

Stochastic Simulation of Inhomogeneous Metocean Fields. Part III: High-Performance Parallel Algorithms

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Abstract. The paper discusses the high-performance parallel algorithms for stochastic simulation of metocean processes and fields. The approaches for parallel representation of sample estimation procedures, linear stochastic systems, Markov chains, periodically correlated processes and inhomogeneous fields are proposed. The speedup of the proposing algorithms is studied in respect to parameters of the models.

1 Introduction

Metocean data fields, like atmospheric pressure, wind speed, ocean waves etc. have a complex spatial and temporal variability. Recently the huge databases of metocean data in the irregular gridpoints are collected (see e.g. [14]). Development of environmental models and use them for data assimilation and reanalysis [10], has allowed to create global information arrays of metocean fields in points of a regular spatial-temporal grid. For the analysis and synthesis of these data the special models, considered in the first [4] and second [5] parts of this paper, has been developed. The modeling procedures often require large amounts of computational resources and are therefore executed on parallel computer systems.

Generally, *parallelization* of statistical computational procedures (including Monte-Carlo techniques) is based on decomposition of sample on the equal sub-volumes (see e.g. [16]). This approach is valid only for independent random values (RV), because in terms of time series (TS) or stochastic fields (SF) the elements of sample are interdependent. Therefore, for the dependent data models, the sophisticated reformulation of the sequential algorithm (and correspondent code) is requires. There are at least two *extensive* ways to solve this problem.

The first way is the automatic translation of sequential code by means of the loop parallelization tools [18]. But if the stochastic algorithm has explicit formalization of interdependence (e.g. – parametrical regression), then the efficiency of this procedure is rather low. The second way concerns the using of the free parallel scientific libraries (as ATLAS, PBLAS, PLAPACK, ScaLAPACK etc. [19]) for the compiling of the code. But the majority of the computational procedures orients on the elected computational tacks (matrix algebra, PDE solving and optimization). Moreover, sometimes

the most labor-consuming part of the algorithm is not respect to any standard procedure.

Thus, the development of the parallel stochastic algorithms is the *creative* problem. The best solution may be obtained using the paradigm of problem “reflection” to parallel architecture of computer [3], take in mind the specifics of data. The main goals of this paper are the follows:

- To illustrate the principles of parallelization for stochastic simulation of metocean processes and fields.
- To study the computational efficiency of the proposed parallel algorithms in respect to parameters of stochastic models.

2 Theoretical Model of Parallel Program

The design of scalable and portable algorithms requires the previous formalization of the theoretical model of parallel program. One of the simple models for computational applications is the BSP (bulk-synchronous parallel) model, associated with simultaneous computation of p parallel threads, with barrier synchronization [8]. It allows consider any parallel program in terms of cortege $\langle p, C, \eta \rangle$. Here $C = (V, E)$ is the communication graph, (where V are the vertexes and E are the edges), and $\eta = \langle L_i, g, f_p \rangle$ are the characteristic of processors loading. The values L_i (associated with V_i) are the times of parallel computations of thread i , and g is the communication time. The value f_p is the part of sequential operations.

There are a few indexes characterizing the performance of parallel algorithms [7]. For statistical application we consider the speedup index $S_p = T_1 / T_p$ (where T_i are the measured time of computations with i parallel threads) as the measure of efficiency $\varepsilon_p = S_p / p$. For maximization of S_p the follows is requires: (1) graph C includes at least p parallel threads, (2) the loadings of the processors are balanced $L_i / L_j \approx 1$, (3) and value g is minimized.

In practice these requirements are not enough for absolute maximization of S_p , because BSP model ignores the platform-dependent features, e.g. caching. Therefore, the validation of proposed algorithms would be controlled by means of computational experiment. We use the on-shell cluster “*Paritet*” (4x2-processor nodes), designed in Institute for High Performance Computing and Data Bases (Russia). In spite of the low number of nodes, this cluster reproduced in scale the *Beowulf* architecture and may be used for *qualitative* analysis of parallel algorithms.

3 Parallelization Principles for Stochastic Models

The paradigm of parallel algorithms design requires the formalization of principles for parallelism detection, based on the features of the stochastic models. Below the three general principles are considered.

3.1 Parallel Algorithms, Based on the Ensemble Decomposition

The principle of ensemble decomposition is based on the data parallelism. For meteocean fields the first level of decomposition technique is result of the *multiscale* hypothesis proposed by Andrey S. Monin [15]. The hypothesis suggests modelling the total variability of process ζ by means of a set of stochastic models for each temporal scale separately, and with the interdependence taken into account parametrically. It allows present the total distribution function $P_\zeta(x)$ over the probability space Ω in terms of combined distribution

$$P_\zeta(x) = \int_{\Omega} G_\zeta(x, y) dF_\zeta(y) dy = \sum_{k=1}^p \int_{\Omega_k} G_\zeta(x, y) dF_\zeta^{(k)}(y) dy. \tag{1}$$

Here G_ζ is the main scale distribution function and F_ζ is the distribution function of above-scale driving process ζ . Eqn. (1) allows consider the probabilistic characteristic of ζ for each sub-volume $\Omega_k = \{ \zeta_k \}$, $\bigcup_{k=1}^p \Omega_k = \Omega$ in parallel. In practice for the

best balancing of the processor loadings it is easy to consider the initial dataset in terms of natural meteocean scales (e.g. day, month, year etc.). For example, in the papers [4,5] the function G_ζ from Eqn. (1) is associated with synoptic variability and F_ζ - with annual and year-to-year variability. Therefore, in simple case (continuous data analysis) the processing of the synoptic data may be carrying out for 12 months in parallel. For the irregular data (series with the data missing) the dynamical balancing is required.

The second level of decomposition is based only on statistical properties of ensemble in terms of RV model. Let us consider the sample estimate Ξ^* of parameter Ξ as any statistical sum $\langle \mathfrak{S}_\zeta(x) \rangle_{\Omega^*}$ over the sample Ω^* [22] (here $\langle \dots \rangle$ is the operation of sample averaging). Such definition allows compute the $\Xi_{(k)}^*$ over the Ω_k^* in the p parallel threads. The obtained sample of estimates $\{ \Xi_{(k)}^* \}_{k=1}^p$ may be used for estimation of the total value Ξ^* and its sample variability, roughly if $N \gg p$:

$$\Xi^* = p^{-1} \sum_{k=1}^p \Xi_{(k)}^*, \quad | \Xi - \Xi^* | \leq t_\alpha(p) \frac{\sigma_\Xi^*}{\sqrt{p}}. \tag{2}$$

Here $t_{\alpha}(p)$ is the $1-\alpha\%$ quantile of Student' distribution, and σ_{Ξ}^* is the estimate of r.m.s., calculated over the sample $\{\Xi_{(k)}^*\}_{k=1}^p$. In the Fig. 1(a) the communication graph of the parallel algorithm is shown. The vertex **A** is the data preparation and storage on the local nodes, vertex **B** – parallel computation the $\Xi_{(k)}^*$, and vertex **D** – computation of total estimate (2).

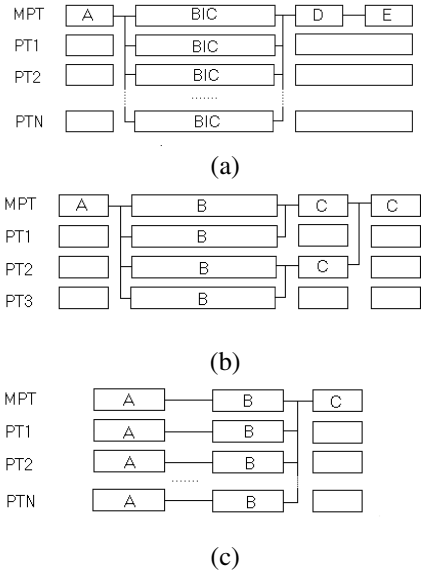


Fig. 1. Communication graphs of the parallel algorithms (Here PT – Parallel thread, MPT – Main parallel thread)

For some statistical parameters another operators are uses instead of $\langle \dots \rangle$. For example, for univariate RV the $q\%$ -quantiles may be estimated as order statistics $\xi_q^* = \text{sort}(\Omega^*)_{[qN]_{J+1}}$. Such definition is clear for parallelism detection: the sample estimates of $x_q^{*(k)} = \text{sort}(\Omega^{(k)})_{[qN_k]_{J+1}}$ for all threads $k = \overline{1, p}$ are considers in parallel (see Fig. 1(a), vertex **C**). For the computation of total estimate the Eqn. (2) may be used also; but for last terms of sample such estimates are biased. Therefore, the total sorting of previously sorted Ω_k^* is required (vertex **E**). In the Fig 1(a) seen, that the most labor-consuming operations: estimation of sums (**B**) and sorting (**C**) are parallel.

In the Fig 2(a) the speedup indexes S_p vs. p for statistical estimation of univariate RV are shown for different volumes N of the sample Ω^* . It is seen, that the scalability of the algorithm is rather good, especially – for high value of N .

Even for RV model, the inverse problem – stochastic simulation by Monte-Carlo technique sometimes require more computational resources, than the estimation. The simulation of random numbers is traditional parallel problem (see e.g. [21]). The parallel scheme of RV simulation is close to Fig. 1(a), when vertex **B** contains the random number generation instead of statistical summation.

3.2 Parallel Algorithms, Based on the Strong Mixing Principle

The ensemble decomposition principle is the best mainly for the RV model. For the TS and SF modeling more sophisticated approaches are require. Here we consider the class of the parallel algorithms, based on the strong mixing principle [11]. In terms of

TS model this expressed as $F_{\zeta(t)\zeta(s)}(x, y) \xrightarrow{|t-s| \rightarrow \infty} F_{\zeta(t)}(x)F_{\zeta(s)}(y)$, where t and s are the time moments. This fact allows design the algorithms on the base of the parallel simulation of p independent time series, and its further sewing.

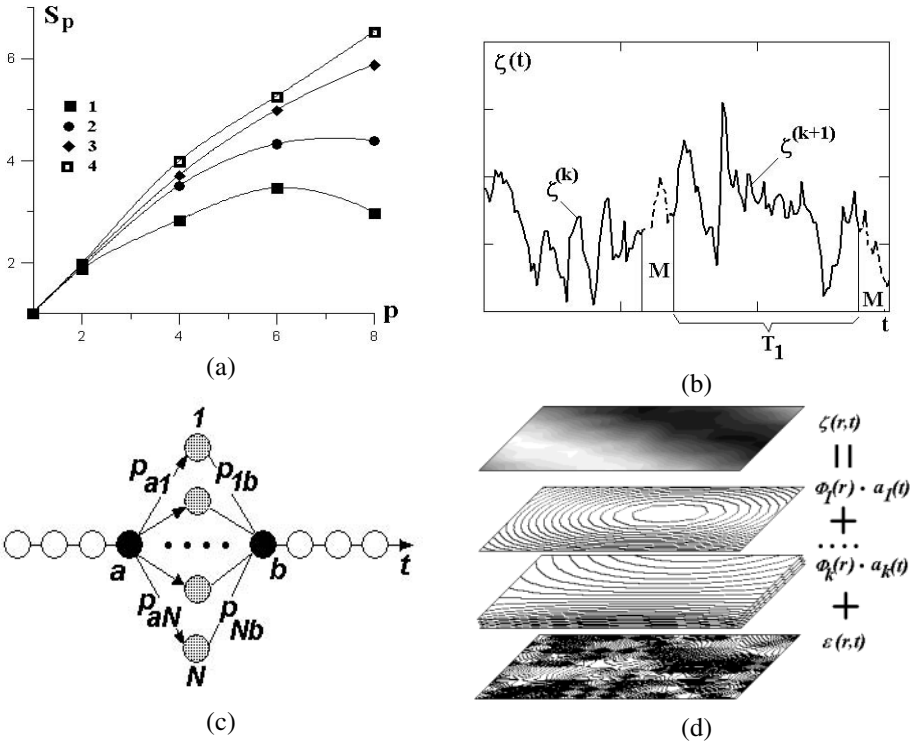


Fig. 2. (a) Speedup of the parallel statistical estimation. Here 1-N=2000, 2-N=4000, 3-N=10000, 4-N=20000.

(b-d) Illustration of the main parallelization principles: (linear stochastic systems **(b)**, Markov chains **(c)** and models of inhomogeneous stochastic fields **(d)**).

3.2.1 Parallel Models of Linear Stochastic Systems

For simulation of Gaussian stationary TS and homogeneous SF $\zeta(\mathbf{u})$ the model of linear stochastic system in terms of partial differential equation may be adopted [1]:

$$\left[\begin{matrix} N \\ * \\ L_k \end{matrix} \right] \zeta(\mathbf{u}) = \left[\begin{matrix} N \\ * \\ E_k \end{matrix} \right] \varepsilon(\mathbf{u}) + \left[\begin{matrix} N \\ * \\ Q_k \end{matrix} \right] \eta(\mathbf{u}). \tag{3}$$

Here $\mathbf{u} = (t, \mathbf{r})$, where \mathbf{r} is vector of spatial coordinates and t is the time, ε is the white noise field, η is the driving stochastic process (input signal) and

$$L_k = \sum_{i=0}^{n_k} l_{ki} \frac{\partial^i}{\partial u_k^i}, E_k = \sum_{i=0}^{m_k} e_{ki} \frac{\partial^i}{\partial u_k^i}, Q_k = \sum_{i=0}^{s_k} q_{ki} \frac{\partial^i}{\partial u_k^i}$$

are the partial differential operators

with constant coefficients (* is the operator composition). When $N = I, q_{ki} = 0, e_{ki} = 0, k \geq I$, the Eqn. (3) reduces to the well-known autoregressive model [9]:

$$\zeta_t = \sum_{i=1}^M \Phi_i \zeta_{t-i} + \sigma_\varepsilon \varepsilon_t, \quad t = \overline{M+1, T}. \tag{4}$$

The parameters $\Phi_i, \sigma_\varepsilon$ are obtains by means of linear equation system

$$\sum_k \Phi_k K_{|i-k|} = K_i, \quad K_i = E[(\zeta_t - m_\zeta)(\zeta_{t-i} - m_\zeta)]. \tag{5}$$

Here K_i is the value of covariance function of ζ_t . It may be estimated by means of parallel algorithm, described in Chapter 3.1. It is seen, that the Eqn. (4) has an explicit recurrence, thus, the direct loop parallelism is impossible here. Taking to account, that $M \ll T$, let us consider the parallelization principle, shown in Fig. 2(b). If we decompose the length of simulated series as $T = pT_1 + (p - 1)M$, the follows steps may be carry out:

- Estimation of the model parameters by Eqn. (5) (vertex **A**)
- Parallel simulation of T_1 -length independent time series $\zeta_t^{(k)}, k = \overline{1, p}$ (vertex **B**)
- Couple sewing of the simulated series by Eqn. (4) (vertex **C**).

Table 1. Speedup indexes for parallel simulation of linear dynamic systems (left part) and Markov chains (right part)

Linear dynamic system (4-6)					Markov chain (7-8)				
T	M	Number of processors p			T	M	Number of processors p		
		2	4	8			2	4	8
2000	10	1.7	1.3	0.8	10 ¹	10	1.0	0.9	0.7
2000	40	1.8	2.9	3.8	10 ¹	100	0.9	0.7	0.4
4000	10	1.7	2.6	3.2	10 ²	10	1.7	2.3	2.7
4000	40	1.9	3.3	4.8	10 ²	100	1.8	2.5	2.7
8000	10	1.8	2.9	3.9	10 ²	10	1.6	2.5	3.3
8000	40	1.9	3.4	5.6	10 ²	100	1.9	3.5	5.8

The algorithm of couple sewing is close to approach for environmental data missing recovering from the paper [20]. It allows present the values of $\tilde{\zeta}_t, t = T_1 + 1, \dots, T_1 + M$ by means of recurrent equation

$$\tilde{\zeta}_t = \sum_{i=1}^M \Theta_i^{(1)} \zeta_{t-i} + \sum_{j=1}^M \Theta_j^{(2)} \zeta_{t+j} + \sigma_\delta \delta_t. \tag{6}$$

Here $\Theta_i^{(*)}, \sigma_\delta$ are the model parameters, and δ_t is the white noise. The Eqn. (6) is the double-side generalization of Eqn. (5), and the values $\{\zeta_{T_1-M+1}^{(k)}, \dots, \zeta_{T_1}^{(k)}\}$ and $\{\zeta_1^{(k+1)}, \dots, \zeta_M^{(k+1)}\}$ of the TS from two parallel threads (k) and ($k+1$) may be consider as the boundary values. The procedure like (5) is used for the estimation of $\Theta_i^{(*)}$. In the Table 1 (left part) the speedup indexes S_p vs. p are present for different values of T

and M . For the short data series the S_p became less 1, but with the increasing of T the speedup became rather better (e.g. for $T = 8000, M = 40$ the $S_p = 5.6$ and $\varepsilon = 70\%$ for 8 processors).

3.2.2 Parallel Markov Models

For stationary Markov chains and processes the strong mixing principle is also valid. Taking to account, that for numerical computations the discrete representation of the continuous Markov processes are traditionally uses, we consider only discrete M -states Markov chains with parameters [2]:

$$\pi = \begin{bmatrix} \pi_1 \\ \vdots \\ \pi_M \end{bmatrix}, \quad \mathbf{P} = \begin{bmatrix} P_{11} & & P_{1M} \\ & \ddots & \\ P_{M1} & & P_{MM} \end{bmatrix}, \quad \sum_{k=1}^M P_{ik} = \sum_{k=1}^M \pi_k = 1, \quad i = \overline{1, M}. \quad (7)$$

Here π is the vector of limit probabilities and \mathbf{P} is the matrix of transient probabilities. The general principle of parallelism is shown in the Fig. 2(c) for first order Markov chain. The parallelization technique is close to the same for linear stochastic systems (the communication graph in the Fig. 1(b)). It consists of three stages:

- Estimation of parameters (7) and data preparation (vertex **A**)
- Parallel simulation of independent sub-chains (vertex **B**)
- *Couple sewing* of the simulated sub-chains (vertex **C**).

The sewing procedure uses the states in the tail of first sub-chain (a) and head of second sub-chain (b) as the boundary conditions for simulation of the sewing Markov state k , with the conditional probability:

$$p_k^{(a,b)} = \frac{P_{ak}P_{kb}}{\sum_{l=1}^M P_{al}P_{lb}}, \quad a, b, k = \overline{1, M}. \quad (8)$$

In the Table 1 (right part) the speedup indexes S_p vs. p for Markov chains with different T and M are shown. For low $T=10^3$ the speedup may be less 1, due to high communication expenses for sewing of the sub-chains. But for high length of the chain ($T=10^5$) the values of S_p increases in respect to M and p . E.g. for Markov chain with the 100 states the $S_p=3.5$ and $S_8=5.8$ times.

3.3 Parallel Algorithms, Based on the Functional Approximation Principle

The principle of functional approximation is based on the classical representation of TS or spatio-temporal SF $\zeta(\mathbf{r}, t)$ in terms of the deterministic function, dependent from the set of random arguments Ξ [12]:

$$\zeta(\mathbf{r}, t) = \zeta(\mathbf{r}, t | \Xi). \quad (9)$$

It allows decompose the spatial (or spatio-temporal) domain on the set of equal sub-volumes. The main advantages of this principle are obvious for the nonstationary TS and inhomogeneous SF, where the strong mixing principle is not valid.

3.3.1 Periodically Correlated Time Series

One of the simplest examples of nonstationary TS is the model of periodically correlated stochastic process (PCSP) $\zeta(t)$, where the mathematical expectation $m_\zeta(t) = m_\zeta(t + \tau)$ and covariance function $K_\zeta(t, s) = K_\zeta(t + \tau, s + \tau)$, τ is the period of correlation (e.g. – one year). The PCSP model is widely used for simulation of the annual variability of different metocean processes [13], e.g. sea waves, wind speed, atmospheric pressure, ice cover, air and water temperature [6] etc. In the book [17] the simulation algorithm for PCSP with explicit formalization of dependence is proposed. Instead of this, let us consider the alternative *parametrical* model of PCSP as expansion [4]:

$$\zeta(t) = \sum_k \alpha_k(t) \exp(iA_k t). \tag{10}$$

Here $\Xi = \{\alpha_k(t)\}$ - the set of parameters, $A_k = 2\pi k / \tau$. The inverse transformation of Eqn. (10) allows obtain the explicit expression for TS $\alpha_k(t)$:

$$\alpha_k(t) = \int_0^t \zeta(s) H(t, s) \exp(-iA_k s) ds. \tag{11}$$

Its covariance function is:

$$K_{\alpha_k \alpha_j}(t, s) = \int_0^t \int_0^s R(t, s, x, y) K_\zeta(x, y) \exp[-i(A_k x + A_j y)] dx dy. \tag{12}$$

Here $H(t, s)$ is the kernel function, $R(t, s, x, y) = H(t, s)H(x, y)$. When $H(t, s)$ is the step function for $s \in [t, t - \tau]$, the time series $\alpha_k(t)$ became stationary and Gaussian [6]. The Eqns. (10,12) allows the domain parallelization of PCSP computation. Communication graph of this algorithm is shown in the Fig. 1(c), where vertex **A** respects to simulation of TS (11) with covariance function (12) by means of multivariate autoregressive model (4), and vertex **B** is the parallel computation of the Eqn. (10) for equal time intervals $[t_k, t_{k+1}]_{k=0}^p$. After the sub-volumes computations all the data send to the main computational thread (vertex **C**).

3.3.2 Inhomogeneous Spatio-Temporal Fields

The principle of functional approximation is applied for simulation of the inhomogeneous spatio-temporal metocean fields. In [4,5] such models are presented as the expansion:

$$\zeta(\mathbf{r}, t) - m(\mathbf{r}, t) = \sum_{k=1}^M a_k(t) \Phi_k(\mathbf{r}, t) + \varepsilon(\mathbf{r}, t). \tag{13}$$

Here $a_k(t)$ are the coefficients, $m(\mathbf{r}, t)$ is the mathematical expectation, $\Phi_k(\mathbf{r}, t)$ is the spatio-temporal basis, $\varepsilon(\mathbf{r}, t)$ is the inhomogeneous white noise. The estimation of $a_k(t)$ is fully discussed in the paper [4]. The general principle of parallelism in Eqn. (13) is shown in the Fig. 2(d). It is seen, that there are at least two alternative ways for parallelization. The first (*horizontal*) way is the domain decomposition on the equal spatial areas, and calculation the Eqn. (13) for each area in parallel. The communica-

tion graph of this algorithm is shown in the Fig. 1(c) and discussed in Section 3.3.1. The second (*vertical*) way is based on the parallel computation of the coefficients (vertex *A* in Fig 1(c)) and the terms $a_k(t)\Phi_k(\mathbf{r},t)$ for all the gridpoints $\{\mathbf{r}_k\}_{k=1}^N$, and finally – summation of Eqn. (13) in the main parallel thread (vertex *C*). Theoretically both schemes are valid, but in practice the real speedup depends from the total numbers of gridpoints N and numbers of basic functions M . In the table 2 the speedup indexes S_p vs. p are present for different values of N and M . Take in mind, that the parameters a_k may be considered as RV, stationary SF or PCSP [4], we carry out all the computations for three classes of complexity (associated with loadings L_A for simulation of coefficients).

Table 2. Speedup indexes for parallel simulation of inhomogeneous metocean fields

Complexity	Horizontal parallelization					Vertical parallelization				
	M	N	Processors p			M	N	Processors p		
			2	4	8			2	4	8
I	4	500	1	1.2	1.2	10	100	0.7	0.4	0.4
	8	1000	1.5	2.1	2.3	100	100	1.0	0.9	0.7
II	4	500	1.5	2.0	1.6	10	100	1.9	1.6	1.8
	8	1000	1.9	3.4	5.7	100	100	~2	1.7	3.2
III	8	500	~2	3.7	6.1	10	100	1.9	3.4	1.9
	16	1000	~2	3.9	7.7	100	100	~2	3.9	5.9

From the table 2 seen, that for horizontal (domain) parallelization the speedup is the highest for the high-complexity models. E.g., for third class of complexity (PCSP model of coefficients) the $S_8=7.7$ (efficiency $\varepsilon_8=96\%$) when $M=16$ and $N=1000$ spatial points. For the complexity class I (RV model, describing only spatial variability), the speedup is low. The vertical (sum) parallelization allows obtain the high speedup only if the number of basic functions is close to number of spatial points. Therefore, this way is not adopts for the reduction of data dimensionality in stochastic models and may be considered only for the specific problems, as the simulation of the fields with very complicated spectral structure.

4 Conclusions

This paper has demonstrated the main principles of parallel algorithms design for computational multivariate statistics of spatio-temporal metocean fields. The principles of ensemble decomposition, strong mixing and functional approximation allow develop the parallel stochastic models for dependent time series and fields (including autoregressive TS, Markov chains, PCSP and inhomogeneous spatio-temporal SF). The analysis of speedup sensitivity to the model parameters shown, that the efficiency of the proposed algorithms is the best for huge model datasets, in practice applying for numerical study of extreme metocean events [5].

Acknowledgment. This research has been partly founded by INTAS 99-0666 Project: “Estimation of extreme metocean events”.

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