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► **To cite this version:**

Nicolas Fressengeas, Hervé Frezza-Buet. Generic method for solving partial differential equations through the design of problem-specific continuous automata. 2007. hal-00107064v4

HAL Id: hal-00107064

<https://hal.science/hal-00107064v4>

Preprint submitted on 26 Jan 2007 (v4), last revised 29 Jan 2010 (v8)

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Generic method for solving partial differential equations through the design of problem-specific continuous automata

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This paper presents an original and generic numerical method for solving partial differential equations. A new mathematical and systematic method stemming from the local very nature of any differential problem is proposed: a custom tailored continuous automaton is purposely derived from any given differential problem so that its steady state yields the solution in a quantitatively correct way. The combined use of formal computing and continuous automata thus offers the unique possibility to completely automate the process from formal problem specification to its numerical solution.

PACS numbers: 02.30.Jr, 02.60.Cb, 02.60.Jh, 02.60.Lj

I. AUTOMATA AND PARTIAL DIFFERENTIAL EQUATIONS

Ever since von Neumann [1], the question of modelling continuous physics with a discrete set of cellular automata has been raised, whether they handle discrete or continuous values. Many answers have been brought forth through, for instance, the work of Stephen Wolfram [2] summarized in a recent book [3]. This problem has been mostly tackled by rightfully considering that modelling physics through Newton and Leibniz calculus is fundamentally different from a discrete modelization as implied by automata.

Indeed, the former implies that physics is considered continuous either because materials and fields are considered continuous in classical physics or because quantum physics wave functions are themselves continuous. On the contrary, modelling physics through automata implies modelling on a discrete basis, in which a unit element called *a cell*, interacts with its surroundings according to a given law derived from local physics considerations. Such discretized automaton based models have been successfully applied to various applications ranging from reaction-diffusion systems [4] to forest fires [5], through probably one of the most impressive achievements: the Lattice Gas Automata [6], where atoms or molecules are considered individually. In this frame, simple point mechanics interaction rules lead to complex behaviors such as phase transition and turbulence. This peculiar feature of automata, making complex group behavior emerge from fairly simple individual rules aroused the interest around them for the past decades.

However, to the best of our knowledge, beside particular solutions [4, 7], the predictions of calculus based, continuous models and those of discrete, automata based ones, are seldom quantitatively identical, though qualitative similarity is often obtained. This is mostly explained by the fact that the two drastically different approaches

are applied to their own class of problems. Attempts at a quantitative link have however been made by showing connexions between an automaton and a particular differential problem [8] or by designing methods for describing automata by differential equations [9, 10, 11] allowing in the way to *assess* the performance of two different *implementations* of the same problem, which are in fact basically two different automata for the description of the same physics.

That is the reason why this paper is devoted to the introduction of a new and systematic method allowing to derive a continuous automaton from any given differential problem whose boundary conditions are of the Dirichlet type. The process of derivation stems from the idea that since differential problems are expressed in a purely local manner, their solution can be computed in an equally local way. However, as will be shown, the locality of the computation is not an *a priori* hypothesis but rather a consequence of the method. Nonetheless, the most interesting aspect of it is the possibility to completely automate the way from the formal expression of the differential problem down to its solution, thanks to formal computing and to a cellular automata based environment, analogous to previously reported ones [12, 13].

II. SOLVING PDE'S THANKS TO CONTINUOUS AUTOMATA

In this section, we will show that the solution seeking scheme of finding a field that meets the requirements of a given differential problem can be transformed into a minimization task. The latter can be implemented by formally computing a cellular automaton which converges to the sought solution.

The very characteristic of continuous physics is its intensive use of *fields*. If we note $(A)^B$ the set of functions from A to B , a field $\xi \in (\mathbb{R}^m)^{\mathbb{R}^n}$ is a mapping of

a given vectorial physical quantity —belonging to \mathbb{R}^n — over a given physical space \mathbb{R}^m , for $(m, n) \in \mathbb{N}^2$. Therefore, a particular local differential problem \mathbb{P} stemming from local relationships, can be expressed in terms of a functional equation $\Phi^{(\xi)} = 0$, where the field ξ is the unknown, and where Φ represents the differential relationships derived from physical considerations, that a field ξ should satisfy to be the solution of \mathbb{P} . Φ can thus be defined as follows, where $p \in \mathbb{N}$ can be thought of as the number of real equations necessary to express the local relationship which are to be satisfied at any point of \mathbb{R}^m :

$$\Phi : (\mathbb{R}^m)^{\mathbb{R}^n} \mapsto (\mathbb{R}^m)^{\mathbb{R}^p} \\ \xi \rightarrow \Phi^{(\xi)}$$

In other words, $\Phi^{(\xi)}$ is a mapping of a vector of p real values over the physical space \mathbb{R}^m . For each point $x \in \mathbb{R}^m$ in space, the i^{th} component of $\Phi^{(\xi)}(x) \in \mathbb{R}^p$, which would be zero if ξ was the solution of \mathbb{P} , actually corresponds to the local amount of violation of the i^{th} real local equation used to describe the problem at x . Using a functional equation instead of considering ξ as a given numerical instantiation, leads us to stress that the mapping $\Phi^{(\xi)}$ depends on ξ intrinsically, whatever its actual instantiation, or value, is. The functional formalism allows to handle the dependency itself, *i.e.* the way all violations $\Phi^{(\xi)}$ over the physical space \mathbb{R}^m depend on the whole field ξ .

The original idea of this paper is that this formalism allows to express, and exploit, the variations of $\Phi^{(\xi)}$ when ξ changes, by using functional derivatives of the mapping Φ with respect to ξ , for driving the resolution process — *i.e.* for finding ξ^* for which $\Phi^{(\xi^*)} = 0$. To make this approach computationally tractable, we need to discretize the problem. This is performed by discretizing Φ on a finite mesh $\Omega \subset \mathbb{R}^m$, the discretized problem being then expressed as $\tilde{\Phi}^{(\tilde{\xi})} = 0$, where $\tilde{\xi}$ is the unknown and $\tilde{\Phi}$ is defined as follows:

$$\tilde{\Phi} : (\Omega)^{\mathbb{R}^n} \mapsto (\Omega)^{\mathbb{R}^p} \\ \tilde{\xi} \rightarrow \tilde{\Phi}^{(\tilde{\xi})} \quad (1)$$

For the sake of clarity, let us illustrate the role of functional formalism with the following example throughout this part of the paper. Let Ω be $\{x_1, x_2, x_3\} \subset \mathbb{R}^m$, where a monodimensional field ξ stands, *i.e.* $n = 1$. Let $\tilde{\Phi}$ be a single real expression, expected to be null on the solution. This corresponds to $p = 1$.

To particularize the notations in the frame of our example, let us give an explicit formulation of $\tilde{\Phi}^{(\tilde{\xi})}$ which highlights the fact that at each x_i , $\tilde{\Phi}^{(\tilde{\xi})}(x_i)$ depends on the whole space Ω . This formulation involves f_1 , f_2 and f_3 in $(\mathbb{R}^3)^{\mathbb{R}}$ and is expressed as follows: $\forall i \in \{1, 2, 3\}$, $\tilde{\Phi}^{(\tilde{\xi})}(x_i) = f_i(\tilde{\xi}(x_1), \tilde{\xi}(x_2), \tilde{\xi}(x_3)) \in \mathbb{R}$. This will be used below to illustrate the formal demonstration.

Getting back to the general case, finding ξ^* for which $\Phi^{(\xi^*)} = 0$ means finding a field $\tilde{\xi}$ for which $\tilde{\Phi}^{(\tilde{\xi})}$ is as

close to the 0 mapping as possible given a distance on the functional space $(\Omega)^{\mathbb{R}^p}$. This, in turn, is equivalent to zeroing all p relations $\tilde{\Phi}^{(\tilde{\xi})}(\omega)$ for *all* $\omega \in \Omega$. Finally, this can be equivalently done by similarly zeroing

$$\mathcal{E}^{(\tilde{\xi})} = \sum_{\omega \in \Omega} \left| \tilde{\Phi}^{(\tilde{\xi})}(\omega) \right| \quad (2)$$

where $|\cdot|$ is any given norm on \mathbb{R}^p . Let us note that $\mathcal{E}^{(\tilde{\xi})}$ can here be understood as a *functional* that measures the sum of the violations of the physical relationships $\tilde{\mathbb{P}}$ by a field $\tilde{\xi}$ given as the formal parameter.

The straightforward method for numerically evaluating the solution $\tilde{\xi}^*$ to $\tilde{\mathbb{P}}$, *i.e.* the value of $\tilde{\xi}$ that best zeroes —*i.e.* that *minimizes*— $\mathcal{E}^{(\tilde{\xi})}$, is the standard Newton method applied to a multidimensional optimization problem. Let us note here however that this minimization process does not ensure the zeroing of $\mathcal{E}^{(\tilde{\xi})}$, which is to be verified *a posteriori* by evaluating $\mathcal{E}^{(\tilde{\xi}^*)}$.

To undertake this optimization task, we previously need to define a canonical basis of the functional space $(\Omega)^{\mathbb{R}^n}$ with respect to which the *gradient* and *Hessian* will be taken. If δ is the Kronecker symbol and $\{r\}_i$ is the canonical basis of \mathbb{R}^n , let us define $\{e\}_{(\omega, i)}$, the canonical basis of $(\Omega)^{\mathbb{R}^n}$ as the set of functions $e_{(\omega, i)}$, for all $\omega \in \Omega$ and all $1 \leq (i \in \mathbb{N}) \leq n$:

$$e_{(\omega, i)} : \Omega \mapsto \mathbb{R}^n \\ \omega' \rightarrow \delta_{\omega\omega'} r_i \quad (3)$$

Let us consider our example again, focusing for instance on the partial derivation with respect to the basis vector $e_{(x_2, 1)}$. It consists in computing a derived

mapping. This mapping is $\lim_{h \in \mathbb{R} \rightarrow 0} \frac{\tilde{\Phi}^{(\tilde{\xi} + h e_{(x_2, 1)})} - \tilde{\Phi}^{(\tilde{\xi})}}{h}$, where the limit is defined according to the following neighbourhood \mathcal{N} in functional space: $\forall \epsilon > 0$, $g \in \mathcal{N}_\epsilon(f) \Leftrightarrow \forall x, |f(x) - g(x)| < \epsilon$. In our example, it can be shown that $\forall i \in \{1, 2, 3\}$, $\partial \tilde{\Phi}^{(\tilde{\xi})} / \partial e_{(x_2, 1)}(x_i) = g_i(\tilde{\xi}(x_1), \tilde{\xi}(x_2), \tilde{\xi}(x_3))$, where $g_i(a, b, c) = \partial f_i(a, b, c) / \partial b$. This depends on partial derivatives of f_i , whatever the actual ξ . As introduced previously, such functional derivatives capture the intrinsic dependency relation between $\tilde{\Phi}^{(\tilde{\xi})}$ and $\tilde{\xi}$, which is the central point of our approach.

Therefore and using these definitions of derivation, the Newton method consists in building a series $\{\tilde{\xi}_i\}_i$ defined as follows, the limit of which should be the sought solution $\tilde{\xi}^*$ to $\tilde{\mathbb{P}}$:

$$\tilde{\xi}_{t+1} = \tilde{\xi}_t - \mu_{\{e\}_{(\omega, i)}}^{(\mathcal{E})}(\tilde{\xi}_t) \\ \mu_{\{e\}_{(\omega, i)}}^{(\mathcal{E})}(\tilde{\xi}_t) = \bar{\mathbb{H}}_{\{e\}_{(\omega, i)}}^{(\mathcal{E})}(\tilde{\xi}_t) \cdot \text{grad}_{\{e\}_{(\omega, i)}}^{(\mathcal{E})}(\tilde{\xi}_t) \quad (4)$$

where $\bar{\mathbb{H}}$ is the inverse of the Hessian matrix.

The above expression requires some derivability conditions on \mathcal{E} , and thus on both $\tilde{\Phi}$ and the chosen norm on \mathbb{R}^n . The former is assumed, since it stems from the problem \mathbb{P} itself. The latter is ensured by the appropriate choice of the used norm. As another precaution to be taken on that choice, the used norm must ensure that no component of the gradient – and thus of the Hessian inverse – neither supersedes the others nor is superseded by them, for this is known to create stability problems in the iteration defined by (4). The conventional $\|\cdot\|_2$ norm, or its square, is for instance a good choice, provided \mathbb{P} is conveniently normalized.

However, the effective computation of such a series implies to compute, for each step t , the gradient and inverse Hessian with respect to $\{e\}_{(\omega,i)}$, which implies getting access to the whole Ω , in contradiction with our initial goal which was to design a *local-only* computational method. To overcome this limitation, we present in the following a method inspired from the stochastic gradient descent method [14], the locality of which will be established in the next section. The stochastic gradient method consists in updating $\tilde{\xi}$ by considering only a few of its components at a time. We choose to consider a single ω in Ω at each step, thus modifying only $\tilde{\xi}^\omega$, the ω -related components of $\tilde{\xi}$. Therefore, the gradient and Hessian appearing in (4) are taken not with respect to the whole $\{e\}_{(\omega,i)}$ but rather with a subset $\{e\}_\omega$ of it, restricted to ω , defined as the set $\{e_{(\omega',i)} : \omega' = \omega \text{ and } 1 \leq i \leq n\}$. One such step is therefore defined as follows:

$$\tilde{\xi}_{t+1}^\omega = \tilde{\xi}_t^\omega - \mu_{\{e\}_\omega}^{(\mathcal{E})}(\tilde{\xi}_t) \quad (5)$$

The above relationship describes a series for a given point ω of Ω . For the series (4) to be completely approximated by the stochastic method, the relationship (5) is of course to be iterated with a random choice of $\omega \in \Omega$ at each step. Thus, provided $\mu_{\{e\}_\omega}^{(\mathcal{E})}$ is somehow local, an issue that will be addressed in the next section, the above considerations allow to consider (5), at ω , as the definition of a *continuous* automaton, which is an extension of classical cellular automata for which the cell states are allowed to take their values in \mathbb{R}^n . This automaton can be implemented for any given differential problem \mathbb{P} by evaluating $\mu_{\{e\}_\omega}^{(\mathcal{E})}$ for this particular problem.

The automaton described by (5) for each ω also departs from the strict definition of a cellular automaton by the fact that the update rule for all cells ω are only the same for a vast majority of them, but not strictly all. Indeed, because of the existing boundary conditions, the H and grad operators will not give the same result for all points, since the boundary conditions are considered as constants. Hence, a Dirichlet boundary is described in the automaton by a constant cell, the value of which is given by the automaton initial state.

At this point of the paper, we have defined an automaton that can be automatically generated from any given

differential problem, thanks to automated formal derivative computing. To ensure the computational efficiency of the automaton, we show in next section that equation (5) actually defines an automaton whose cells can be updated using the values of their neighbors only.

III. LOCALIZATION OF EACH CELL NEIGHBORHOOD

The definition of the *neighborhood* \mathcal{V} of a given function $\zeta \in \left((\Omega)^{\mathbb{R}^n}\right)^{\mathbb{R}}$ is to be understood as being the set of all the points ω needed in the evaluation of ζ :

$$\mathcal{V} : \left((\Omega)^{\mathbb{R}^n}\right)^{\mathbb{R}} \mapsto \mathcal{P}(\Omega) \\ \zeta \rightarrow \left\{ \omega \in \Omega : \exists \tilde{\xi} : \text{grad}_{\{e\}_\omega}^{(\zeta)}(\tilde{\xi}) \neq 0 \right\}$$

The automaton described in the previous section is thus practically usable if the calculations needed to evaluate it are *local*, *i.e.* expression (5) can be evaluated without requiring access to Ω as a whole. This can be formally stated as $\mathcal{V}\left(\left|\mu_{\{e\}_\omega}^{(\mathcal{E})}\right|\right) \neq \Omega$. This can happen only if some kind of locality condition on \mathbb{P} is assumed.

To show that this is indeed the case, let us first define the *reciprocal neighborhood* $\bar{\mathcal{V}}$ for a given $\omega \in \Omega$ and a given $\tilde{\Phi}$: $\bar{\mathcal{V}}(\omega, \tilde{\Phi}) = \left\{ \omega' : \omega \in \mathcal{V}\left(\left|\tilde{\Phi}(\omega')\right|\right) \right\}$. Given the definition (4) of $\mu_{\{e\}_\omega}^{(\mathcal{E})}$, the gradient can be linearly distributed over the additive components of \mathcal{E} :

$$\mu_{\{e\}_\omega}^{(\mathcal{E})} = \sum_{\omega' \in \bar{\mathcal{V}}(\omega, \tilde{\Phi})} \bar{\text{H}}_{\{e\}_\omega}^{(|\mathcal{E}|)} \text{grad}_{\{e\}_\omega}^{(|\tilde{\Phi}(\omega')|)} \quad (6)$$

$$= \left(\sum_{\omega' \in \bar{\mathcal{V}}(\omega, \tilde{\Phi})} \text{H}_{\{e\}_\omega}^{(|\tilde{\Phi}(\omega')|)} \right)^{-1} \sum_{\omega' \in \bar{\mathcal{V}}(\omega, \tilde{\Phi})} \text{grad}_{\{e\}_\omega}^{(|\tilde{\Phi}(\omega')|)} \quad (7)$$

The summation term appearing in 6 has been restricted to those ω' in Ω for which the gradient does not vanish. The summations product in 7 is obtained by similarly distributing the Hessian. The neighborhood of a product being included in the union of its operands neighborhoods, the neighborhood of $\mu_{\{e\}_\omega}^{(\mathcal{E})}$, according to 7, can be limited to

$$\mathcal{V}\left(\left|\mu_{\{e\}_\omega}^{(\mathcal{E})}\right|\right) \subset \mathcal{V}\left(\left|\sum_{\omega' \in \bar{\mathcal{V}}(\omega, \tilde{\Phi})} \text{H}_{\{e\}_\omega}^{(|\tilde{\Phi}(\omega')|)}\right|\right)^{-1} \\ \cup \mathcal{V}\left(\left|\sum_{\omega' \in \bar{\mathcal{V}}(\omega, \tilde{\Phi})} \text{grad}_{\{e\}_\omega}^{(|\tilde{\Phi}(\omega')|)}\right|\right) \quad (8)$$

For obvious reasons, the neighborhood of a derivative, or a gradient, is included in the neighborhood of its operand. The same holds for the neighborhood of a Hessian since any line or column of the Hessian is a derivative of the gradient. Therefore, the right-hand term of the above union is included in $\bigcup_{\omega' \in \bar{\mathcal{V}}(\omega, \tilde{\Phi})} \mathcal{V}\left(\left|\tilde{\Phi}(\omega')\right|\right)$.

Furthermore, the neighborhood of a matrix norm $|M|$ is obviously included in the union of the neighborhoods of all its components. The same holds for the inverse matrix $\left|(M)^{-1}\right|$ since each of its components can be obtained by a combination of the components of M . We can therefore conclude that the left-hand term of the union in (8) is also a subset of $\bigcup_{\omega' \in \bar{\mathcal{V}}(\omega, \tilde{\Phi})} \mathcal{V}\left(\left|\tilde{\Phi}(\omega')\right|\right)$.

Therefore, provided we can assume that $\mathcal{V}\left(\left|\tilde{\Phi}(\omega)\right|\right)$ is small enough for all $\omega \in \Omega$ —which is ensured if the differential problem \mathbb{P} is defined locally—, the calculations to be undertaken to evaluate $\mu_{\{e\}_\omega}^{(\mathcal{E})}$ for each cell ω are local to some extended neighborhood of that cell:

$$\mathcal{V}\left(\left|\mu_{\{e\}_\omega}^{(\mathcal{E})}\right|\right) \subset \bigcup_{\omega' \in \bar{\mathcal{V}}(\omega, \tilde{\Phi})} \mathcal{V}\left(\left|\tilde{\Phi}(\omega')\right|\right)$$

IV. APPLICATION EXAMPLE

As hinted before, we have implemented the continuous automaton described in the previous sections with the help of an off-the-shelf formal computing software and a cellular automata environment analogous to those reported in [12, 13]. We have thus automated the computation from the specification of the discrete differential

problem $\tilde{\mathbb{P}}$ to the design of the adequate continuous automaton.

We have applied this method to the difficult problem of guided electromagnetic propagation *without the paraxial approximation*. Indeed, we have computed the coupling of a Gaussian laser beam into a half-waist wide and off centered Gaussian shaped waveguide of modulation depth 10^{-2} .

The non paraxial propagation equation is thus solved by deriving two real equations from it, discretizing them with finite difference centered derivatives except along the propagation direction where left-handed derivatives are needed because of the impossibility to give a boundary condition on both sides of the propagation axis. The adequate continuous automaton is then computed from the discretized problem (too complicated to show here). When launched on a $30 \times 30 \times 30$ network, it stabilizes to a steady state showing, as expected, the partial coupling of the beam in the waveguide. The *a posteriori* remaining error is computed to be less than 10^{-10} .

V. CONCLUSION

We have described and successfully assessed what we believe to be the first method allowing to tailor a Continuous Automaton so that its steady state *quantitatively* solves a given differential problem. We believe that this method can be applied to most continuous differential problems. The accompanying formal computing automation thus offers the unique possibility to reduce differential problem solving to the mere specification of the problem with an adequate formal language and its feeding to a specifically designed Continuous Automaton.

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