not illustrated.
 On the other hand, if the data were considered to be subject to noise characterized by a
 variance σ_n^2 , then the approximate response curve would depend on the ratio σ_p^2/σ_n^2 and
 it would not be required to pass through the data, and the hyperparameters could be
 adjusted so that the envelope might provide a more quantitative assessment of the accuracy
 of the interpolation.

¹⁷Recall that the polynomial interpolation illustrated in figure 5 lead to physically
 impossible negative values for surface oil concentration.

Figure 8: Same as figure 6 except that the response is approximated using a Gaussian process with mean set to the mean of the data and with a covariance function that is a squared exponential with length scale of $30\mu\text{m}$, which is the same as the standard deviation characterizing the uncertainty of droplet size.

387 probability density: $30 \mu\text{m}$; and the variance parameter was set to $1 \text{ kg}^2/\text{m}^4$.
 388 Because the Gaussian process regresses toward the prior mean when extrap-
 389 olating beyond the data, the histogram describing possible surface oil con-
 390 centration does not show the heavy tail corresponding to unreasonably high
 391 concentrations. Otherwise, given this characterization of the uncertainty of
 392 the input, this histogram provides essentially the same information about
 393 the uncertainty of the response as those in figures 4 and 6. There is every
 394 reason to expect that additional samples from further into the tails of the in-
 395 put distribution might give an excellent approximation to the response curve
 396 over the extended range of the data, but given the low probability associated
 397 with this extension, the computationally costly simulations providing such
 398 samples could not be justified, as they would not substantially impact our
 399 understanding of the uncertainty of the surface oil concentration.

400 7. Discussion.

401 The examples presented here illustrate how the uncertainty of a model's
 402 response can be analyzed as an interaction between the shape of its response
 403 curve and the probability density of its input. The plots show how colored
 404 segments of a response curve are related to the bins of the response his-
 405 togram and how the probability associated with a particular bin reflects the
 406 probability of the input contributing to the corresponding segments. While
 407 these examples involve only a single input, the analysis is appropriate for any
 408 number of inputs. For example, with two inputs a response surface replaces
 409 the response curve and intervals between contours replace segments.

410 In most practical situations the shape of the response function is un-

known and the only access to it is via model simulations. While response functions for computationally demanding oceanic and meteorological models cannot be exhaustively sampled, they might be usefully approximated by interpolating a manageable number of simulations. How many simulations are needed is not known in advance and must be determined through exploratory sampling. At the same time, little information is generally available for characterizing input uncertainty, so alternative views should be explored and this influences the simulations that are needed. The expense of each simulation dictates using as few as possible to interpolate the response over the region of likely inputs while adding a few more, as needed, to extend the region to accommodate alternate views of which inputs are likely. It was the lack of flexibility in choice of simulations when using a standard non-intrusive polynomial chaos approach to uncertainty quantification that motivated this study.

The response curve considered here is highly nonlinear: the response first increases, then decreases, and then increases again as the input varies over the explored range, indicating three separate quasi-linear regimes. All inputs within this highly nonlinear range were initially assumed to be equally likely for technical reasons: the range encompassed all reasonable values of the input and the uniform density allowed for the use of sparse quadrature for exploring the impact of several uncertain inputs. The two sets of archived simulations, corresponding to two polynomial approximations of the response curve were ideal for this study, as they could be combined to provide sufficient sampling to explore different interpolations and different views of which input values are likely. The nonlinearity of the response and the uniformity of the

436 density resulted in a histogram of possible responses that was multi-modal.
437 Furthermore, the shape of the histogram was sensitive to the accuracy of the
438 interpolation: different views of the smaller-scale wiggles (nonlinearities) of
439 the response curve leading to different assessment of the relative likelihood
440 of possible responses.

441 Such multi-modal histograms might be expected in a wide range of mod-
442 eling situations where the range of likely inputs spans a region of highly
443 nonlinear response. It is important to understand that the detailed structure
444 of a response histogram is significant only if there is an important practical
445 question that it can help answer. Given that the analysis is conditioned on
446 the particular model's formulation and on the uncertainties of many other in-
447 puts, the individual peaks and valleys of the response histogram are not likely
448 to be sufficiently robust to provide a basis for answering practical questions.
449 This suggests that seeking a more accurate response surface would not be
450 worth the computational effort. The useful information conveyed by these
451 histograms is the possible range of responses resulting from the assumed
452 range of uniformly likely inputs.

453 On the other hand, different assessments of input uncertainty can have
454 significant practical consequences. By limiting the range of possible inputs,
455 their responses might be confined to quasi-linear sections of the response
456 function. As a linear response function preserves the shape of the density, the
457 response could be expected to be more nearly unimodal with departures from
458 linearity contributing primarily to skewness. This was illustrated by replacing
459 the initial uniform density by two alternative views of input uncertainty, both
460 Gaussian but with different centers and different spreads.

461 In most situations little information is available to provide an accurate
462 picture of input uncertainty, and when information does exist transforming
463 it into a probability density can be a lot of work. The process is much like
464 that of data assimilation, as it involves using Bayesian inference to extract
465 information from observations to update a prior view of the density¹⁸. When
466 accurate information about input uncertainty is unavailable, the only option
467 is to explore the impact of different assumed densities, as illustrated here.

468 The bulk of this paper treats the technical problem of interpolating the
469 responses, which becomes important when model simulations are limited by
470 their computational expense. The rigidity of the sampling necessitated by the
471 use of quadrature as part of a popular noninvasive polynomial chaos approach
472 for propagating uncertainty motivated our desire for more flexible alternative.
473 We tracked the cause of this rigidity to the exploitation of orthogonality and
474 to the desire to approximate the response globally, both of which stem from
475 the introduction of polynomial chaos by Wiener (1938) before the advent
476 of the computer. We illustrated that orthogonality and quadrature were
477 not essential to the nonintrusive polynomial chaos approach and that the
478 polynomial approximation to the response function could be determined by
479 a standard method for polynomial interpolation. This minor change removes
480 the rigidity and allows the freedom to sample the possible inputs much more
481 flexibly.

482 Once these parts of the polynomial chaos tradition had been abandoned, it

¹⁸See, for example the discussions of Sraj et al. (2013) and Sraj et al. (2014) on using observations of temperature in the upper ocean to quantify the uncertainty of parameters charactering wind drag on the sea surface.

483 was clear that all that remained was its use of polynomial interpolation. But
484 what is special about polynomials? Over a small enough interval a smooth
485 function is approximately linear and over a bit larger interval its curvature
486 might be described as quadratic or cubic, but variations over larger regions
487 are likely to require polynomials of higher degree and sufficient data to define
488 them. Gaussian process interpolation was demonstrated as an alternative,
489 as it provides the same sampling flexibility as polynomial interpolation. And
490 through the specification of a prior mean response function it provides a way
491 to avoid unreasonable responses in data voids where interpolation is more
492 like extrapolation and where polynomial interpolation can behave poorly.

493 One issue that deserves further attention is finding an optimal strategy
494 for choosing which simulations to interpolate. Clearly, when little is known
495 about the response function, the strategy would be exploratory and iterative,
496 using a few simulations to get a first impression and additional simulations
497 as needed and when affordable. When using Gaussian process interpolation,
498 the posterior covariance function could be used to indicate which subsequent
499 simulations might be most effective, as it indicates where the emulator benefit
500 least from the simulations that are already available. Of course, the nature of
501 the variability that is discovered during such an exploration should be used
502 to reassess initial judgment about the choice of the covariance function when
503 using Gaussian process interpolation or the number of terms to retain when
504 using polynomial interpolation.

505 Another issue deserving attention is the construction of emulators for
506 models incorporating random processes, as repeated simulations using the
507 same inputs produce different responses. Exact interpolation of the simu-

lated responses is inappropriate and the smoothing capability of regression is needed. Polynomial regression, which is a natural extension of polynomial interpolation when there are more data than the minimum required to determine the coefficients, would allow the response curve to average out the noise. Similarly, Gaussian process regression can smooth out the response through the use of a noise covariance matrix.

A third issue left for the future is identifying a good approach to exploring the uncertainty of multiple inputs. Given the curse of dimensionality, there is a limit to how well the uncertainties of very many inputs can be handled simultaneously. This is an issue that confronts data assimilation, where sampling can never explore all uncertain inputs. Within the context of this paper, there are questions of how many simulations might be needed for sampling in several dimensions, how they should be chosen, and how to best interpolate them. There is also the question of the relative merit of treating the multiple inputs simultaneously, which is expensive, individually, which is more practical, or pairwise, which is a compromise.

Appendix A. Non-intrusive polynomial chaos.

Wiener (1938) solved a set of coupled differential equations for the coefficients of the polynomial approximation to the response function. Their derivation is similar to the derivation of the equations for a spectral model of the atmosphere with the polynomial basis being the analogue of the spherical harmonics.¹⁹ When generalized from his model, which was based on a single

¹⁹Shen et al. (2010) have used this approach to quantify the growth of uncertainty for a Lorentz model.

530 ordinary differential equation, to models based on systems of coupled partial
 531 differential equations, solving for the expansion coefficients has an overhead
 532 cost similar to that of constructing a new numerical model, and it is termed
 533 *intrusive* because it requires intimate knowledge of the model’s source code.
 534 For this reason the intrusive approach is not considered in this paper.

535 The *non-intrusive* alternative treats the model as a black box and deter-
 536 mines the expansion coefficients by interpolating responses found by running
 537 the forecast model multiple times; with n coefficients to be determined, n
 538 forecast runs are needed²⁰. Here we are interested in the situation where
 539 available computational resources limit the number of runs, which in turns
 540 limits the number of coefficients that can be determined and thus the de-
 541 gree of the interpolating polynomial. Appendix B and Appendix C provide
 542 technical details for two non-intrusive approaches, which differ in how the
 543 expansion coefficients are computed.

544 **Appendix B. Determining polynomial coefficients via quadrature.**

545 The polynomial-chaos approach to propagating uncertainty starts by rep-
 546 resenting the response function with an infinite series of orthogonal polynomi-
 547 als $P_j(x)$, which are chosen based on the probability density $\rho(x)$ describing

²⁰Webster and Sokolov (2000) have used a non-intrusive polynomial chaos approach for characterizing responses of climate models. Our groups previous work (Thacker et al., 2012; Alexanderian et al., 2012; Sraj et al., 2013; Winokur et al., 2013; Sraj et al., 2014) using a non-intrusive polynomial chaos approach to propagate uncertainties through the hybrid coordinate ocean model (HYCOM) motivated this study.

548 the uncertainty of the input x :

$$r(x) = \sum_{j=0}^{\infty} a_j P_j(x) , \quad (\text{B.1})$$

549 where $P_0(x) = 1$, $P_1(x) = x$, and the other polynomials depend on $\rho(x)$ via
 550 orthogonality. The expression for the orthogonality of the polynomials $P_n(x)$
 551 is:

$$\int P_j(x) P_k(x) \rho(x) dx = \delta_{j,k} N_k , \quad (\text{B.2})$$

552 where the integral extends over the entire support of the input density $\rho(x)$,
 553 where N_k is a normalization constant, and where $\delta_{j,k}$ is the Kronecker delta.
 554 Multiplying the response function by $P_k(x)\rho(x)$ and integrating thus yields
 555 an expression for each coefficient:

$$a_k = \frac{1}{N_k} \int r(x) P_k(x) \rho(x) dx . \quad (\text{B.3})$$

556 If the response function is sufficiently smooth, it can be approximated
 557 with a polynomial of degree n by truncating the expansion:

$$\hat{r}(x) = \sum_{j=0}^n a_j P_j(x) . \quad (\text{B.4})$$

558 In the two examples of figure 1, where the input density is uniform and the
 559 expansion is in Legendre polynomials, one curve corresponds to $n = 6$ and
 560 the other to $n = 20$.

561 As the response function is expensive to evaluate, the strategy is to ap-
 562 proximate the integrals for the coefficients in (B.3) by efficient quadrature

563 formulae using the values of the response evaluated for only a few values
 564 x_q . In this way the integral becomes a sum over an ensemble of quadrature
 565 points with the corresponding quadrature weight w_q appearing as a factor in
 566 each term, so that:

$$a_k \approx \frac{1}{N_k} \sum_q r(x_q) P_k(x_q) w_q . \quad (\text{B.5})$$

567 For Gaussian quadrature, the quadrature ensemble and weights are chosen
 568 so that using $n + 1$ points yields the exact integral whenever the integrand
 569 is a polynomial of degree $2n$ or less²¹. So using $n + 1$ quadrature points to
 570 evaluate all coefficients $a_1, \dots, a_n$ guarantees that the approximate response
 571 function will be a polynomial passing through each of the quadrature points.

572 As the integral in (B.3) extends over the entire support of the input den-
 573 sity ρ , *i.e.* over *all possible* values of the input and the coefficients guarantee
 574 global polynomial exactness, the quadrature points tend to accumulate far
 575 from the center of the region of highly likely inputs. Furthermore, the lo-
 576 cations of the quadrature points depend sensitively on the input density ρ ,
 577 which is poorly known. Given the expense of the quadrature simulations,
 578 it might be wise to seek an approximation to the response function that is
 579 less strongly tied to the input density and that is less concerned with global
 580 polynomial exactness.

581 Once the coefficients have been evaluated, multiplying appropriate ex-
 582 pressions involving $\hat{r}(x)$ by $\rho(x)$ and integrating yields expressions for the
 583 statistical moments of the response. For example, because all of the poly-
 584 nomials except for the constant average to zero, $\bar{\hat{r}} = a_0$, and because the

²¹See, *e.g.*, Abramowitz and Stegun (1970) or Davis and Rabinowitz (2007).

585 polynomials are orthogonal, $\overline{(r - \hat{r})^2} = \sum_{j=1}^n a_j^2 N_j$. Such expression for the
 586 moments can provide a useful and inexpensive characterization of the uncer-
 587 tainty of the response — but only if $\rho(x)$ provides an adequate description
 588 of the input uncertainty.

589 A general feature of the quadrature ensembles used to build surrogates is
 590 that they include simulations for inputs that are significantly different than
 591 the default values that gave rise to the forecasts. In fact, some of the quadra-
 592 ture simulations might fail, because the model cannot handle such extreme
 593 inputs. This is the consequence of the expressions for the polynomial coef-
 594 ficients, which require integrating over all possible inputs, however unlikely,
 595 together with quadrature attempting to guarantee polynomial exactness. In
 596 other words, it is a result of the global way in which the problem has been
 597 formulated. As a result, the tails of a poorly known approximate input dis-
 598 tribution can play a much larger role than they should in the design of the
 599 quadrature ensemble of model runs that comprise the overwhelming bulk
 600 of the computation effort. An alternative to quadrature, which allows the
 601 ensemble to be chosen more flexibly, is described in Appendix C.

602 **Appendix C. Determining polynomial coefficients by solving a** 603 **linear system of equations.**

604 The polynomial-chaos strategy of polynomial interpolation does not re-
 605 quire that the polynomial coefficients be determined by quadrature (B.5).
 606 A straight-forward alternative is to solve for the coefficients algebraically.
 607 Rather than using simulated responses to evaluate an expression based on
 608 the orthogonality of the polynomials (B.3), just solve an algebraic system

609 that expresses the fact that the polynomial passes through the simulations.
610 As this alternative does not exploit orthogonality of the terms comprising
611 the polynomial, it lessens the bond between the approximating polynomial
612 and the probability density describing the uncertainty of the input and al-
613 lows the simulations to be chosen more flexibly. When they are chosen at
614 the quadrature points, the polynomial response curve is exactly the same as
615 you would get using quadrature. But if they are chosen to focus the accuracy
616 more locally, the different coefficients can be expected and remote parts of
617 the response curve might differ substantially.

618 While the response can be represented as a sum of orthogonal polynomial
619 terms, since orthogonality is not exploited, this is not necessary. Instead, it
620 can be represented simply in terms of powers of the input. If the response is
621 to be approximated by a polynomial of degree n :

$$\hat{r}(x) = c_0 + c_1x + c_2x^2 + \dots + c_nx^n, \quad (\text{C.1})$$

622 then its coefficients $c_j, j = 0, \dots, n$ can be determined from $n + 1$ simulated
623 responses $r_i, i = 1, \dots, n + 1$ to inputs $x_i, i = 1, \dots, n + 1$ by solving a system
624 of linear equations:

$$\mathbf{r} = \mathbf{D}\mathbf{c}, \quad (\text{C.2})$$

625 stating that the vector of responses $\mathbf{r}$ is the product of the vector of coef-
626 ficients $\mathbf{c}$ and a design matrix²² $\mathbf{D}$, each column of which corresponds to a

²²Within the context of polynomial interpolation, this matrix is often referred to as the *Vandermonde matrix*. *Design matrix* is terminology most often used in the context of regression modeling where there are more data than unknowns. In that case the polynomial would not be expected to agree with all the data, so an additional term is added to the

627 power of the input and each row to a simulated response²³.

628 The solution for the coefficients $\mathbf{c} = \mathbf{D}^{-1}\mathbf{r}$ requires $\mathbf{D}$ to be invertible.
629 In other words, the simulations must be chosen so that they are able to dis-
630 tinguish between the different powers of the input. While this was not an
631 issue for the simulations used in our examples, it is something that deserves
632 attention. Fortunately, the design matrix can be examined before any simu-
633 lations are computed to insure that the planned simulations correspond to a
634 well-conditioned design matrix.

635 Solving a linear system for the polynomial's coefficients does *not* preclude
636 the possibility of obtaining simple expressions for statistics of the response.
637 If the input probability density ρ can be approximated by a density that
638 serves as an orthogonality weight for a set of orthogonal polynomials, then
639 it is quite straightforward to re-express the powers of the input in (C.1) as
640 linear combinations of those polynomials in order to find the coefficients in
641 which the statistics are expressed. In the examples of figures 5 and 6, which
642 are based on Gaussian densities, Hermite polynomials would be appropriate.

643 Because the more flexible approach to computing the polynomial coef-
644 ficients is not based on the integral expressions, which were derived by ex-
645 ploiting the orthogonality of the polynomials, the strong coupling between
646 the polynomial approximation of the response function and the assumed in-

right-hand side of (C.1) to characterize the misfit, and the statistics of the misfit can be used to quantify the error of the polynomial fit to the data. The least-squares coefficients would be given by $\mathbf{c} = (\mathbf{D}^T\mathbf{D})^{-1}\mathbf{D}^T\mathbf{r}$ rather than by $\mathbf{c} = \mathbf{D}^{-1}\mathbf{r}$.

²³If the polynomial approximation had been expressed as a sum of orthogonal polynomials rather than simply powers of the inputs, then the columns of the design matrix would be the polynomials evaluated at the values of the inputs and the coefficient vector would contain the coefficients a_k used for the polynomial chaos expansion.

put density is broken. Most of the polynomial chaos formalism is no longer needed. All that remains is the fact that the response is approximated as being polynomial.

The next step is to consider other approximations. An obvious choice is Gaussian process interpolation, because it limits the influence of the simulated responses to the region of likely values without trying to extrapolate to the tails of poorly determined input densities. Appendix D describes how it works.

Appendix D. Gaussian processes.

Gaussian process regression is just another term for objective mapping or optimal interpolation where point observations are used to approximate continuous fields, and Gaussian process interpolation is just the limit where the observations are treated as being noise-free. Within our current context, simulations provide the counterparts of the data that are to be optimally interpolated and the response function is the counterpart of the fields that are to be corrected²⁴.

Gaussian process interpolation is conceptually quite different from polynomial interpolation: its error is described statistically rather than being relegated to the discarded terms of an infinite series, and the choice of its statistical description replaces the choice of the interpolating polynomial's degree. Furthermore, the statistics are best regarded as Bayesian. The process is defined by a mean function $m(x)$ and a covariance function $K(x, x')$,

²⁴For an overview of Gaussian processes, see Rasmussen and Williams (2006) and for a discussion of optimal interpolation see Daley (1993).

669 which provide the prior statistical description. The data to be interpolated
670 are used to update the prior with the resulting posterior mean providing the
671 interpolating function. The posterior covariance function reflects the inter-
672 polating function's exact agreement with the data as well as the error away
673 from the data²⁵.

674 The interpolated response $\hat{r}(x)$ for any possible input x is the posterior
675 mean of the Gaussian process after taking into account the information pro-
676 vided by the simulations. It can be regarded as a correction to the prior mean
677 that can be computed as a linear combination of the corrections needed to
678 make the prior mean function agree with the simulated responses r_j for inputs
679 x_j :

$$\hat{r}(x) - m(x) = \sum_{j=1}^n \alpha_j(x)(r(x_j) - m(x_j)) , \quad (\text{D.1})$$

680 where the differences $r(x_j) - m(x_j)$ are often called *innovations*. In this pa-
681 per the mean function is taken to be a constant and set to the mean of the
682 simulated responses. The coefficients α_j that define the liner combination
683 are determined by the covariance function $K(x', x'')$ of the Gaussian process,
684 which relates responses for all pairs of inputs x' and x'' . Typically, a covari-
685 ance function is chosen to be a function of the distance $|x' - x''|$ between
686 the input pairs and, even then, a wide variety of different function can be

²⁵While the posterior covariance function can also be used to measure the error of the interpolation away from the data, this measure only reflects the choice for the prior covariance function, which imposes a view of the smoothness in much the same way as truncation of an infinite series would. It should be regarded not as a quantitative measure of interpolation error but as a qualitative indication of the limits of the influence of the data given the assumptions of correlation length. Error envelopes could have been added to the plots in figures 5 and 6, but would not have added significantly to the discussion.

used. Here we restrict our attention to the squared exponential covariance function:

$$K(x', x'') = \sigma_p^2 \exp \left(-\frac{|x' - x''|^2}{2\Delta^2} \right) , \quad (\text{D.2})$$

where σ_p^2 is a constant variance and Δ scales the distance.

Central to the computation of the linear combinations is the $n \times n$ covariance matrix $\mathbf{K}$ relating the n simulations that are to be interpolated:

$$\mathbf{K}_{i,j} = K(x_i, x_j) . \quad (\text{D.3})$$

Its inverse converts the elements of the innovation vector $\mathbf{r} - \mathbf{m}$ into a vector $\delta = \mathbf{K}^{-1}(\mathbf{r} - \mathbf{m})$ having components that represent the relative influence of each of these n simulations. For any input x the response is approximated by weighting δ_j by the covariances $K(x, x_j)$ and then summing over the simulations. If interpolated values are desired for N inputs x_k where simulations may or may not be available, then it is useful to introduce the $N \times n$ covariance matrix relating these inputs to those where simulation are available:

$$\mathbf{K}^*_{k,j} = K(x_k, x_j) . \quad (\text{D.4})$$

Then the vector of N interpolated responses $\hat{\mathbf{r}}$ can be written compactly as:

$$\hat{\mathbf{r}} = \hat{\mathbf{m}} + \mathbf{K}^* \mathbf{K}^{-1}(\mathbf{r} - \mathbf{m}) , \quad (\text{D.5})$$

where vector $\hat{\mathbf{m}}$ contains the estimated mean responses before interpolation, i.e., the prior mean given by the mean function of the Gaussian process evaluated at the target points of the interpolation, and the second term is

704 the correction provided by the simulations.

705 Note that the predicted responses do not depend on the magnitude of the
 706 covariance function but only on its shape, as the variance σ_p^2 cancels out in
 707 equation (D.5) ²⁶. Note also that, when there are the same number of target
 708 points as simulations and when those points are chosen to coincide with the
 709 inputs of the simulations, $\mathbf{K}^*$ becomes identical to $\mathbf{K}$ and $\hat{\mathbf{m}}$ to $\mathbf{m}$, so the
 710 interpolating function passes through all of the simulated values. In other
 711 words, the prior variance σ_p^2 , is replaced by a posterior variance of zero.

712 Just as the simulations provide information for replacing the Gaussian
 713 process's mean function with a posterior mean function that can be evaluated
 714 pointwise, they also provide a posterior covariance function that indicates
 715 zero variance at the simulations and reduced variance at interpolated values.
 716 For the N interpolated points the elements of the $N \times N$ prior covariance
 717 matrix $\mathbf{K}^\dagger$ are just the Gaussian process covariance function evaluated at for
 718 pairs of target points $\mathbf{K}^\dagger_{k,k'} = K(x_k, x_{k'})$. The posterior covariance matrix:

$$\hat{\mathbf{K}}^\dagger = \mathbf{K}^\dagger - \mathbf{K}^* \mathbf{K}^{-1} \mathbf{K}^* \quad (\text{D.6})$$

719 reflects a reduced uncertainty due to the information provided by the simula-
 720 tions. When the target points are the same as the inputs for the simulations,
 721 the poster covariance matrix is zero, confirming that the posterior mean
 722 function reproduces the simulations. For target points that are very close to
 723 the simulations, the covariance matrix doesn't quite vanish, but its diagonal

²⁶In the limit of $\sigma_p^2 \rightarrow 0$, where this cancellation may be problematic, the covariance function (D.2) no longer makes sense.

724 elements are small, indicating a reduction in variance in the neighborhood
725 of the simulations. But at points far enough from the simulations for prior
726 correlations to be tiny, its diagonal elements, i.e. the posterior variances, are
727 approximately the same as the prior variance.

728 If the covariance function were a true characterization of uncertainty of
729 what the model might produce at the target points for interpolation, then
730 the posterior covariances would provide an estimate of interpolation error.
731 But this is not the case. The covariance function should be regarded simply
732 as a prescription for interpolating and its choice is analogous to the choice
733 of where to truncate the polynomial series. Just as the posterior mean func-
734 tion, which prescribes the interpolation, is independent of the scaling of the
735 prior variance, the reduction in variance shown in (D.6) is proportional to
736 σ_p^2 . A large σ_p^2 would show greater reduction in variance than a small one,
737 but without information about how to set its size, what to use is arbitrary.
738 So error estimates based on the posterior covariances provide only a qual-
739 itative indication of interpolated values that have benefited little from the
740 information provided by the simulations.

741 Because this paper addresses the issue of propagating uncertainty through
742 computationally demanding numerical models, the emphasis has been on us-
743 ing as few simulations as possible to provide inexpensive emulators. Discus-
744 sion of regression-based approaches did not seem appropriate, as they require
745 more simulations for approximating the response function. However, in some
746 cases regression might be justified. For example, the model might contain
747 stochastic processes and give different results when run repeatedly for the
748 same inputs. In that case the desired response is a function that filters the

749 stochastic noise much as a straight line provides a useful summary of data
 750 presented as a scatter plot. Even without stochastic processes the model
 751 might involve iterations with convergence criteria chosen to provide reason-
 752 able results with few iterations. In that case the number of iterations might
 753 change as an input parameter is varied causing the response function to ap-
 754 pear noisy. Again, some filtering is desirable. Another motivation might be
 755 to accommodate the fact that the numerical model is inexact. But whatever
 756 the reason, the response is desired to be smoother than the simulated data.
 757 This mention of regression has been added in response to a question about
 758 the possibility of using the posterior variance of a Gaussian process to char-
 759 acterize interpolation error. Just as the standard deviation of the scatter of
 760 data about a regression line provides an envelope within which data are most
 761 likely to fall, the same is true for Gaussian process regression. And just as
 762 the noise variance is not known before building the linear regression model but
 763 is determined after fitting to the data, the hyperparameters of the Gaussian
 764 process can be adjusted to make its error envelope meaningful.

765 When data have noise centered about posterior mean of the Gaussian
 766 process with covariance matrix $\Sigma_n = \sigma_n^2 \mathbf{I}$, then the posterior mean function
 767 is not given by (D.5) but by:

$$\hat{\mathbf{r}} = \hat{\mathbf{m}} + \mathbf{K}^* (\mathbf{K} + \Sigma_n)^{-1} (\mathbf{r} - \mathbf{m}) , \quad (\text{D.7})$$

768 so the posterior mean function for Gaussian process regression is *not* in-
 769 dependent of the value of σ_p^2 and it does *not* pass through the simulated
 770 responses. Similarly, the expression for the posterior covariance function

771 (D.6) is replaced by:

$$\hat{\mathbf{K}}^\dagger = \mathbf{K}^\dagger - \mathbf{K}^* (\mathbf{K} + \Sigma_n)^{-1} \mathbf{K}^* . \quad (\text{D.8})$$

772 The hyperparameters for variance σ_p^2 , σ_n^2 and correlation length Δ can be
773 adjusted, e.g., by cross-validation, to obtain an error envelope encompassing
774 the bulk of the data.

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