# The Computational Science of Klaus Hasselmann

Patrick Heimbach, *University of Texas at Austin, Austin, TX, 78712, USA*

***We review the work of Klaus Hasselmann, one of three recipients of the Nobel Prize in Physics 2021, from the perspective of computational science and engineering (CSE). In addition to highlighting Hasselmann's extensive contributions to climate science, we shine a light on his groundbreaking work in ocean surface wave dynamics and prediction, which preceded his career in climate research. Early on, Hasselmann also gained a strong interest in elementary particle physics, which led him to develop, in his spare time, a unified theory of particles and fields, and which we outline here. With this review we hope to entice computational scientists to delve deeper into Hasselmann's extraordinarily broad work at the interface of climate physics, mathematics, and scientific computing, and to appreciate the central role that CSE continues to play in climate research.***

The Nobel Prize in Physics 2021 was awarded to Klaus Hasselmann, Syukuro Manabe, and Giorgio Parisi "for groundbreaking contributions to our understanding of complex systems."[1] The two climate scientists, Hasselmann and Manabe, shared one half of the prize "for the physical modelling of Earth's climate, quantifying variability and reliably predicting global warming." The award recognizes the fundamental physical insights underlying climate science, and, as such, affirms climate science as a core discipline of physics.[2] Equally important, their work represents a triumph of the role of computational science and engineering in today's research enterprise. Extensive monographs have recently been published on Hasselmann's[3] and Manabe's[4] careers. The following is a subjective account of Klaus Hasselmann's work, viewed from a computational science perspective and in the context of his early contributions to geophysics. This focus is in no way meant to diminish the groundbreaking contributions of Syukuro Manabe and Giorgio Parisi, but merely reflects interactions of the author with Hasselmann during his time as a Ph.D. student in Hamburg.

Like most branches of the geosciences, climate science[a] has been, over the course of the 20th century, and arguably remains to date, a *sparse data* science, at least from an observational perspective. It is true that stunning advances in satellite remote sensing and autonomous, uncrewed *in situ* sensing are providing us today with an unprecedented wealth of Earth observations. But in the face of the wide range of physical processes acting on a continuum of space and time scales (from seconds to millennia) observational sampling of most geophysical variables remains sparse geographically and temporally. For the ocean, in particular, which is opaque to electromagnetic radiation, remote sensing techniques that have revolutionized everything from Earth science to astrophysics have been of limited use in revealing the properties of its interior, with those vast, barely observed water masses representing an essential flywheel of the climate system.

In view of the above, climate science is a compelling candidate for productive applications of developments

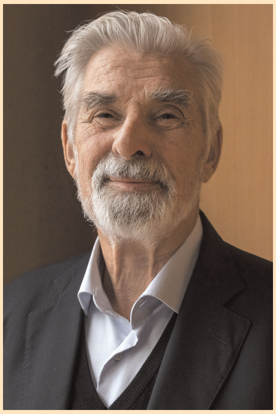

Digital Object Identifier 10.1109/MCSE.2022.3195105
Date of current version 4 January 2023.

[a]In the early days "climate science" was restricted to the study of long-term evolution of the atmosphere, but today consisting of the coupled dynamics and physics of the atmosphere, ocean, cryosphere, land, and biosphere, sometimes referred to collectively as Earth system science, but not (yet) including solid Earth and geodetic processes.

## FROM THE EDITOR-IN-CHIEF

This review article comes to you by invitation of the EiC, with a personal perspective on the phenomenal life and career of a multi-faceted researcher and Nobel laureate who was also a pioneer of computational science. **Klaus Hasselmann** and Syukuro Manabe were awarded the 2021 Nobel Prize in Physics (jointly with Giorgio Parisi) "for the physical modelling of Earth's climate, quantifying variability and reliably predicting global warming." In this account by Patrick Heimbach, we discover how Hasselmann's trajectory shows the impact that interdisciplinary science can have in the world. *CiSE* is proud to bring you this fascinating account of his contributions.

Lorena A. Barba
*Editor-in-Chief*



Klaus Hasselmann. Credit: Julia Knop/Max-Planck-Gesellschaft.

in computational science and engineering (CSE), which according to Rüde et al. (2018)[5] is

> *an essential driving force for progress in science when classical experiments or conventional theory reach their limits, and in applications where experimental approaches are too costly, slow, dangerous, or impossible.*

Their characterization of CSE as "rooted in the mathematical and statistical sciences, computer science, the physical sciences, and engineering," reflects in many ways Hasselmann's broad groundbreaking body of work. Through implicit or explicit advances in CSE, Hasselmann has made not one, but (at least) two major contributions, namely in the fields of ocean wave research and climate research. It is instructive to sketch both of these developments, as both of their fundamental descriptions rely on the embedding of the governing dynamics within a stochastic framework and applying judicious approaches of model reduction to render the problem at hand tractable. Arguably, Hasselmann's deep dive into ocean wave physics and stochastic dynamics provides a fertile canvas for much of his thinking about, and work in climate dynamics, as well his ideas on fundamental physics, pursued on the side.

## OCEAN WAVE RESEARCH

Hasselmann made his first major impact in geophysics with his solution to the long-sought problem of ocean swell modeling and its prediction. Some progress had been made in the prediction of wind-generated surface waves with the ground-breaking work by Sverdrup and Munk (1943, declassified 1947)[6] to support Allied landing operations in Europe during World War II. Although this work introduced fundamental statistical descriptions of *mean* wave field properties and empirical relationships between these and the surface wind field, a satisfactory theory for ocean swell generation remained elusive at the time.

### Formulating the General Governing Equations

Setting the stage for a flurry of papers, Hasselmann (1960)[7] argued that the largely empirical or parametric relationships between the local wind and wave properties should give way to a comprehensive energy balance (or radiative transfer) equation for the local two-dimensional (horizontal) spectral energy density $F(\mathbf{k}, \mathbf{x}, t)$ characterizing the wave field as a function of horizontal wavenumber $\mathbf{k}$, horizontal position $\mathbf{x}$, and time $t$

$$\begin{aligned}\frac{DF}{Dt} &= \frac{\partial F}{\partial t} + \dot{x}_i \frac{\partial F}{\partial x_i} + \dot{k}_i \frac{\partial F}{\partial k_i} \\ &= S_{in} + S_{nl} + S_{ds} \\ &= S\end{aligned} \tag{1}$$

with Hamilton's equations for the phase space coordinates $\mathbf{k}$, $\mathbf{x}$,

$$\dot{x}_i = \frac{\partial}{\partial k_i} \sigma(\mathbf{k}, \mathbf{x}), \qquad \dot{k}_i = -\frac{\partial}{\partial x_i} \sigma(\mathbf{k}, \mathbf{x}) \tag{2}$$

and where $\sigma = (gk \tanh kH)^{1/2}$ is the dispersion relationship for surface gravity waves in water of depth $H$. Unknown to Hasselmann at the time, a similar proposition had been made by Gelci et al. in 1957[8] but not further explored.

The energy balance equation accounts for a fundamentally statistical description of ocean (surface) waves.[b] The local spectral wave energy density then evolves under the influence of the following three main "source" terms in (1).

1) A term $S_{\text{in}}$ describing the physics of energy input from the atmosphere to the surface wave field (air-sea interactions).
2) A term $S_{\text{nl}}$ describing the redistribution of spectral energy due to resonant nonlinear wave–wave interactions among different spectral components.
3) A term $S_{\text{ds}}$ capturing all processes that lead to spectral energy dissipation, such as white-capping, wave–bottom interactions and dissipation in shallow water.

The sum of these source terms, $S$, represents the net energy transfer at wavenumber $\mathbf{k}$ due to all sources, sinks, and transfer processes affecting $\mathbf{k}$.

Although the functional form of each of these terms remained virtually unknown at the time (and for two of these terms remains subject to considerable uncertainty today), the very structure of the equations, along with certain invariance principles provided strong constraints on the general functional form, thus offering the prospect of predictive modeling of the surface wave field via integration of the spectral energy balance equation. Importantly, such a dynamical wave field description could account for the integrated effect of wave field evolution back in time, everywhere in the domain, on the local wave spectral energy at the current time.

## From Invariance to a Closed Nonlinear Interaction Theory

Within the spectral energy balance framework, Hasselmann[9–11] cast a conservative weak nonlinear interaction theory that described the gradual growth of long swell from short windsea through nonlinear resonant wave–wave interactions, which preserved overall energy, but led to a redistribution of energy within the wave spectrum. The theory borrowed concepts from the description of nonlinear interactions between lattice vibrations in solids[12] and applied in quantum scattering theory of nonlinearly interacting particles.

First, a Hamiltonian is formulated for the linear system in terms of generalized momenta and transformed into normal mode variables for free waves akin to those of the quantized linear harmonic oscillator. The full nonlinear Hamiltonian may then be expressed as a Taylor series expansion around the linear system, where symmetry and invariance principles impose constraints on the coupling coefficients of the higher order terms. At each order of the Hamiltonian's Taylor series expansion, resonance conditions are encountered among a set of $N$ interacting wave components, which produce dominant contributions due to the secular energy redistribution over finite times. Previously, Phillips (1960)[13] and Longuet-Higgins (1962)[14] had carried out perturbation expansions to third order and showed that the dispersion relationship for surface gravity waves did not admit any resonance among three interacting waves. Carrying out a perturbation expansion to fifth order, Hasselmann (1962)[9] demonstrated that the resonant wave–wave interaction among four waves represented a feasible nonlinear interaction that could account for the growth of long-wavelength swell by redistributing energy within the wave spectrum.

Through a wave–particle duality the spectral energy can be related to the number density of the wave group in $(\mathbf{k}, \mathbf{x})$ phase space. This establishes an analogy between nonlinear resonant wave–wave interaction and particle–particle scattering.[10] This, in turn, led Hasselmann to the description of the perturbation expansion series through Feynman diagrams representing the various processes in the conservative perturbation expansion.[15] In this picture, resonance of a wave quadruplet implied the scattering among three wave components to a fourth. Hasselmann (1967)[16] extended this formalism to include nonconservative wave–atmosphere turbulence, wave–ocean turbulence, and wave–ocean current interactions. His initial dive into the conceptual framework of Feynman diagrams would raise his interest in fundamental particle physics, as he saw it as an avenue to make progress on a unified theory of particles and fields. He would pursue this interest in his free time over the course of his career, as detailed below.

Concluding an initial flurry of research on surface waves, Hasselmann (1968)[17] proposed a "complete"[c] weak nonlinear interaction theory including all expansible

[b]Analogy with geometric ray theory enables an interpretation as the continuity equation for the number density of wave groups in phase space, along with the application of Liouville's theorem.

[c]The theory is "complete" in that it accounts for all expansible processes, including local wave generation, wave–wave interaction/scattering, and parametric damping by turbulent processes. Nonexpansible processes, in particular dissipation due to white-capping and turbulent bottom friction cannot be strictly accounted for within this framework.[17]

terms for wave growth, wave dissipation, conservative nonlinear wave–wave coupling, as well as nonconservative wave–external field interactions. This work proved foundational to this day for the development of skillful global ocean wave modeling and prediction.

### Approximate Solutions and Experimental Evidence

Solving the perturbation expansion involved a five-dimensional Boltzmann collision integral for an ensemble of interacting particles. Initial numerical solutions needed to be carried out in highly approximate form and for different empirical wave spectral shapes.[11] Encouraging qualitative agreement was found with data obtained during the classic field campaign to measure ocean swell that originated in the Southern Ocean during austral winter storms off New Zealand, propagating across the Pacific Ocean, and detected at several stations set up along great circle paths all the way to the coast of Alaska.[18]

The critical role of nonlinear wave–wave interactions in extracting energy from the central part of the spectrum and redistributing it at low and high frequencies was further corroborated in the Joint North Sea Wave Project, a field campaign held during the summers of 1968 and 1969 (JONSWAP).[19] It was the first of many efforts organized by Hasselmann to bring together the community to solve complex scientific problems. JONSWAP enabled the study of wave growth under quasicontrolled conditions, which led to a more accurate description of the growth term of windsea spectra, $S_{in}$ of (1). It was another scientific milestone that has withstood the test of time.

### From Theory to Numerical Prediction

Moving on from ocean swell and JONSWAP, Hasselmann laid the foundation to modern ocean surface wave prediction. Together with his wife, Susanne, he guided the community in the development of the third-generation WAve Model WAM (WAMDI Group 1988).[20] The model was run at the time on early supercomputers, such as Cray Research's Cray-1 and Control Data Corporation's Cyber-205. The most important progress compared to earlier wave model generations was an improved numerical representation of the full five-dimensional Boltzmann transfer integral underlying the nonlinear wave–wave interactions, $S_{\mathrm{nl}}$ of (1), work that Hasselmann undertook again with his wife.[65] Exploiting a number of symmetries among the interaction terms, their work led to a both faster and more accurate approximation to the full transfer integral. The numerical algorithms underlying WAM form the backbone of most operational wave forecasting models in use to this day at leading numerical weather prediction centers worldwide, including at ECMWF ("HRES-WAM") in Europe and at NOAA (WAVEWATCH-III) in the U.S. The wide interest in, and impact of this work is evidenced by the fact that it was supported by entities ranging from the European Space Agency to the U.S. Office of Naval Research.

In parallel, Hasselmann recognized that forthcoming, ocean-dedicated Earth observing satellites, notably the first European Remote Sensing satellite ERS-1, offered the prospect of quasisynoptic wave data for forecasting applications. Having also published on radar backscatter modulation from sea surface waves as early as 1971,[22] he once again convened the community in the Marine Remote Sensing field campaign in 1979,[21] during which radar remote sensing techniques were explored in preparation for ERS-1. In 1980 Hasselmann became a member of the European Space Agencies' High-level Earth Observation Advisory Committee. He and his wife went on to derive a computationally efficient algorithm for inverting the nonlinear mapping between wave spectra and the distorted SAR image spectra, which was eventually implemented for ERS-1.[23] To overcome the practical issues of limited data transmission, Hasselmann also devised the so-called ERS-1 SAR "imagette mode," which operated over the ocean, taking smaller subimages ("imagettes").[24] Finally, as early as 1985, he laid out a framework for assimilating the satellite retrievals into a numerical model, preempting modern data assimilation schemes in operation today at numerical weather prediction centers.[25,26]

## CLIMATE RESEARCH

It is not hard to imagine that Hasselmann's approach to surface wave modeling and forecasting strongly influenced his thinking about the problem of climate dynamics and prediction. Similarly to recognizing the statistical nature of the evolution of, and nonlinear interaction among surface waves, Hasselmann considered the climate system to require a basic description within a stochastic dynamical framework. His approach was to proceed from simple conceptual models capturing salient features—in part due to severe computational limitations early on—to models of increasing complexity, always seeking to find methods within which reduction in complexity was paired with retaining—or exposing—mathematical structure and physical insight in the reduced-order models.

### Stochastic Climate Models

To understand the origin of natural climate variability, Hasselmann's initial goal was to obtain a basic description spanning the vast range of time scales, from seasonal anomalies to that of Pleistocene ice age cycles. To do so required a description of spectral properties of climate variations, in particular an explanation of the substantial variance found at low frequencies. Deterministic feedback models proposed at the time tended to produce, according to Hasselmann, artificial "flip-flop" transitions in discord with the observed quasicontinuous spectrum of climate variability.[d] In his foundational 1976 article[27] Hasselmann proposed instead to describe climate variations in terms of stochastic processes, such as captured in the theory of *Brownian motions*[28,29] or *random walks*.[30] According to this description,

> *the variability of climate is attributed to internal random forcing by the short time scale 'weather' components of the system. Slowly responding components of the system, such as the ice sheets, oceans, or vegetation of the Earth's surface, act as the integrators of this random input much in the same way as heavy particles embedded in an ensemble of much lighter particles integrate the forces exerted on them by the light particles.*[27]

It is important to note that while general circulation models (GCMs) that integrated approximate forms of the Navier–Stokes equations were beginning to come online at the time in the developing field of numerical weather prediction,[31,32] integrating such "GCMs" over climate-relevant time scales (tens to thousands of years) remained out of reach initially, despite the seminal work being pursued beginning with Manabe and colleagues at the NOAA Geophysical Fluid Dynamics Laboratory (GFDL).[33–35] Alternative methods were thus required to quantify climate variations on time scales of years to millennia. So-called *Statistical Dynamical Models* were being devised, which integrated slow time-scale behavior while averaging fast time-scale processes using some closure assumptions. These resulted, however, despite their naming, in *deterministic* solutions of the slow time-scale variables, which were used to investigate the response of the climate system to external forcing, but which were limited in their ability to produce "red noise" behavior of the climate variance spectrum.

The stochastic modeling approach proposed by Hasselmann overcame this limitation by explicitly accounting for the fast, high-frequency turbulent weather fluctuations as stochastic forcing in what is in practice a stochastic differential equation. An important result of such processes is that a stationary random (white noise) forcing may produce a red noise response.[e] As a remarkable consequence, Hasselmann pointed out that

> *the problem of climate variability is not to discover positive feedback mechanisms which enhance the small variations of external inputs or produce instabilities, but rather to identify the negative feedback processes which must be present to balance the continual generation of climate fluctuations by the random driving forces associated with the internal 'weather' interactions.*[27]

Such negative feedback processes have subsequently been studied.[37,38] The stochastic climate model may be reinterpreted as a first-order autoregressive process that is characterized by a stationary mean, but whose variance may grow linearly in time.[39] Such behavior is characteristic of Brownian motions[28,29,40] or random walk processes.[30]

With his 1976 work, Hasselmann formulated the generic statistical null hypothesis of *natural climate fluctuations:* in order to test whether observed low-frequency or secular changes in the climate record were due to external forcing (anthropogenic or otherwise), one had to demonstrate that such changes could not be explained (to some degree of confidence) by natural climate variability, whereby low-frequency, red-noise variations were generated internally (as opposed to forced externally) due to high-frequency, white-noise fluctuations.

From here on, a climate research programme needed to tackle two major issues.

1) A better representation of *natural* climate variability beyond simple autoregressive models through the development and maturation of sophisticated GCMs that were able to integrate approximations of the Navier–Stokes equations for fluids on a rotating sphere, representing the

[d]This seemingly subtle distinction has implications for potential tipping-point behavior of nonlinear systems described as either deterministic or stochastic processes.

[e]Hasselmann[27] draws an explicit connection between the stochastic climate model framework and that of a weak nonlinear interaction theory (see previous section) by noting that the time-scale separation into a fast time scale of an ensemble of independent random fluctuations and slow response time scale on the one hand and the weak nonlinear interaction among components of a field of independent random motions on the other hand. Much more has since been studied within the stochastic climate modeling framework.[36]

atmospheric circulation (later coupled to an ocean, cryosphere, and land model) over long time periods relevant to climate variations.

2) A quantitative approach for detecting changes in the climate system that were due to *external forcing processes* within the noise of *internal* (i.e., natural) fluctuations of the stochastic climate system.

Syukuro Manabe, hired by GFDL's founding director Joseph Smagorinsky in 1959,[41] and colleagues (among which oceanographer Kirk Bryan, hired in 1961), building on modeling work in the context of early numerical weather prediction by Norman Phillips, John von Neumann, and Jules Charney,[31] made initial ground-breaking contributions to the development of comprehensive GCMs of the coupled climate system[35] (for a detailed account, see the recent monograph by Manabe and Broccoli, 2020[4]), thus addressing issue 1). With regard to issue 2), soon after formulating the null-hypothesis of natural climate variability that produces internally generated low frequency variations on all climate-relevant time scales, Hasselmann developed another computational framework within which to undertake the formal detection of externally forced, i.e., human-made climate change and the attribution of specific patterns of change to specific external forcing mechanisms, such as from greenhouse gas emissions versus aerosol forcing. More on this in the following.

## From Stochastic to Reduced-Order Dynamical Models

Complementing efforts to develop comprehensive GCMs of the global climate system that required substantial computational resources, Hasselmann recognized a need for reduced order models for at least two reasons: first, by analogy with nonlinear wave–wave interaction theory and stochastic dynamics, Hasselmann posited that the complex interactions between a broad range of time scales of the different components of the climate system would remain out of reach of cutting-edge GCMs and available supercomputers for the foreseeable future, thus limiting the spectral bandwidth of simulated climate variability by GCMs; second, identifying a low-order representation of the full climate system along with associated "patterns" would lead to considerable understanding of the underlying dynamics governing large-scale, low-frequency climate variability. It would also pave the way for making pattern detection tractable.

To proceed, Hasselmann[42] sought a representation that would go beyond accounting only for an optimal spatial covariance structure among a set of "modes" over time, as afforded by the principal component analysis (also known as empirical orthogonal function (EOF) analysis, proper orthogonal decomposition, or Karhunen–Loève decomposition). Instead, the derived "modes" should also be an optimal representation for the *time-evolution of the reduced-order system*. To accomplish this, Hasselmann[42] introduced the framework of *principal interaction patterns* (PIPs), which sought to combine and extend two concepts: 1) the concept of EOFs to represent low-order aspects of high-dimensional statistical fields, and 2) the autoregressive moving average concept for constructing dynamical models of systems with a few degrees of freedom.

The PIP concept consists of determining (either jointly or separately) an optimal set of spatial patterns and coefficients of a general linear or nonlinear dynamical system, represented via a set of ordinary differential equations (ODEs), through a least squares minimization of a misfit between the time derivative of the full system (either from observations or simulation) $\dot{\mathbf{\Phi}} = d\mathbf{\Phi}/dt$ and its low-order representation $\dot{\hat{\mathbf{\Phi}}} = d\hat{\mathbf{\Phi}}/dt$. Concretely, the full state vector $\mathbf{\Phi}$ is approximated by a reduced-order system $\hat{\mathbf{\Phi}}$ of time-independent PIPs $\mathbf{p}_i$ with residual error $\boldsymbol{\rho}$, such that

$$\mathbf{\Phi} = \hat{\mathbf{\Phi}} + \boldsymbol{\rho} \tag{3}$$

where

$$\hat{\mathbf{\Phi}} = \sum_{i=1}^{m} z_i(t)\, \mathbf{p}_i. \tag{4}$$

The time-varying expansion coefficients $z_i(t)$ obey a set of (in general nonlinear, time-dependent) dynamical systems equations with noise $n_i$

$$\frac{dz_i(t)}{dt} = G_i(z(t); \alpha_1, \ldots, \alpha_p) + n_i. \tag{5}$$

Determining the reduced-order system then consists in finding a set of unknown model parameters $\alpha_j,\ j = 1, \ldots, p$ and PIPs $\mathbf{p}_i,\ i = 1, \ldots, m$, which minimize the the mean square error

$$\epsilon = ||\dot{\hat{\mathbf{\Phi}}} - \dot{\mathbf{\Phi}}||^2. \tag{6}$$

Substituting the evolution (5), a general solution to the problem, i.e., optimal spatial patterns (PIPs) and dynamical system parameters, may be obtained via gradient-based optimization, exploiting the gradient of $\epsilon$ with respect to the parameters $\alpha_j$ and PIPs $\mathbf{p}_i$. The approach has several striking features: First, an approach for a general solution involves the adjoint operator of the dynamical systems operator to efficiently compute the gradient. Hasselmann explicitly refers to adjoint gradient techniques as a solution method. As such, the PIPs may be viewed as low-order dynamical systems versions of PDE-constrained optimization of inverse problems (e.g., atmospheric data assimilation[43] or ocean parameter and state estimation[44]). Second, a broad analogy exists to the concept of neural ODEs[45] if the dynamical systems operator is replaced by a neural ODE operator or neural network. In this case, the adjoint of the dynamical systems operator (gradient of the misfit error with respect to the parameters) is replaced by the mathematically "equivalent" notion of "backpropagation" (gradient of the misfit error $\epsilon$ with respect to the network weights).

These examples highlight the way in which Hasselmann's 1988 proposed PIP framework presaged today's "data science" or "data driven" algorithms, notably that of dynamical mode decomposition,[46] with the PIP concept retaining important properties of a dynamical system. Like many of the reduced-order modeling approaches, whether PIPs lend themselves to capturing the stringent constraints imposed by conservation laws remains unclear.

The operator $G_i$ arising in (5) is in general nonlinear. Hasselmann also considered the special case in which $G_v$ is linear, and the corresponding optimal patterns he termed *principal oscillation patterns* (POPs). The linear approach has subsequently been used extensively in climate diagnostics [see, e.g., the review by von Storch et al. (1995)[47]] and more recently in the disguise of "linear inverse models."[48] In contrast, only very few direct but noteworthy applications of the nonlinear PIP framework have been conducted.[49,50]

## Detection and Attribution of Anthropogenic Climate Change

With the stochastic climate model providing an effective "null-hypothesis" of natural climate variability that is well described by a red noise or Markov process, a question becomes how to distinguish between apparent signals due to external forcing and the low-frequency "noise" generated by natural fluctuations. Hasselmann recognized the conceptual similarity between this problem and that of the use of optimal filters for signal extraction from noisy data encountered in various areas of engineering and signal processing. His initial proposition to solving this signal-to-noise maximization problem in the context of climate change detection[51] received little attention. This was likely due in part to the lack of appreciation by the community of its significance, as well as to the fact that an important ingredient, namely that of robust estimates of long-term climate variability were not available at the time. Hasselmann perceived a central role for climate models in solving this problem not only in the simulation of "signal patterns" of externally forced, i.e., anthropogenic climate change, but also—and equally important—in the provision of long records of (simulated) natural climate variability that provide an adequate low-frequency "noise" statistics (in terms of spectral characteristics and magnitude) against which to conduct signal detection studies.

The advent of such long (millennial) coupled atmosphere–ocean climate model simulations in the 1990s opened the door to conducting such rigorous detection studies. Hasselmann (1993)[52] revisited and extended his 1979 treatment to a time-dependent multivariate climate signal, while also simplifying its mathematical formulation. He laid out a mathematical framework for

> *constructing an optimal space-time dependent filter*—a fingerprint—*that maximizes the signal-to-noise ratio for the associated detector for any multi-variate, space-time-dependent climate signal.*

The framework has the following three ingredients.

1) A time-dependent (forced) climate change signal pattern.
2) A statistical estimate of natural climate variability (noise pattern), e.g., from an ensemble of simulations or from a long integration (and assuming ergodicity).
3) Construction of an optimal detection variable (detector) and associated optimal fingerprint.

Given a climate trajectory (either from observations or from a simulated response to external forcing), represented by a state vector $\boldsymbol{\Psi}$ (which need not be spatially or temporally complete, as is typically the case for measurements) the detection problem consists of determining whether the trajectory can be distinguished from the statistical ensemble of natural variability trajectories. Assuming a known space-time signal pattern $\psi$ of the deterministic signal trajectory $\boldsymbol{\Psi}^s = c\,\psi$ with unknown amplitude $c$, and separability between signal and noise trajectory, $\boldsymbol{\Psi}^s$, $\boldsymbol{\Psi}^n$ (with the latter a realization of the ensemble of natural variability), we can write

$$\boldsymbol{\Psi} = \boldsymbol{\Psi}^s + \boldsymbol{\Psi}^n \,.$$

An optimal (scalar-valued) detection variable $d$ with associated optimal fingerprint $\boldsymbol{f}$ is sought, such that

$$d \;=\; \boldsymbol{f}^T\boldsymbol{\Psi} \;=\; d^s + d^n$$

where $d^s = f^T \Psi^s$ and $d^n = f^T \Psi^n$ represent the signal and natural variability components, respectively. For the fingerprint $f$ to be optimal, the signal-to-noise ratio

$$R^2 = \frac{(d^s)^2}{< (d^n)^2 >}$$

is maximized over all possible patterns $f$. Application of the Lagrange multiplier method leads to a solution for the optimal fingerprint in terms of the signal pattern $\psi$

$$f = \mathrm{C}^{-1} \psi \,. \tag{7}$$

Here, C is the covariance matrix of natural climate variability, inferred from climate model simulations under unforced conditions. If the problem is recast in a reduced order basis with statistical orthogonal eigenvectors, such as EOFs or the POPs introduced earlier, (7) simplifies considerably to

$$f_i' = \sigma_i^{-2} \psi_i' \,, \quad i = 1, \ldots, m.$$

The result has the following important consequences.

1) Having access to a robust estimate of natural climate variability to obtain an estimate of $\mathrm{C}^{-1}$ is critical.
2) The optimal fingerprint direction is generally not parallel to the assumed signal direction.[52] Instead, each component of the signal vector is weighted by the variance (or, more generally, covariance) of the estimated natural climate variability. Regions of large natural fluctuations may mask information carried in the climate signal pattern.
3) With respect to the EOF or POP basis functions, large variances act to down-weight corresponding components, thus shifting patterns from high-noise to low-noise directions.

Another important ingredient to increase significance in the detection is the dimension reduction of the complex space-time-dependent natural variability.[53] Here, the previous development of POPs[42] plays an important role at rendering the problem tractable.

Hasselmann (1993)[52] proceeded with generalizing the framework to a multipattern detection problem, which lays the foundation for solving another key problem of climate science, namely that of signal *attribution*, beyond its *detection*. The general multipattern fingerprint method for detection and attribution of climate change was presented in 1997.[54] The breakthrough application of the optimal fingerprint method to detecting greenhouse-gas induced climate change was conducted by Hegerl et al.[55,56] and, using a related method, by Santer et al.[57,58] They are considered as milestones leading the Intergovernmental Panel on Climate Change to conclude, in its Second Assessment Report (1995) that "The balance of evidence suggests a discernible human influence on global climate."[59] A number of detection and attribution studies were conducted in the following years.[60]

An important aspect of early detection and attribution studies is the fact that optimal fingerprints are most likely associated with large-scale patterns. As Hasselmann pointed out,[61] policymakers are interested in assessing local changes, which may not be reliably represented in global climate models. Overcoming the challenge in moving from global scale to regional or local detectors requires both higher resolution climate models[62] that more reliably capture highly localized probability distributions of climate-relevant variables and extended approaches of extreme event attribution.[63,64]

## TOWARD A UNIFIED THEORY OF FIELDS AND PARTICLES

Hasselmann's work on nonlinear resonant wave–wave interactions during the 1960s and his realization that the perturbation expansion within a nonlinear interaction theory, which he developed could be cast in terms of Feynman diagrams developed for particle–particle scattering[15] raised his interest in elementary particle physics. Being deeply immersed in expressing the nonlinear interactions among a set of wave packets in terms of particle collision probabilities for the purpose of practical computation,[65] he became suspicious about the established quantum mechanical interpretation of the fundamental wave–particle duality. In particular, the inability to give a precise description of microscopic objects (either as particles or fields), but instead to resort to the *wave function* as a fundamentally probabilistic description of such objects was at odds with his intuition, as was the "imprecise demarcation" between classical and quantum phenomena. While accepting the many astonishing successes that quantum mechanics and quantum field theory have had—and continue to have—in describing a wide range of experimental phenomena, he posited nevertheless that it remained unsatisfactory. In particular, he shared the skepticism regarding the exhaustive description of reality by a wave function as expressed in the Einstein, Podolsky, and Rosen (EPR) paradox[66] and was convinced that the unfinished program pursued by Einstein of a complete unified theory would hold the key to a deeper understanding of fundamental physics. As a prominent example, he pointed to the Standard Model of elementary particle physics with its 18 free parameters and which failed to explain the mass hierarchy of elementary particles from first principles. Particle physics thus became an intellectual passion of Hasselmann since the late 1960s, one which he chose to pursue in his spare time instead of as a professional career, because of his worry that running against mainstream theoretical physics would be unsustainable. The following summary follows that of von Storch and Heimbach (2022).[67]

Hasselmann set out to develop a unified deterministic theory of particles and fields, which he termed the "metron model" and which he only published some three decades after embarking on this work.[68–71] He was guided in his ideas by Einstein's notion of a *unified field theory*, which Einstein had pursued since the early 1920s.[72] A starting point of this model was the concept introduced by Theodor Kaluza (1921)[73] and Oskar Klein (1926)[74] of a five-dimensional generalization of Einstein's equation of general relativity which unified electromagnetism and general relativity within a higher dimensional field theory. [Previously, Hermann Minkowski (1909)[75] had formally combined special relativity and electromagnetism within a four-dimensional geometric theory.] Hasselmann's fundamental equations of motion would consist of a ($4 + D$) dimensional generalization of Einstein's nonlinear equations in matter-free space.

Crucial to Hasselmann's programme is the existence of soliton solutions to the generalized nonlinear field equations. These solitons would manifest in different ways, dependent on their near-field and far-field properties. In the soliton's localized core or near field, it would behave strongly nonlinear, a manifestation of particle-like properties (mass, charge, spin, weak, and strong coupling constants). In contrast, its far field manifestation would be linear, i.e., exhibit wave-like superposition properties consistent with classical gravitational and electromagnetic fields.

In giving precise meaning to microscopic properties of wave-like and particle-like behavior, the soliton solution as a single object thus resolves the wave–particle duality, avoiding the need for a probabilistic interpretation of wave functions. Hasselmann termed such soliton solutions *metric solitons* or *Metrons*. Furthermore, drawing from his experience in nonlinear resonant wave–wave interactions he surmised that all quantization phenomena could be described by resonant interactions between scattered far-field waves and particle trajectories. In today's parlance, quantum mechanics could then be regarded as an emergent property of the generalized nonlinear (classical) field equations (some theories currently under debate are pursuing an opposite approach of gravity as an emergent property from quantum mechanics).

Other features of Hasselmann's metron programme worth noting are the following.

1) All four fundamental forces should emerge geometrically from the curvature of the spacetime components, the extra-dimension components, and mixed spacetime-extra dimension components. This generalizes the five-dimensional Kaluza–Klein theory, within which the energy–momentum field tensor arises as a geometric property (i.e., from the metric tensor and its derivatives).
2) The generalized equations (Einstein's gravitational field equations in higher dimension) would have no source term (i.e., matter free), such that "the curvature is not produced by prescribed mass fields, but is a self-generated feature of the nonlinear field equations themselves."[68]
3) The "coupling constants and symmetries are not postulated in the basic field equations, but follow from the specific geometrical properties of the metron solutions."[68] Avoiding the use of physical constants in the $D$-dimensional nonlinear vacuum equations, Hasselmann's ambition was to overcome the perceived shortcomings of the Standard Model and to derive these constants, in particular the hierarchy of observed particle masses, from solutions to the equations.
4) Addressing the concept of entanglement, the metron theory regards fermions, bosons, and gravitons as not independent, but instead as different manifestations of a single particle. As example, Hasselmann[76] invokes the emission of a photon from an atom as simply the electromagnetic far field of an electron as it transitions from one orbital state to another in its interaction with the atom's nucleus.

In order for the metron programme to be viable, a number of challenges need to be solved, some of which Hasselmann's addressed, others remaining open questions. An immediate concern is the metron model's apparent violation of Bell's theorem (a generalization of the EPR paradox) on the nonexistence of deterministic hidden-variable theories (Bell, 1964).[77] Hasselmann solved this seeming contradiction by pointing to the fact that the basic field equations are invariant under time reversal at the microscopic level, but which is at odds with Bell's theorem which postulates the existence of an arrow of time (see Hasselmann, 2013,[76] for a detailed discussion in the context of entanglement). A key stepping stone of the metron programme is the ability to find nontrivial soliton solutions to the generalized nonlinear vacuum field equations. Searching for such solutions has been a major occupation of Hasselmann, together with his wife Susanne, since their retirement. Initial progress has been made and documented for the simplest possible particle, the electron,[76,78] however much of this project remains outstanding. Another explicit goal of the metron programme is the ability to derive the observed, discrete particle spectrum as solution of the field equations, which at present remains an unsolved problem.

A compelling test of the metron theory would be its ability to predict *new* phenomena in elementary particle physics or astrophysics that are not being predicted by established theories and that could be verified experimentally. Such a test is certainly elusive at the present time, as is a confirmation (or falsification) of the metron programme. Hasselmann himself invoked the scientific process to be the ultimate judge of his programme in his 2006 interview, in which he states

> *Once the theory is published in accepted journals, it will become either accepted or rejected. This is as it should be. I am not really concerned about the outcome, which is beyond my control." (von Storch and Olbers, 2007, reproduced in von Storch's work[3]).*

The challenges ahead are likely as much theoretical as they are in terms of bringing to bear computational solution approaches. In light of Hasselmann's groundbreaking achievements, it is hoped that physicists will be compelled to examine the metron programme and its potential merits more closely.

## FINAL THOUGHTS

This review covers some, but by far not all of Hasselmann's contributions to climate science, geophysics, and physics more broadly. Several aspects of his work have been left unmentioned, notably his work on internal waves in the ocean, and his leadership as founding director of the Max-Planck-Institute for Meteorology in the development of a comprehensive coupled climate model that has been among the world's leading climate modeling enterprises since the 1980s. In his quest for tackling the problem of anthropogenic climate change, Hasselmann also recognized that beyond a sufficient level of scientific consensus regarding its reality, which was reached by the late 1990s (despite some lingering "noise"[79]), the largest uncertainty became the climate system's connection with environmental and socio-economic issues. Once again, Hasselmann's conviction rested on the need for obtaining some basic quantitative understanding of the underlying issues through the incorporation of socio-economic models into Earth system models in order to estimate optimal emission path scenarios, as well as the exploration of game-theoretic approaches for understanding multiactor behavior in climate negotiations.[80–82] Whether such integrated assessment models are useful tools has remained subject for debate, but which prompted Hasselmann to pose as a challenge to the science community to mature such approaches into tools that are useful and used in practice.[83] Nevertheless, his work on quantifying feedbacks between the climate, environmental, socio-economic, and human systems to infer optimal greenhouse gas emission paths, led Hasselmann to the conviction that the climate change problem "is quite solvable," provided that adequate investments in available and emerging renewable energy technologies are made.

In all of the work reviewed in this article, Hasselmann's foundational contributions are based on pairing physical insight with extracting essential features from complex systems through salient mathematical properties of the governing equations, which permitted the development of a hierarchy of simulation approaches, from simple conceptual models to comprehensive models, which today harness some of the world's fastest supercomputers.[62] Arguably, he also presaged the era of "data science" as he sought to develop data-calibrated reduced-order models for fast computation, pattern detection methods to uncover signals in noisy data, and inverse methods (data assimilation) to learn from the incomplete knowledge reservoirs of sparse observational data and models. In developing these, he was guided closely by the underlying governing dynamics of the systems at hand which, he recognized, provided powerful constraints on the solution manifold.

It is hoped that this review will raise the curiosity of computational scientists and engineers to dive deeper into Hasselmann's extraordinarily broad work at the interface of climate physics, mathematics, and computational science. They will find that their expertise remains essential for thinking outside the box and for making further progress in today's and tomorrow's climate modeling enterprise.[84]

## ACKNOWLEDGMENTS

I wish to thank Lorena Barba for initiating this review. I benefited from discussions with Hans von Storch, Carl Wunsch, and Susanne Hasselmann. All errors are mine.

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**PATRICK HEIMBACH** is a computational oceanographer, professor in the Jackson School of Geosciences, and W. A. "Tex" Moncrief, Jr., chair III in simulation-based engineering and sciences in the Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin, Austin, TX, 78712, USA. He is an expert in the use of inverse methods and automatic differentiation applied to ocean and sea ice model parameter and state estimation, uncertainty quantification, and observing system design. Heimbach received his Ph.D. degree from the Max-Planck-Institute for Meteorology, University of Hamburg, Hamburg, Germany. He is member of the WCRP Lighthouse Activity on Explaining and Predicting Earth System Change and the U.S. CLIVAR Ocean Uncertainty Quantification working group. Contact him at heimbach@utexas.edu.