observation of the acceleration of characteristic X-ray radiation with transitions from the L_{III} electron shell appears possible even if in the X-ray photon counting mode.

Acceleration of the second-forbidden capture is easier to realize. The necessary intensities of laser radiation can be achieved even by focusing radiation from powerful continuous wave lasers. Equally possible are experiments in a constant electric field of 10–100 MV cm^{-1}, i.e., in a field lower than the breakdown field voltage of many pure dielectrics containing nuclei of interest.

Finally, considerable acceleration of the neutrinoless double capture of electrons, as well as verification of Majorana's hypothesis for the nature of neutrino, is possible in an experiment with a plasma consisting of electrons and neonlike $^{74}Se^{24+}$ ions. Also, the use of heavy ^{168}Yb ions offers great prospects.

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Computational physics and testing theoretical predictions

L N Shchur

1. Introduction

Computational physics was born simultaneously with the creation of the first electronic computers.[1] Physicists used computers to achieve a practical goal important at that moment: to develop thermonuclear weapons. One of the first computational tasks needed for peaceful applications was the work of Fermi, Pasta, and Ulam [1] on simulating the dynamics of the one-dimensional nonlinear chain; the work was done on the MANIAC 1 mainframe computer in Los Alamos [2]. The opinion prevalent at the beginning of the 1950s was that nonlinearity should lead to equipartition of energy over degrees of freedom, i.e., to stochastization. Contrary to expectations, numerical experiments revealed quasiperiodic behavior. This phenomenon was explained in 1965 by Zabusky and Kruskal [3], who numerically identified solitons (and introduced the very term 'soliton') and found their inelastic scattering. This result led to the discovery of the inverse scattering problem method [4] which, in turn, became the key to obtaining exact solutions of nonlinear problems (see, e.g., monograph [5]). This is an impressive example of the

[1] The author uses the Russian term 'electronic computing machine' (EVM in *Russ. abbr.*) interchangeably with the currently widespread term 'computer' in those section of the text where it was historically justifiable. The English translation uses the term 'computer' throughout.

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success of computational physics and, in particular, of the computational experiment — the first case of a numerical experiment generating new knowledge.

Another important method created at about the same time was the Monte Carlo method developed by Metropolis in collaboration with Rosenbluth and Teller for modeling thermodynamic phenomena [6]. The Monte Carlo method lies at the basis of virtually the entire current research in computational statistical physics.

The distinguishing characteristic of computational physics consists in using computers for the study of physical phenomena. Important aspects of the successful application of computers are the algorithms and methods of calculation and simulation, as well as methods of processing the results obtained, thereby extracting new knowledge.

This report presents the author's experience in applying the methods of computational physics to testing theoretical predictions and hypotheses. As an illustration we have selected several specific examples of solving problems of nonlinear physics and statistical mechanics; they develop and demonstrate the current status of these historically first fields to which computational physics was applied.

2. Testing integrability of nonlinear models

In the 1960s–1980s, progress in the inverse scattering problem method led to explosive growth in the number of exactly solved models of theoretical and mathematical physics. For example, attempts were made to exactly solve equations of two-dimensional hydrodynamics, Yang–Mills equations, cosmological problems, and some others. Applications of computational physics can suggest arguments in favor of the integrability of the model or give a definite conclusion of nonintegrability of the model in question, and in some cases achieve results at the level of a 'computer-assisted proof', i.e., the level of rigorousness of a theorem.

2.1 Nonintegrability of two-dimensional hydrodynamics

There is an elegant reply to the question about integrability of two-dimensional hydrodynamics [7]. The energy of a two-dimensional vortex diverges logarithmically. Let us compose a pair of vortices with different signs but equal absolute vorticity κ. The energy of this vortex pair is finite, and its momentum (both projections) is conserved, i.e., a vortex pair exhibits the properties of a particle. This particle is not at rest and, when alone, it moves along a straight line with the constant velocity $v = \kappa/a$, where a is the distance between the vortices. We can analyze numerically the problem of scattering of vortex particles with vorticities κ and $\kappa + \epsilon$ ($\epsilon \ll \kappa$) on one another. The resulting dependence of the scattering angle on the impact parameter is irregular, with accumulation points presenting. The lifetime of the captured state, in which all four vortices are at a finite distance from each other on the order of $\kappa a/\epsilon$, increases in the vicinity of these accumulation points. The divergence of the capture time is analogous to the known phenomenon of the capture of three bodies in celestial mechanics; its nonintegrability was proved by Poincaré [8]. The hope that additional integrals of motion exist in the scattering of vortex pairs (in addition to the above-mentioned energy and momenta) is incompatible with the phenomenon of stochasticity of their scattering. Notice that paper [7] appears to be the first ever computational work on stochastic scattering.

2.2 Nonintegrability of the classical Yang–Mills fields

The problem of integrability of classical Yang–Mills fields, in particular via the numerical solution of equations, was formulated by V E Zakharov and was widely discussed in the scientific literature. An unambiguous answer to the question was obtained in paper [9]. The original Yang–Mills equations can be reduced by an admissible substitution to a dynamical system described by a Hamiltonian with two degrees of freedom. The phase space of the dynamical system $(x, \dot{x}, y, \dot{y})$, where (x, y) are two coordinates, and $(\dot{x}, \dot{y})$ are the corresponding momenta, is four-dimensional. The fixed value of the energy integral $E = -(1/2)\{\dot{x}^2 + \dot{y}^2 + x^2y^2\} = \text{const}$ defines a three-dimensional hypersurface in four-dimensional space. The phase portrait of the system is now numerically constructed in the Poincaré cross section, i.e., the cross section of the three-dimensional hypersurface by the half-plane $y = 0$, $\dot{y} > 0$. If an additional integral of motion I_1 existed, the initial values would fix the value of the integral $I_1 = \text{const}$ and the points of the Poincaré cross section would be isolated or would lie in closed curves defined by this value $I_1 = \text{const}$. Numerical analysis established that invariant curves (or separatrices) of the fixed points intersect at a nonzero angle. For example, trivial periodic solutions $x = y = +F$ and $x = y = -F$, where $F = \text{cn}\,(t, 1/\sqrt{2}\,)$ is the Jacobi elliptic cosine, correspond to fixed points in the Poincaré cross section with coordinates $(0; 1/\sqrt{2}\,)$ and $(0; -1/\sqrt{2}\,)$. The linearized Poincaré map in the vicinity of these points is hyperbolic, and its eigenvalues are $\lambda_1 = 129{,}647014\ldots$ and $\lambda_2 = 1/\lambda_1$. The numerically constructed separatrices of these points intersect at an angle of about 72°. Under the conditions of the numerical calculations, the obtained value of the angle greatly exceeds possible calculation errors. This constitutes the proof of the nonintegrability of Yang–Mills equations in the style of the computer-assisted proof.

2.3 The exact solution of the interchange of Kasner epochs

The next example belongs to the study of statistical properties of the oscillatory evolution [10] of homogeneous cosmological vacuum Bianchi Type-IX models [11]. The duration n of the epoch is measured in the number of oscillations k_n of the epoch. The infinite sequence k_n ($n = 0, 1, 2, \ldots$) is determined by the numbers $x_{-1}, x_0, x_1, x_2, \ldots$ ($0 < x_s < 1$) related to one another by the transformation $x_{s+1} = \{1/x_s\}$, where the braces stand for the fractional part of a number. Note that the durations (lengths) are $k_s = [1/x_{s-1}]$, where the brackets denote the integer part of a number. We can write down an expression for x_s in terms of k_s as a continued fraction $x_{s-1} = 1/(k_s + 1/(k_{s+1} + 1/(k_{s+2} + \ldots \equiv x_s^+$. This law of interchange of epoch lengths results in stochastization of the behavior of the model as it evolves to a singularity. The probability density distribution on the segment $(0, 1)$ of the values $x_s \equiv x$ is given by the Gauss formula $w(x) = 1/(1 + x)\ln 2$. Let us denote the moment when the sth epoch begins by Ω_s; we can now derive the following recurrence formulae relating the characteristics of the two successive epochs:

$$\frac{\Omega_{s+1}}{\Omega_s} = 1 + \delta_s k_s \left(k_s + x_s + \frac{1}{x_s} \right),$$

$$\frac{\delta_{s+1}}{\delta_s} = 1 - \frac{k_s/x_s + 1}{\Omega_{s+1}/\Omega_s}\,.$$

Numerical solution of these equations [12] showed that the quantity $\delta_s \equiv \delta$ has a stable distribution $P(\delta)$ whose plot is approximated well by the function

$$P(\delta) = 1\big(|1 - 2\delta| + 1\big) \ln 2 \,.$$

Analytical studies gave evidence that the problem can be solved by the introduction of a continued fraction with a reverse sequence of denominators

$$x_s^- = 1/(k_{s-1} + 1/(k_{s-2} + 1/(k_{s-3} + \dots \,.$$

It turns out that the joint probability distribution for x_s^+ and x_s^- is given by the formula $P(x^+, x^-) = 1/(1 + x^+ x^-)^2 \ln 2$, which provides the exact solution to the initial problem and confirms that the approximating function given above comprises a solution of the problem, and that it is the exact solution.

This example is significant in that a carefully worked out solution of the problem may lead to discovering the exact result [12]. In its time, it has greatly changed the attitude of theoreticians to work on computational physics.

3. Monte Carlo methods

We have mentioned in the Introduction that, already at the dawn of the computer era, the Monte Carlo method was developed for solving problems of statistical physics. The name itself indicates that the method leans upon randomness (e.g., in choosing values of a random variable from a specific distribution). Computers follow strictly deterministic algorithms, so that randomness cannot be achieved in the course of executing a program. Two approaches appear inescapable, and both have been used ever since the first days of computers: an algorithmic approach to generating a pseudorandom sequence, and an approach using an external source of real noise. In the former, researchers initially applied the middle-square method proposed by J von Neumann. An integer of n bits is squared. This generally gives $2n$ bits, of which the left- and rightmost $n/2$ bits are dropped, while the middle n bits are used as the next pseudorandom number. It was understood rather soon that this method does not generate a sequence that meets the requirements of intuitively expected randomness. In essence, the algorithms for generating random numbers define a mapping of a certain number of equally spaced points of a unit segment onto itself. In other words, the algorithm for generating random numbers is equivalent to a dynamical system in the set of rational numbers of the unit segment. Keeping in mind the lesson of the first computational experiment by Fermi, Pasta, and Ulam on stochastization, one should not be surprized by the fact that the development of algorithmic methods for generating pseudorandom numbers is a serious scientific issue requiring special attention. We shall not engage in a discussion of this largely mathematical problem in this report, referring the reader to detailed discussions of the issue in our papers [13–15]. The second method consists in using a device in which the generation of randomness is based on a physical principle. For instance, a method has recently been proposed to digitize the fluctuating intensity of a chaotic semiconductor laser [16].

In this section, we turn our attention to methods of numerical analysis of models in statistical physics. The main purpose of this analysis is to test theoretical hypotheses and predictions.

3.1 Two-dimensional Ising model with impurities

The effect of impurities on the critical behavior of systems is one of the most interesting features, from both the theoretical and the practical points of view. The critical behavior of the two-dimensional Ising model was studied exactly by Onsager in one of the most beautiful theoretical works [17], published in 1944. At the beginning of the 1980s, the brothers Vladimir and Victor Dotsenko found that the critical behavior of specific heat is modified by a logarithmic correction [18]. Their theory was for a long time the object of intense discussions, with conflicting claims. It was decided to carry out extensive numerical studies.

3.2 Dedicated SPP-1 and SPP-2 processors

In the 1980s, the computational power of supercomputers was insufficient for the numerical study of the fine points of the logarithmic behavior. A group of researchers at the L D Landau Institute for Theoretical Physics (ITF) designed two dedicated processors to attack the problem which presented huge difficulties at the time.

In 1990, they built a processor [19] implementing the Monte Carlo method with Metropolis's algorithm [6] and a pseudorandom number generator of the shift register R250 type [20]. The researchers applied the method of programming with a soldering iron. The algorithm was analyzed and formulated in the form of logical operations with integers and with WRITE and READ memory operations. It was in the end possible to create a computer with an architecture of ideal performance characteristics — all the operations of one Monte Carlo step were performed in one memory cycle. As a result, the performance of the system exceeded that of the Cray 1 supercomputer. Alas, methodological mistakes caused by the order in which generated random numbers were used made it impossible to arrive at any significant results.

In 1994, the second dedicated processor was built [21], which for the first time realized the cluster Monte Carlo method that eliminated the danger of critical slowdown inherent in the Metropolis method. This processor was applied to studying the critical behavior of magnetization, magnetic susceptibility, and specific heat with an accuracy sufficient for reliable confirmation of logarithmic corrections to the three physical quantities mentioned above [22]. The results can be interpreted in the following manner. The correlation length of the pure Ising model, $\xi \propto 1/|\tau|$, where $\tau = (T - T_c)/T$ is the reduced temperature, is modified by impurities in the way that

$$\xi \propto \frac{\sqrt{1 + (4/\pi) g_0 \ln (1/|\tau|)}}{|\tau|} \,.$$

Note that thermodynamic quantities such as magnetization, susceptibility, and specific heat show identical functional dependence on the correlation length both in the pure model and in the impurity model.

Owing to capacity greater than that of the Cray 2 supercomputer, the dedicated processor made it possible for the first time to analyze numerically the correlation function both of pure and impurity Ising models [23], in full agreement with the above interpretation.

The dedicated computer hardware was thus able to successfully conclude the work on the long-standing problem of testing the presence of logarithmic corrections to the thermodynamic functions of the two-dimensional Ising model with impurities.

3.3 The central charge of the Ising model with impurities

Plechko [24] computed the central charge g of the theory for the Ising model with nonmagnetic impurity sites (see also Ref. [25]) as a function of the concentration q of site impurities: $g = 4.843q/(1-q)$. The central charge is included in the dependence of the magnetic susceptibility in the critical region on reduced temperature $\tau = (T - T_c)/T$ as a coefficient of the logarithm:

$$\chi(\tau) = \Gamma|\tau|^{-7/4}(1 + 0{,}07790315\tau)(1 - g\ln|\tau|)^{7/8}\,.$$

Approximating numerical data for the dependence of magnetic susceptibility on temperature by this expression yields the values of two parameters: the amplitude Γ, and the central charge g. The solid curve in Fig. 1 plots the theoretical dependence of the central charge and the results of approximation of the magnetic susceptibility on both sides of the critical point. Both approximations give identical values of the central charge, within computational errors. Both coincide with the theoretical prediction up to the impurity concentration $q \approx 0.1$. This magnitude can be estimated as follows. In addition to the two scales of the pure Ising model, namely the correlation length $\xi \propto 1/|\tau|$ and the size L of the system, the impurity model exhibits two more scales: the mean spacing between impurities $l_i \propto \exp(-1/g)$ [18], and the percolation length $\xi_p \propto (q_c - q)^{4/3}$ [26]. Curiously enough, the last two lengths coincide at $q \approx 0.1$. This can be physically interpreted as indicating that the size of a cluster of nonmagnetic impurities has reached the mean distance between impurities, after which impurities cannot be considered independent, i.e., disorder ceases to be weak.

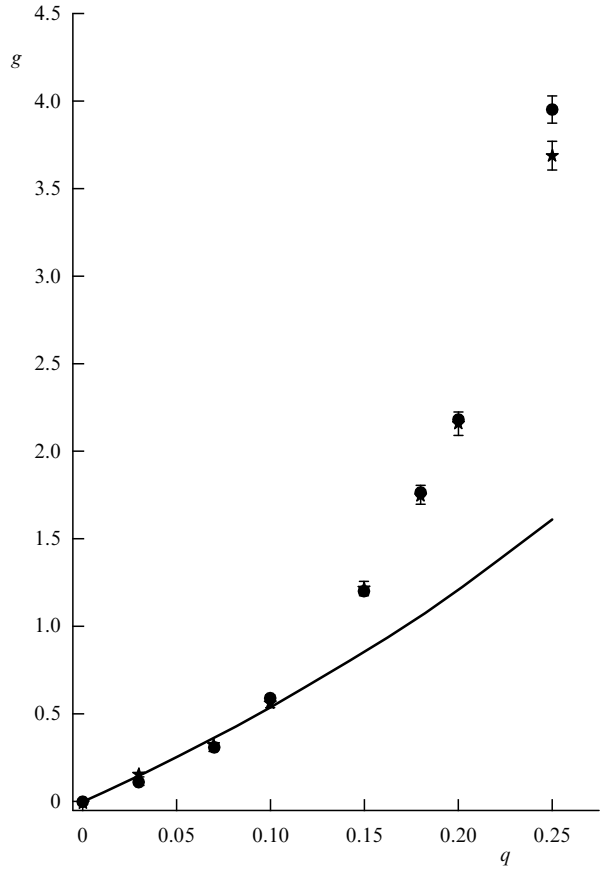

Figure 1. The central charge g as a function of the concentration of site impurities q. The curve traces Plechko's theoretical prediction [24]. Black dots (stars) correspond to an approximation of the numerical data for susceptibility in the low-temperature (high-temperature) field.

3.4 Three-dimensional Ising model and dedicated processors

Attempts to find the exact solution of the three-dimensional Ising model have so far been unsuccessful. This work involves approximate analytical methods and numerical simulation. To test the theoretical hypotheses, one needs to evaluate the critical temperature and critical exponents. Numerical methods for simulation of the three-dimensional Ising model are similar to those discussed above for the two-dimensional model. Evaluation of critical exponents using the renormalization-group methods [27]: $y_t = 1.587(4)$ and $y_h = 2.485(2)$, yields less accurate values than, for example, the values obtained by numerical analysis of high-temperature series [28]; $y_t = 1.5869(4)$ and $y_h = 2.48180(15)$. Early estimates obtained using Monte Carlo techniques [29]: $y_t = 1.590(2)$ and $y_h = 2.482(7)$, yielded rather poor agreement with the predictions of the analytical renormalization group theory.

In the mid-1990s, ITF researchers, together with H Blöte of the University of Delft, developed a cluster processor for studying the three-dimensional Ising model [30]. They implemented the single-cluster Wolff algorithm, which we used successfully in the past to realize a processor for studying the Ising model with impurities [21]. A programmable block was developed to generate random numbers; it allowed us to implement number generator algorithms of the shift register type up to 16,384 in length. Each processor has two such blocks (the two layers at the top left in Fig. 2) which work in parallel, and a random number is obtained by modulo 2 addition. This approach has allowed us to eliminate all reported systematic errors [13, 31]. The spin memory contains 16,777,216 spins, and the boundary conditions are programmable. In all, we manufactured 12 processors controlled by three servers. The accuracy of the numerical estimates achieved with these processors by the Monte Carlo method for the critical temperature of the three-dimensional Ising model, $1/T_c = 0.62358(15)$, and for the values of critical exponents [32] $y_t = 1.5865(14)$ and $y_h = 2.4814(5)$ still remains record-best in the field.

3.5 The critical percolation

In 1995, Aizenman [33] formulated a conjecture at a conference on statistical physics that in the thermodynamic limit the probability of observing two infinite percolating clusters occurring in critical percolation is finite. This inference was counterintuitive. However, numerical simulation gave evidence that this is indeed the case, even though this event is observed very infrequently. For example, out of a thousand square samples of *infinite* linear size, 13 samples, on average, contain two percolating clusters. In a million samples three contained three percolating clusters. We conducted numerical experiments in which a 100 million clusters were generated for each sample size, and analyzed the limiting case of lattices of an infinite size. The resulting numerical estimates were published [34] before John Cardy's analytical solution of the problem became known [35]. The assessments and the analytical solution were found to coincide quite well.

Later simulation of the critical percolation [36] confirmed the complete Aizenman conjecture on the dependence of the

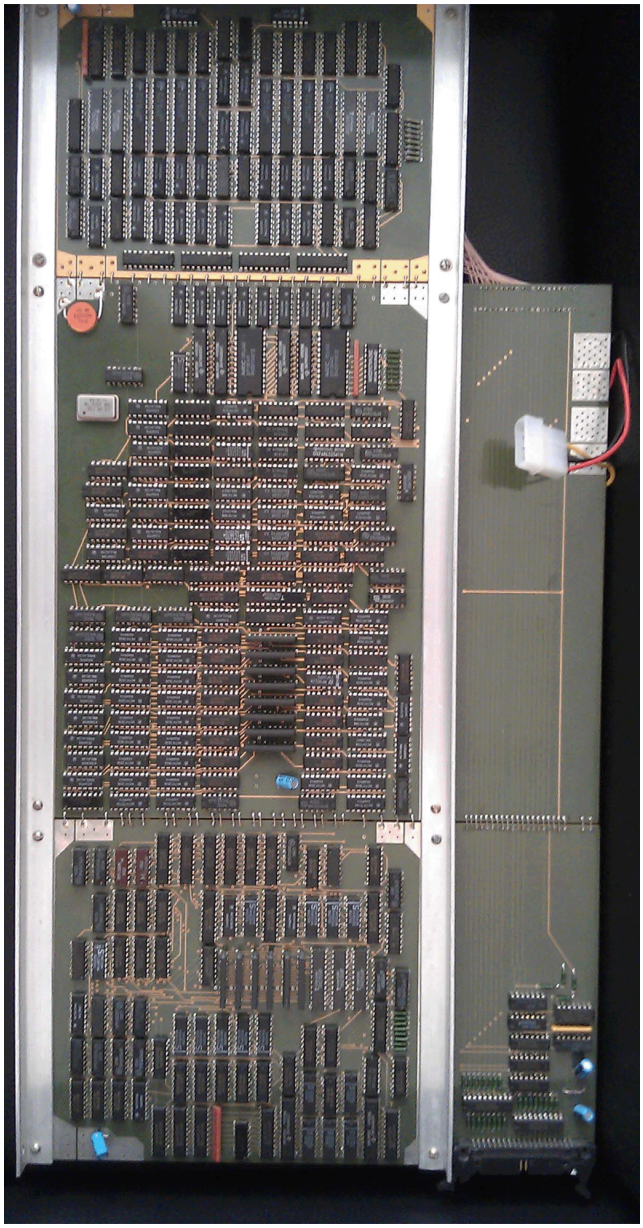

Figure 2. Photograph of the processor board of one of the dedicated processors for the numerical study of the three-dimensional Ising model. From upper left down: random number generator block, single-cluster algorithm block, and spin memory. On the right: I/O block with sockets for connection to server computers.

critical exponent ζ_d of cluster percolation multiplicity on the space dimension $2 < d < 6$: $\zeta_d = d/(d-1)$.

3.6 Duality of critical interfaces

Critical clusters constitute fractal objects [37]. Conformal field theory [38] provides predictions for the critical exponents of two-dimensional objects [39]. Applying this theory, one can compute the fractal dimensions of critical clusters of two-dimensional Potts models, the $O(N)$ model, and some others. The method of analytical calculation of the fractal dimension of boundaries of such clusters (so-called critical interfaces) has been developed fairly recently [40], and accurate results have already been obtained for some models [41]. At the same time, Duplantier [42] advanced a conjecture on the duality of critical interfaces based on some qualitative reasoning and analogies.

Verification of the duality hypothesis for critical interfaces using numerical simulation requires identification of interfaces on the lattice. Analysis of numerical results for Potts models with the number of components from 1 to 4 (not necessarily an integral number!) showed that boundaries of the clusters of two types are dual [43]. The first is the geometric cluster, which consists of neighboring spins of identical color. The second is the Fortuin–Kasteleyn cluster, which contains a smaller number of spins and is sparser than the geometric cluster, since some nearest-neighbor spins are unaligned (uncorrelated) owing to interaction with the heat bath. Identification of these clusters on the medial lattice is unambiguous and uses a well-defined algorithm [43]. Many scenarios for defining the boundaries of clusters on a lattice have been discussed in the literature on random fractal clusters. They are essentially reducible to the above-described boundaries of two clusters.

3.7 Critical amplitudes

I will briefly mention the work on the computation of universal ratios between critical amplitudes, which has been progressing very vigorously in recent years. This field requires a special review. A brief overview of the current status of numerical studies can be found in Ref. [44].

3.8 Problem of diffusion-limited aggregation

The problem of structure growth through diffusion is well defined in the two-dimensional case. It can be formulated as a random walk in an infinite plane with a particle sticking to the growing seed on contact. The probability of the particle escaping to infinity is zero, i.e., during the random walk (which can be arbitrarily long) the particle will eventually come in contact with the cluster boundary, so the cluster grows by one particle. This formulation allows the construction of an algorithm which ensures any required accuracy of obeying boundary conditions. This is important, because such a walk is described by the solution of the two-dimensional Laplace equation with two boundary conditions: on the boundary of the growing cluster, and at infinity; we know that this solution may lead to explosive instability. An algorithm was suggested in Ref. [45] which accurately implements such boundary conditions for simulating random diffusion-limited aggregation (DLA) [46].

To compute the fractal dimension of such clusters, we need to analyze a great number of large-sized clusters. Such simulation can be successfully realized in a computing cluster, specially designed for the type of problems in which every node possesses a large amount of RAM (4 gigabytes per thread), which makes it possible to commit to memory the entire computational structure of a cluster comprising up to a billion particles. For each value of the parameter, we generated a thousand clusters containing a hundred million particles each. An analysis of these clusters using a specially developed probe particle technique [47] made it possible to build a morphological histogram, shown in Fig. 3 and providing a qualitative description of the first-order phase transition between symmetrically arranged clusters and random clusters in the plane of two parameters — the coefficient of adhesion, and the symmetry of the external crystal field (such as that of the crystalline substrate on which diffusion unfolds) [48].

An investigation of the probability of growth of the emerging clusters allowed us to disprove in the DLA framework the hypothesis of multiscaling of random growth

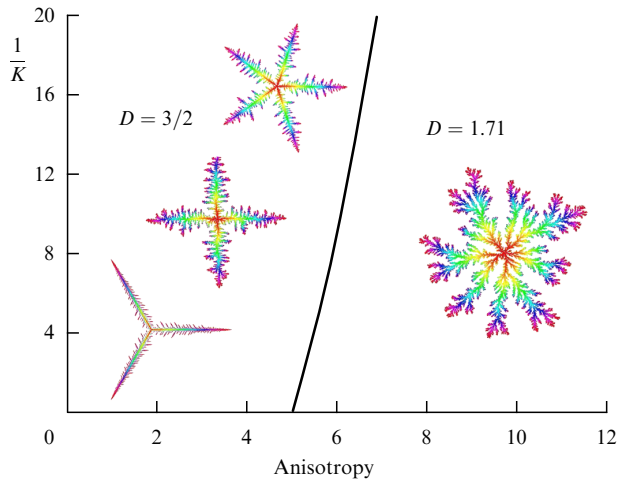

Figure 3. Morphological diagram of growth patterns of random clusters through diffusion. The horizontal axis specifies the symmetry of the external crystal field. The vertical axis is the inverse coefficient of particle adhesion. The solid line fits the line of first-order phase transition. D denotes the value of the fractal dimension of clusters in the thermodynamic limit.

clusters and to identify a scale-invariant form of the probability of a particle attachment to a cluster [49].

4. Conclusion

The examples given above conclusively demonstrate that computational physics can be successfully applied to testing theoretical hypotheses and predictions in various fields of physics.

The application of specialized computing machines has proved to be very successful in a number of cases. It should be noted that an elevated level of specialization, demanding a relatively high investment of intellectual effort, leads to the creation of machines whose usefulness for research is limited in time. However, even though their effective employment does not stretch beyond five or six years, during which they outperform all other computational systems, they may help in obtaining important scientific results much earlier than by using other approaches.

In 1996, the International Union of Pure and Applied Physics (IUPAP) created Commission C20 on Computational Physics [50]. Its task is to conduct annual conferences on computational physics. Conferences are held alternately in three geographic sectors — North and South America, Asia and Oceania, and Europe and Africa. Next year, in 2013, the conference will be conducted by the Russian Academy of Sciences in Moscow, which will give Russian scientists a chance to present to the international community their achievements in the field of computational physics.

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