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Wave Equation Numerical Resolution: Mathematics and Program

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Thème : Programmation, vérification et preuves
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Abstract: We formally prove the C program that implements a simple numerical scheme for the resolution of the one-dimensional acoustic wave equation. Such an implementation introduces errors at several levels: the numerical scheme introduces method errors, and the floating-point computation leads to round-off errors. We formally specify in Coq the numerical scheme, prove both the method error and the round-off error of the program, and derive an upper bound for the total error. This proves the adequacy of the C program to the numerical scheme and the convergence of the effective computation. To our knowledge, this is the first time a numerical analysis program is fully machine-checked.

Key-words: Formal proof of numerical program , Convergence of numerical scheme , Proof of C program , Coq formal proof , Acoustic wave equation , Partial differential equation , Rounding error analysis

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Résolution numérique de l'équation des ondes : mathématiques et programme

Résumé : Nous prouvons formellement le programme C implémentant un schéma numérique simple pour la résolution de l'équation des ondes acoustiques en dimension 1. Une telle implémentation introduit différents types d'erreurs : l'erreur de méthode due au schéma numérique et les erreurs d'arrondi dues aux calculs en virgule flottante. Nous spécifions formellement en Coq le schéma numérique, nous prouvons les deux types d'erreur et nous dérivons une majoration de l'erreur totale. Cela prouve l'adéquation du programme C avec le schéma numérique et la convergence des calculs effectifs. À notre connaissance, c'est la première fois qu'un programme d'analyse numérique est complètement vérifé mécaniquement.

Mots-clés : preuve formelle d'un programme numérique, convergence d'un schéma numérique, preuve de programme C, preuve formelle en Coq, équation des ondes acoustiques, équation aux dérivées partielles, analyse d'erreurs d'arrondi.

1 Introduction

Ordinary differential equations (ODE) and partial differential equations (PDE) are ubiquitous in engineering and scientific computing. They show up in nuclear simulation, weather forecast, and more generally in numerical simulation, including block diagram modelization. Since solutions to nontrivial problems are non-analytic, they must be approximated by numerical schemes over discrete grids.

Numerical analysis is mainly interested in proving the *convergence* of these schemes, that is, to prove that the approximation quality increases as the size of the discretization steps decreases. The approximation quality represents how close to the exact continuous solution is the approximated discrete solution; this distance must tend toward zero in order for the numerical scheme to be useful.

Once a numerical scheme has been proven to be convergent, it is implemented as a C/C++ or Fortran program that performs floating-point computations. This now adds an extra level of uncertainty to the confidence one can give to the computation result. Indeed, three kinds of unfortunate issues can arise. First, the numerical scheme might not converge as fast as expected (if there were an oversight or a mistake in its convergence proof). Second, even if the scheme is formally proven, the floating-point computations introduce round-off errors that could lead to completely irrelevant results. Third, the program must be written with extreme care to ensure that it effectively implements the scheme and is immune from runtime errors, out-of-bound accesses, overflows, and so on.

The purpose of mechanically-checked verification is to prevent all these issues and to ensure the overall correctness of the program. This work is a first step toward the development of a set of formal tools for dealing with numerical schemes, their convergence, and their implementation: we present the formal verification of a C program that implements a simple numerical scheme.

It would have been sensible to start with some classical scheme for ODE, such as the Euler or Runge-Kutta method. But we decided to directly validate the feasibility of the approach on more complicated PDE. Indeed, this opens the door to a wider variety of applications, as PDE appear in many realistic problems from industry. Also, this is a better test case to check whether current formal tools are sufficient to verify a real program from numerical analysis.

We chose the domain of wave propagation because it is one of the most common physical phenomena one can experiment in everyday life: directly through sight and hearing, but also via telecommunications, radar, medical imaging, etc. Industrial applications are numerous and range from aeroacoustics to music acoustics (acoustic waves), from oil prospection to non-destructive testing (elastic waves), from optics to stealth technology (electromagnetic waves), and even include the stabilization of ships and offshore platforms (surface gravity waves).

We consider an archetypal model for all kinds of waves: the acoustic wave equation in a one-dimensional space domain. The equation describes the propagation of pressure variations (or sound waves) in a fluid medium; it also models the behavior of a vibrating string. Among the wide variety of numerical schemes for approximately solving the 1D acoustic wave equation, we chose the simplest one: the second order centered finite difference scheme, also known as the *three-point scheme*. To keep it simple, we assume an homogeneous media (meaning that the propagation velocity is a constant), and consider discretization over regular grids with constant discretization steps for time and space.

As expected, the resulting C program is simple: it contains a few functions and loops, manipulates matrices (arrays of arrays) of numbers, and performs floating-point computations. In addition, there are some textual comments, called *annotations*, that state what we claim the program is computing, namely an approximation of the solution to the wave equation. In particular, we assert a bound on the approximation error. This program is then submitted to Frama-C, a framework [1] for verifying C programs. Combined with Jessie/Why, it generates *proof obligations*. If these theorems can be proved, either automatically or by the user, then the program is

[1] Tools cited in this paragraph are presented in Section 3

guaranteed to satisfy the specifications expressed by the annotations and to be free from runtime errors.

Part of the proof obligations are discharged by automated provers, *e.g.* Alt-Ergo, CVC3, Gappa, and Z3. The more complicated ones, such as the one related to the convergence of the numerical scheme, are left to the user. We have proved these obligations with Coq, an interactive proof assistant. In the end, we have formally verified all the properties of the C program. To our knowledge, this is the first time this kind of verification is machine-checked. The annotated C program and the Coq sources of the formal development are available from

`http://fost.saclay.inria.fr/wave_total_error.html`

There is an abundant literature about the convergence of numerical schemes, *e.g.* see [43, 45]. In particular, the convergence of the three-point scheme for the wave equation is well-known and taught relatively early [7]. Unfortunately, no article goes into all the details needed for a formal proof. These mathematical "details" may have been skipped for readability, but some mandatory details may have also been omitted due to an oversight.

In the fields of automatic provers and proof assistants, few works have been done for the formalization and mechanical proofs of mathematical analysis, and even fewer works for numerical analysis. Indeed, real analysis developments are relatively new. The first developments on real numbers and real analysis are from the late 90's [25, 30, 27, 36, 28]. Some intuitionist formalizations have been realized by a team at Nijmegen [29, 20]. Still, analysis results are available in provers such as ACL2, Coq, HOL Light, Isabelle, Mizar, or PVS; regarding numerical analysis, we can also cite a work by one of the author which deals with the formal proof of an automatic differentiation algorithm [37]. An extensive work has been done by Harrison regarding $\mathbb{R}^n$ and the dot product [31]. Concerning the big O operator for asymptotic comparison, a decision procedure has been developed in [4]; unfortunately, those results were not applicable since we needed a more powerful big O.

Runtime errors and convergence properties have been mentioned above. The third task to tackle in order to guarantee the correctness of the program is to bound the round-off errors. As explained by Rosinger in 1985, old methods were based on "unrealistic linearizing assumptions" for round-off errors and the convergence was proved excellent [39]. Further work was done under more realistic assumptions about round-off errors [39, 40], but none of these assumptions were proved correct with respect to the actual round-off errors of the numerical schemes.

As Roy and Oberkampf, we believe that round-off errors should not be treated as random variables and that traditional statistical methods should not be used [41]. Proposed methods are the use of interval arithmetic or a precision increase to control the accuracy. Note that their example of hypersonic nozzle flow is converging so fast that round-off errors are neglected [41].

Another use of interval arithmetic is to include the method error [42]. Then the final interval is guaranteed to contain the mathematical exact solution as both the method error and the rounding error have been added at each step. Note that this fact has not been formally proved. Also, the width of the final interval is not guaranteed.

The previous methods are dedicated to numerical schemes. There are also some generic tools for bounding round-off errors. Some successful approaches are based on abstract interpretation [19, 24]. In our case, they would have been of little help, since there is a complex phenomenon of error compensation during the computations. Ignoring this compensation would lead to bounds on round-off errors growing as fast as $O(2^k)$ (k being the number of time steps). That is why we had to thoroughly studied the propagation of round-off errors in this numerical scheme to get much tighter bounds. It also means that most of the proofs had to be done by hand to achieve this part of the formal verification.

Section 2 presents the PDE, the numerical scheme, and their mathematical properties. Section 3 describes the software tools used in the formalization. Section 4 is devoted to the formal proof of the convergence of the numerical scheme, and Section 5 contains the formal proof of the upper bound for the round-off error. The total error for a particular solution of the wave equation is studied in Section 6. Details about the annotations and the proofs are in Section 7.

2 Numerical Scheme for the Wave Equation

A partial differential equation (PDE) modeling an evolution problem is an equation involving partial derivatives of an unknown function of several independent space and time variables. The uniqueness of the solution is obtained by imposing initial conditions, which are the value of the function and of some of its derivatives at the initial time. The problem of the vibrating string tied down at both ends, among many other physical problems, is formulated as an *initial-boundary value problem* where the boundary conditions are additional constraints set on the boundary of the supposedly bounded domain [43].

This section, as well as the steps taken at Section 4 to conduct the proof of the convergence of the numerical scheme, is inspired by [7].

2.1 The continuous equation

The chosen PDE models the propagation of waves along an ideal vibrating elastic string which is tied down at both ends, see [1, 15], see also Figure 1. The PDE is obtained from Newton's laws of motion [38].

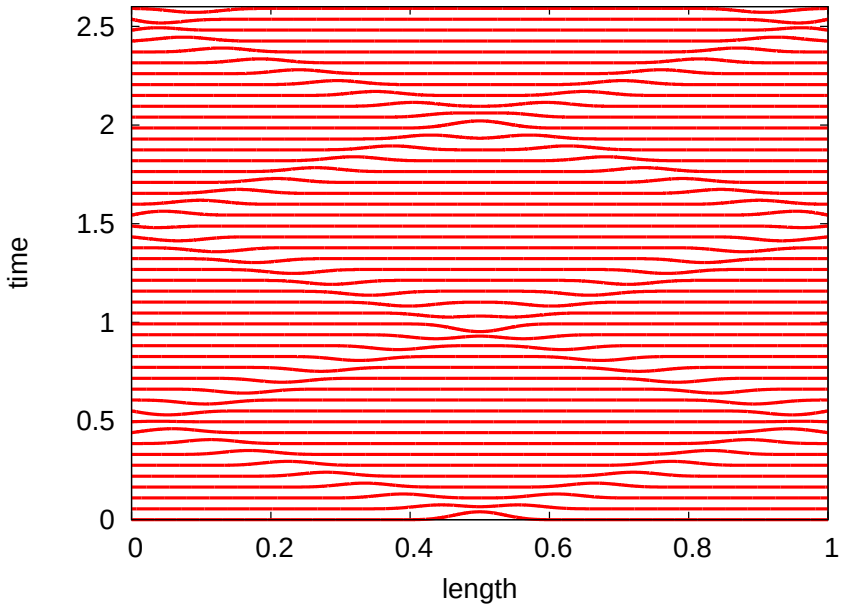


Figure 1: Space-time representation of the signal propagating along a vibrating string. Each curve represents the string at a different time step.

The gravity is neglected, so the string is supposed rectilinear when at rest. Let $x_{\min}$ and $x_{\max}$ be the abscissas of the extremities of the string. Let $\Omega = [x_{\min}, x_{\max}]$ be the bounded space domain. Let $p(x,t)$ be the transverse displacement of the point of the string of abscissa x at time t from its equilibrium position. It is a (signed) scalar. Let c be the constant propagation velocity. It is a positive number that depends on the section and density of the string. Let $s(x,t)$ be the external action on the point of abscissa x at time t; it is a source term, such that $t = 0 \Rightarrow s(x,t) = 0$. Finally, let $p_0(x)$ and $p_1(x)$ be the initial position and velocity of the point of abscissa x. We

consider the initial-boundary value problem

$$\forall t \geq 0,\ \forall x \in \Omega, \qquad (L(c)\,p)(x,t) \stackrel{\text{def}}{=} \frac{\partial^2 p}{\partial t^2}(x,t) + A(c)\,p(x,t) = s(x,t), \tag{1}$$

$$\forall x \in \Omega, \qquad (L_1\,p)(x,0) \stackrel{\text{def}}{=} \frac{\partial p}{\partial t}(x,0) = p_1(x), \tag{2}$$

$$\forall x \in \Omega, \qquad (L_0\,p)(x,0) \stackrel{\text{def}}{=} p(x,0) = p_0(x), \tag{3}$$

$$\forall t \geq 0, \qquad p(x_{\min},t) = p(x_{\max},t) = 0 \tag{4}$$

where the differential operator $A(c)$ is defined by

$$A(c) \stackrel{\text{def}}{=} -c^2 \frac{\partial^2}{\partial x^2}. \tag{5}$$

This simple partial derivative equation happens to possess an analytical solution given by the so-called d'Alembert's formula [33], obtained from the method of characteristics and the image theory [32], $\forall t \geq 0$, $\forall x \in \Omega$,

$$p(x,t) = \frac{1}{2}(\tilde{p}_0(x-ct) + \tilde{p}_0(x+ct)) + \frac{1}{2c}\int_{x-ct}^{x+ct} \tilde{p}_1(y)dy + \frac{1}{2c}\int_0^t \left(\int_{x-c(t-\sigma)}^{x+c(t-\sigma)} \tilde{s}(y,\sigma)dy\right) d\sigma \tag{6}$$

where the quantities $\tilde{p}_0$, $\tilde{p}_1$, and $\tilde{s}$ are respectively the successive antisymmetric extensions in space of p_0, p_1, and s defined on Ω to the entire real axis $\mathbb{R}$.

We are in the process of formally verifying d'Alembert's formula as a separate work. But for the purpose of the current work, we have just admitted that under reasonable conditions on the Cauchy data p_0 and p_1 and on the source term s, there exists a unique solution p to the initial-boundary value problem (1)–(4) for each $c > 0$. Simply supposing the existence of a solution instead of exhibiting it, opens the way to scale our approach to more general cases for which there is no known analytic expression of a solution, *e.g.* in the heterogeneous case.

For such a solution p, it is natural to associate at each time t the positive definite quadratic quantity

$$E(c)(p)(t) \stackrel{\text{def}}{=} \frac{1}{2}\left\|\left(x \mapsto \frac{\partial p}{\partial t}(x,t)\right)\right\|^2 + \frac{1}{2}\left\|(x \mapsto p(x,t))\right\|_{A(c)}^2 \tag{7}$$

where $\langle q, r\rangle \stackrel{\text{def}}{=} \int_\Omega q(x)r(x)dx$, $\|q\|^2 \stackrel{\text{def}}{=} \langle q, q\rangle$ and $\|q\|_{A(c)}^2 \stackrel{\text{def}}{=} \langle A(c)\,q, q\rangle$. The first term is interpreted as the kinetic energy, and the second term as the potential energy, making E the mechanical energy of the vibrating string.

2.2 The discrete equations

Let n_i be the positive number of intervals of the space discretization. Let the space discretization step be $\Delta x \stackrel{\text{def}}{=} \frac{x_{\max}-x_{\min}}{n_i}$ and define the discretization function $i_{\Delta x}(x) \stackrel{\text{def}}{=} \left\lfloor \frac{x-x_{\min}}{\Delta x} \right\rfloor$.

Let us consider the time interval $[0, t_{\max}]$. Let $\Delta t \in]0, t_{\max}[$ be the time discretization step, define $k_{\Delta t}(t) \stackrel{\text{def}}{=} \left\lfloor \frac{t}{\Delta t} \right\rfloor$, and set $n_k \stackrel{\text{def}}{=} k_{\Delta t}(t_{\max})$.

Now, the compact domain $\Omega \times [0, t_{\max}]$ is approximated by the regular discrete grid defined by

$$\forall k \in [0..n_k],\ \forall i \in [0..n_i], \quad \mathbf{x}_i^k \stackrel{\text{def}}{=} (x_i, t^k) \stackrel{\text{def}}{=} (x_{\min} + i\Delta x, k\Delta t). \tag{8}$$

For a function q defined over $\Omega \times [0, t_{\max}]$ (resp. Ω), the notation q_{h} denotes any discrete approximation of q at the points of the grid, *i.e.* a discrete function over $[0..n_i] \times [0..n_k]$ (resp. $[0..n_i]$). By extension, the notation q_{h} is also a shortcut to denote the matrix $(q_i^k)_{0\leq i\leq n_i, 0\leq k\leq n_k}$ (resp. the vector $(q_i)_{0\leq i\leq n_i}$). The notation $\bar{q}_{\text{h}}$ is reserved to the approximation defined on $[0..n_i] \times [0..n_k]$ by $\bar{q}_i^k \stackrel{\text{def}}{=} q(\mathbf{x}_i^k)$ (resp. $\bar{q}_i \stackrel{\text{def}}{=} q(x_i)$).

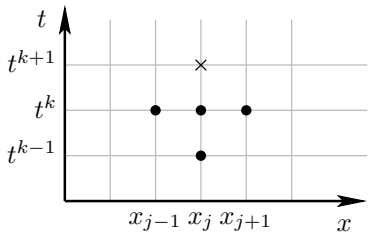


Figure 2: Three-point scheme: p_i^{k+1} (at $\times$) depends on p_{i-1}^k, p_i^k, p_{i+1}^k, and p_i^{k-1} (at $\bullet$).

Let $p_{0\mathrm{h}}$ and $p_{1\mathrm{h}}$ be two discrete functions over $[0..n_i]$; let s_h be a discrete function over $[0..n_i] \times [0..n_k]$. Then, the discrete function p_h over $[0..n_i] \times [0..n_k]$ is said to be the solution of the three-point[2] finite difference scheme, as illustrated in Figure 2, when the following set of equations holds:

(9) $\forall k \in [2..n_k]$, $\forall i \in [1..n_i - 1]$,

$$(L_\mathrm{h}(c)\, p_\mathrm{h})_i^k \stackrel{\text{def}}{=} \frac{p_i^k - 2p_i^{k-1} + p_i^{k-2}}{\Delta t^2} + (A_\mathrm{h}(c)\,(i' \mapsto p_{i'}^{k-1}))_i = s_i^{k-1},$$

(10) $$\forall i \in [1..n_i - 1], \qquad (L_{1\mathrm{h}}(c)\, p_\mathrm{h})_i \stackrel{\text{def}}{=} \frac{p_i^1 - p_i^0}{\Delta t} + \frac{\Delta t}{2}(A_\mathrm{h}(c)\,(i' \mapsto p_{i'}^0))_i = p_{1,i},$$

(11) $$\forall i \in [1..n_i - 1], \qquad (L_{0\mathrm{h}}\, p_\mathrm{h})_i \stackrel{\text{def}}{=} p_i^0 = p_{0,i},$$

(12) $$\forall k \in [0..n_k], \qquad p_0^k = p_{n_i}^k = 0$$

where the matrix $A_\mathrm{h}(c)$, a discrete analog of $A(c)$, is defined for any vector q_h, by

(13) $$\forall i \in [1..n_i - 1], \quad (A_\mathrm{h}(c)\, q_\mathrm{h})_i \stackrel{\text{def}}{=} -c^2 \frac{q_{i+1} - 2q_i + q_{i-1}}{\Delta x^2}.$$

A discrete analog of the energy is also defined by[3]

(14) $$E_\mathrm{h}(c)(p_\mathrm{h})^{k+\frac{1}{2}} \stackrel{\text{def}}{=} \frac{1}{2}\left\| \left(i \mapsto \frac{p_i^{k+1} - p_i^k}{\Delta t} \right) \right\|_{\Delta x}^2 + \frac{1}{2} \left\langle (i \mapsto p_i^k), (i \mapsto p_i^{k+1}) \right\rangle_{A_h(c)}$$

where, for any vectors q_h and r_h,
$\langle q_\mathrm{h}, r_\mathrm{h} \rangle_{\Delta x} \stackrel{\text{def}}{=} \sum_{i=0}^{n_i} q_i r_i \Delta x$, and $\|q_\mathrm{h}\|_{\Delta x}^2 \stackrel{\text{def}}{=} \langle q_\mathrm{h}, q_\mathrm{h} \rangle_{\Delta x}$,
$\langle q_\mathrm{h}, r_\mathrm{h} \rangle_{A_h(c)} \stackrel{\text{def}}{=} \langle A_\mathrm{h}(c)\, q_\mathrm{h}, r_\mathrm{h} \rangle_{\Delta x}$, and $\|q_\mathrm{h}\|_{A_h(c)}^2 \stackrel{\text{def}}{=} \langle q_\mathrm{h}, q_\mathrm{h} \rangle_{A_h(c)}$.

Note that the three-point scheme is parametrized by the discrete Cauchy data $p_{0\mathrm{h}}$ and $p_{1\mathrm{h}}$, and by the discrete source term s_h. Of course, when these discrete inputs are respectively approximations of the continuous functions p_0, p_1, and s (e.g., when $p_{0\mathrm{h}} = \bar{p}_{0\mathrm{h}}$, $p_{1\mathrm{h}} = \bar{p}_{1\mathrm{h}}$, and $s_\mathrm{h} = \bar{s}_\mathrm{h}$), then the discrete solution p_h is an approximation of the continuous solution p.

2.3 Convergence

Let ξ be in $]0, 1[$. The CFL(ξ) condition (for Courant-Friedrichs-Lewy, see [18]) states that the discretization steps satisfy the relation

(15) $$\frac{c\Delta t}{\Delta x} \leq 1 - \xi.$$

[2] In the sense "three spatial points", for the definition of matrix $A_\mathrm{h}(c)$.

[3] By convention, the energy is defined between steps k and $k+1$, hence the notation $k + \frac{1}{2}$.

The convergence error e_h measures the distance between the continuous and discrete solutions. It is defined by

$$\forall k \in [0..n_k],\ \forall i \in [0..n_i], \quad e_i^k \stackrel{\text{def}}{=} \bar{p}_i^k - p_i^k. \tag{16}$$

Note that when $p_{0\mathrm{h}} = \bar{p}_{0\mathrm{h}}$, then for all i, $e_i^0 = 0$. The truncation error ε_h measures at which precision the continuous solution satisfies the numerical scheme. It is defined by

$$\forall k \in [2..n_k],\ \forall i \in [1..n_i - 1], \qquad \varepsilon_i^k \stackrel{\text{def}}{=} (L_\mathrm{h}(c)\,\bar{p}_\mathrm{h})_i^k - \bar{s}_i^{k-1}, \tag{17}$$

$$\forall i \in [1..n_i - 1], \qquad \varepsilon_i^1 \stackrel{\text{def}}{=} (L_{1\mathrm{h}}(c)\,\bar{p}_\mathrm{h})_i - \bar{p}_{1,i}, \tag{18}$$

$$\forall i \in [1..n_i - 1], \qquad \varepsilon_i^0 \stackrel{\text{def}}{=} (L_{0\mathrm{h}}\bar{p}_\mathrm{h})_i - \bar{p}_{0,i}. \tag{19}$$

Again, note that when $p_{0\mathrm{h}} = \bar{p}_{0\mathrm{h}}$ and $p_{1\mathrm{h}} = \bar{p}_{1\mathrm{h}}$, then for all i, $\varepsilon_i^0 = 0$ and $\varepsilon_i^1 = \frac{e_i^1}{\Delta t}$. Furthermore, when there is also $s_\mathrm{h} = \bar{s}_\mathrm{h}$, then the convergence error e_h is itself solution of the same numerical scheme with inputs defined by, for all i, k,

$$p_{0,i} = \varepsilon_i^0 = 0, \quad p_{1,i} = \varepsilon_i^1 = \frac{e_i^1}{\Delta t}, \quad \text{and } s_i^k = \varepsilon_i^{k+1}.$$

The numerical scheme is said to be convergent of order 2 if the convergence error tends toward zero at least as fast as $\Delta x^2 + \Delta t^2$ when both discretization steps tend toward zero.[4] More precisely, the numerical scheme is said to be convergent of order (m,n) uniformly on the interval $[0, t_{\max}]$ if the convergence error satisfies[5]

$$\left\| \left(i \mapsto e_i^{k_{\Delta t}(t)} \right) \right\|_{\Delta x} = O_{[0,t_{\max}]}(\Delta x^m + \Delta t^n). \tag{20}$$

The numerical scheme is said to be consistent with the continuous problem at order 2 if the truncation error tends toward zero at least as fast as $\Delta x^2 + \Delta t^2$ when the discretization steps tend toward 0. More precisely, the numerical scheme is said to be consistent with the continuous problem at order $(m,\ n)$ uniformly on interval $[0, t_{\max}]$ if the truncation error satisfies

$$\left\| \left(i \mapsto \varepsilon_i^{k_{\Delta t}(t)} \right) \right\|_{\Delta x} = O_{[0,t_{\max}]}(\Delta x^m + \Delta t^n). \tag{21}$$

The numerical scheme is said to be stable if the discrete solution of the associated homogeneous problem (*i.e.* without any source term, $s(x,t) = 0$) is bounded independently of the discretization steps. More precisely, the numerical scheme is said to be stable uniformly on interval $[0, t_{\max}]$ if the discrete solution of the problem without any source term satisfies

$$\begin{aligned} \exists \alpha, C_1, C_2 > 0,\ \forall t \in [0, t_{\max}],\ \forall \Delta x, \Delta t > 0, \quad & \sqrt{\Delta x^2 + \Delta t^2} < \alpha \Rightarrow \\ & \left\| \left(i \mapsto p_i^{k_{\Delta t}(t)} \right) \right\|_{\Delta x} \leq (C_1 + C_2 t)(\|p_{0\mathrm{h}}\|_{\Delta x} + \|p_{0\mathrm{h}}\|_{A_h(c)} + \|p_{1\mathrm{h}}\|_{\Delta x}). \end{aligned} \tag{22}$$

The result to be formally proved at Section 4 states that if the continuous solution p is regular enough on $\Omega \times [0, t_{\max}]$ and if the discretization steps satisfy the CFL(ξ) condition, then the three-point scheme is convergent of order (2, 2) uniformly on interval $[0, t_{\max}]$.

We do not admit (nor prove) the Lax equivalence theorem which stipulates that for a wide variety of problems and numerical schemes, consistency implies the equivalence between stability and convergence. Instead, we establish that consistency and stability implies convergence in the particular case of the one-dimensional acoustic wave equation.

2.4 Program

The main part of the C program is listed in Listing 1.

[4] Note that Δx tending toward 0 actually means that n_i goes to infinity.

[5] See Section 4.1 for the definition of a big O notation that is uniform with respect to time.

Listing 1: The main part of the C code, without annotations.

```
/* Compute the constant coefficient of the stiffness matrix. */
a1 =  dt/dx*v;
a  = a1*a1;

/* First initial condition and boundary conditions. */
/* Left boundary. */
p[0][0] = 0.;
/* Time iteration -1 = space loop. */
for (i=1; i<ni; i++) {
  p[i][0] = p0(i*dx);
}
/* Right boundary. */
p[ni][0] = 0.;

/* Second initial condition (with p1=0) and boundary conditions. */
/* Left boundary. */
p[0][1] = 0.;
/* Time iteration 0 = space loop. */
for (i=1; i<ni; i++) {
  dp = p[i+1][0] - 2.*p[i][0] + p[i-1][0];
  p[i][1] = p[i][0] + 0.5*a*dp;
}
/* Right boundary. */
p[ni][1] = 0.;

/* Evolution problem and boundary conditions. */
/* Propagation = time loop. */
for (k=1; k<nk; k++) {
  /* Left boundary. */
  p[0][k+1] = 0.;
  /* Time iteration k = space loop. */
  for (i=1; i<ni; i++) {
    dp = p[i+1][k] - 2.*p[i][k] + p[i-1][k];
    p[i][k+1] = 2.*p[i][k] - p[i][k-1] + a*dp;
  }
  /* Right boundary. */
  p[ni][k+1] = 0.;
}
```

The grid steps Δx and Δt are respectively represented by the variables dx and dt, the grid sizes n_i and n_k by the variables ni and nk, and the propagation velocity c by the variable v. The initial position $p_{0\mathrm{h}}$ is represented by the function p0. The initial velocity $p_{1\mathrm{h}}$ and the source term s_{h} are supposed to be zero and are not represented. The discrete solution p_{h} is represented by the two-dimensional array p of size $(n_i + 1) * (n_k + 1)$ (this is a simple naive implementation, a more efficient implementation would only require the storage of two time steps).

To assemble the stiffness matrix $A_{\mathrm{h}}(c)$, we only have to compute the square of the CFL coefficient $\frac{c\Delta t}{\Delta x}$ (lines 1–2). Then, we recognize the space loops for the initial conditions: Equation (11) on lines 6–8, and Equation (10) with $p_{1\mathrm{h}} = 0$ on lines 14–17. The space-time loop on lines 23–28 for the evolution problem comes from Equation (9). And finally, the boundary conditions of Equation (12) are spread out on lines 9–10, 18–19, and 29–30.

3 Tools

Several softwares are used in this work. The formal proof of the method error has been made in Coq. The formal proof of the round-off error has been made in Coq, and using Gappa tactic. The certification of the C program has used Frama-C (with Jessie plug-in), and to prove the produced goals, we used Gappa, SMT provers and the preceding Coq proofs. This section is devoted to present these tools and some necessary libraries.

3.1 Coq

Coq[6] is a formal system that provides an expressive language to write mathematical definitions, executable algorithms, and theorems, together with an interactive environment for proving them [8]. Coq's formal language is based on the Calculus of Inductive Constructions [17] that combines both a higher-order logic and a richly-typed functional programming language. Coq allows to define functions or predicates, that can be evaluated efficiently, to state mathematical theorems and software specifications, and to interactively develop formal proofs of these theorems. These proofs are machine-checked by a relatively small *kernel*, and certified programs can be extracted from them to external programming languages like Objective Caml, Haskell, or Scheme [34].

As a proof development system, Coq provides interactive proof methods, decision and semi-decision algorithms, and a tactic language for letting the user define its own proof methods. Connection with external computer algebra system or theorem provers is also available.

The Coq library is structured into two parts: the initial library, which contains elementary logical notions and data-types, and the standard library, a general-purpose library containing various developments and axiomatizations about sets, lists, sorting, arithmetic, real numbers, etc.

In this work, we mainly use the Reals standard library [36], that is a classical axiomatization of an Archimedean ordered complete field. We chose Reals to make our numerical proofs because it is the simplest axiomatization and also because we do not need an intuitionistic formalization.

For floating-point numbers, we use a large Coq library[7] initially developed in [21] and extended with various results afterwards [10]. It is a high-level formalization of IEEE-754 with gradual underflow. This is expressed by a formalization where floating-point numbers are pairs (n, e) associated with real values $n \times \beta^e$. The requirements for a number to be in the format $(e_{\min}, \beta^p)$ are:

$$|n| < \beta^p \quad \wedge \quad e_{\min} \leq e.$$

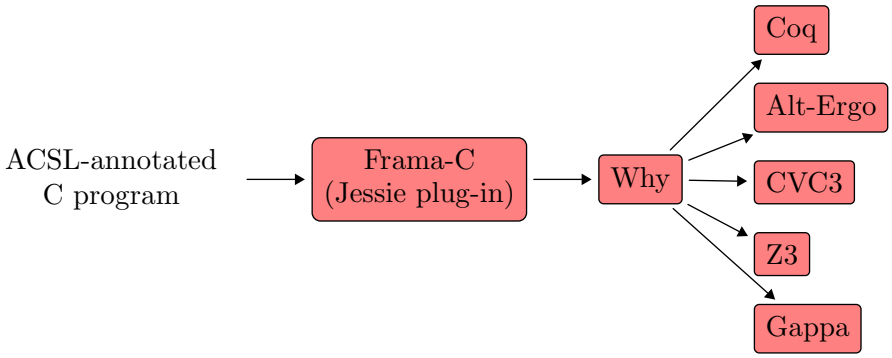
This formalization is convenient for human interactive proofs as testified by the numerous proofs using it. The huge number of lemmas available in the library (about 1400) makes it suitable for a large range of applications.

[6] http://coq.inria.fr/

[7] http://lipforge.ens-lyon.fr/www/pff/

3.2 Frama-C/Jessie/Why/SMT solvers

We use the Frama-C platform[8] to perform formal verification of C programs at the source-code level. Frama-C is an extensible framework which combines static analyzers for C programs, written as plug-ins, within a single tool. In this work, we use the Jessie plug-in for deductive verification. C programs are annotated with behavioral contracts written using the *ANSI C Specification Language* (ACSL for short) [6]. The Jessie plug-in translates them to the Jessie language [35], which is part of the Why verification platform [26]. Finally, the Why platform computes verification conditions, using traditional techniques of weakest preconditions, and emits them to a wide set of existing theorem provers, ranging from interactive proof assistants to automated theorem provers. In this work, we use the Coq proof assistant (Section 3.1), SMT solvers Alt-Ergo [16], CVC3 [5] and Z3 [23], and the automated theorem prover Gappa (Section 3.3). The dataflow from C source code to theorem provers can be depicted as follows:



In ACSL, annotations are using first-order logic. Following the *programming by contract* approach, the specifications involve preconditions, postconditions, and loop invariants. Contrary to other approaches focusing on run-time assertion checking, ACSL specifications do not refer to C values and functions, even if pure, but refer instead to purely logical symbols. In the following contract for a function computing the square of an integer x

```
//@ ensures \result == x * x;
int square(int x);
```

the postcondition, introduced with ensures, refers to the return value \result and argument x. Both are denoting mathematical integer values, for the corresponding C values of type int. In particular, x * x cannot overflow. Of course, one could give function square a more involved specification that handles overflows, *e.g.* with a precondition requiring x to be small enough. Simply speaking, we can say that C integers are reflected within specifications as mathematical integers, in an obvious way.

Reflection of C floating-point numbers is more subtle. Following previous work by two of the authors [13], a floating-point number f is modeled in the logic as a triple of real numbers (r, e, m). Note that infinite and *Not-a-Number* values are not taken into account as we always prove they do not happen. Value r simply stands for the real number which is immediately represented by f; value e stands for the *exact* value of f, as obtained if no rounding errors had occurred; finally, value m stands for the *model* of f, which is a placeholder for the value intended to be computed and filled by the user. The latter can be seen as a ghost variable attached to each-floating point number.

In ACSL, the three components of the model of a floating point number f can be referred to using f, \exact(f), and \model(f), respectively. \round_error(f) is a macro for the rounding error, that is, \abs(f - \exact(f)).

For instance, the following is from our C program, regarding error on dx which represent the grid steps Δx (see Section 2).

[8] http://www.frama-c.cea.fr/

```
dx = 1./ni;
/*@ assert
  @   dx > 0. && dx <= 0.5 &&
  @   \abs(\exact(dx) - dx) / dx <= 0x1.p-53;
  @ */
```

Note that 0x1.p-53 is a valid C statement meaning 2^{-53}.

3.3 Gappa

The Gappa tool[9] adapts the interval-arithmetic paradigm to the proof of properties that occur when verifying numerical applications. The inputs are logical formulas quantified over real numbers whose atoms are usually enclosures of arithmetic expressions inside numeric intervals. Gappa answers whether it succeeded in verifying it. In order to support program verification, one can use *rounding* functions inside expressions. These unary operators take a real number and return the closest real number in a given direction that is representable in a given binary floating-point format. For instance, assuming that operator $\circ$ rounds to the nearest binary64 floating-point number, the following formula states that the relative error of the floating-point addition is bounded:

$$\forall x, y \in \mathbb{R},\ \exists \varepsilon \in \mathbb{R},\ |\varepsilon| \leq 2^{-53} \wedge \circ(\circ(x) + \circ(y)) = (\circ(x) + \circ(y)) \times (1 + \varepsilon).$$

Converting straight-line numerical programs to Gappa logical formulas is easy and the user can provide additional hints if the tool were to fail to verify a property. The tool is specially designed to handle codes that are performing convoluted manipulations. For instance, it has been successfully used to verify a state-of-the-art library of correctly-rounded elementary functions [22]. In the current work, Gappa has been used to check much simpler properties. (In particular, no user hint was needed to discharge a proof automatically.) But the length of their proofs would discourage even the most dedicated users if they were to be manually handled. One of the properties is the round-off error of a local evaluation of the numerical scheme (Section 5.1). Other properties mainly deal with proving that no exceptional behavior occur while executing the program: due to the initial values, all the computed values are sufficiently small to never cause overflow.

Some formulas would require long and intricate reasonings, hence casting some doubts on whether Gappa actually succeeded in verifying them. That is why the tool also generates a formal certificate that can be mechanically checked by a proof assistant. This feature has served as the basis for a Coq tactic for automatically solving goals related to floating-point and real arithmetic [14]. The tactic reads the current goal, generates a Gappa goal, executes Gappa on it, recovers the certificate, and converts it to a complete proof term that Coq matches against the current goal. This tactic has been used whenever a verification condition would have been directly proved by Gappa, if not for some confusing notations or encodings of matrix elements. We just had to apply a few basic Coq tactics to put the goal into the proper form and then call the Gappa tactic to discharge it automatically.

4 Method Error

We start by presenting in Section 4.1 the required notions necessary to formalize and to prove the method error. In the following sections, we detail how the method error proof works: we establish the consistency, the stability and the fact that they imply convergence in the particular case of the one-dimensional acoustic wave equation.

4.1 Big O, Differentiability, and Regularity

When considering a big O equality $a = O(b)$, one usually assumes that a and b are two expressions defined over the same domain and its interpretation as a quantified formula comes naturally. Here

[9] http://gappa.gforge.inria.fr/

the situation is a bit more complicated. Consider

$$f(\mathbf{x}, \mathbf{\Delta x}) = O(g(\mathbf{\Delta x}))$$

when $\|\mathbf{\Delta x}\|$ goes to 0. If one were to assume that the equality holds for any $\mathbf{x} \in \mathbb{R}^2$, one would interpret it as

$$\forall \mathbf{x}, \exists \alpha > 0, \exists C > 0, \forall \mathbf{\Delta x}, \quad \|\mathbf{\Delta x}\| \leq \alpha \Rightarrow |f(\mathbf{x}, \mathbf{\Delta x})| \leq C \cdot |g(\mathbf{\Delta x})|,$$

which means that constants α and C are in fact functions of $\mathbf{x}$. Such an interpretation happens to be useless, since the infimum of α may well be zero while the supremum of C may be $+\infty$.

A proper interpretation required us to define the notion of uniform big O relation with respect to the additional variable $\mathbf{x}$:

$$\exists \alpha > 0, \exists C > 0, \forall \mathbf{x} \in \Omega_{\mathbf{x}}, \forall \mathbf{\Delta x} \in \Omega_{\mathbf{\Delta x}}, \|\mathbf{\Delta x}\| \leq \alpha \Rightarrow |f(\mathbf{x}, \mathbf{\Delta x})| \leq C \cdot |g(\mathbf{\Delta x})|. \tag{23}$$

To emphasize the dependency on the two subsets $\Omega_{\mathbf{x}}$ and $\Omega_{\mathbf{\Delta x}}$, uniform big O equalities are now written

$$f(\mathbf{x}, \mathbf{\Delta x}) = O_{\Omega_{\mathbf{x}}, \Omega_{\mathbf{\Delta x}}}(g(\mathbf{\Delta x})).$$

Usual mathematical pen-and-paper proofs switch from one interpretation to the other depending on which one is the most adapted, without noticing that they may not be equivalent. The formal development was helpful in bringing into light the erroneous reasoning hidden by the usage of big O notations [12]. Since we are not considering the case of the infinite string in this paper, both interpretations of the big O notation are in fact equivalent for compactness reasons. But we still used the second one as it allows to share more proofs between the finite and infinite cases.

Now that we have a full-fledged notation for the big O, we can express the needed requirement on the solution of the continuous equation, denoted by a "sufficiently regular" function. We introduce two operators that, given a real-valued function f defined on the 2D plane and a point of it, return the values $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial t}$ at this point. Given these two operators, we can define the usual 2D Taylor polynomial of order n of a function f:

$$\mathrm{TP}_n(f, \mathbf{x}) \stackrel{\text{def}}{=} (\Delta x, \Delta t) \mapsto \sum_{p=0}^{n} \frac{1}{p!} \left(\sum_{m=0}^{p} \binom{p}{m} \cdot \frac{\partial^p f}{\partial x^m \partial t^{p-m}}(\mathbf{x}) \cdot \Delta x^m \cdot \Delta t^{p-m} \right).$$

Let $\Omega_{\mathbf{x}} \subset \mathbb{R}^2$. We say that the previous Taylor polynomial is a uniform approximation of order n of f on $\Omega_{\mathbf{x}}$ when the following uniform big O equality holds

$$f(\mathbf{x} + \mathbf{\Delta x}) - \mathrm{TP}_n(f, \mathbf{x})(\mathbf{\Delta x}) = O_{\Omega_{\mathbf{x}}, \mathbb{R}^2}\left(\|\mathbf{\Delta x}\|^{n+1} \right).$$

A function f is then said to be *sufficiently regular* of order n uniformly on $\Omega_{\mathbf{x}}$ when all its Taylor polynomials of order smaller than n are uniform approximations of f on $\Omega_{\mathbf{x}}$.

As long as we were studying only the method error, we did not have to define the differential operators nor assume anything about them [12]. Their only properties appeared through their usage: function p is a solution of the partial differential equation and it is sufficiently regular. This is no longer possible for the annotated C program. Indeed, due to the underlying logic, the annotations have to define p as a solution of the PDE by using first-order formulas stating differentiability, instead of second-order formulas involving differential operators. Since the formalization of Taylor approximations has been left unchanged, the natural way to relate the C annotations with the Coq development is therefore to define the operators as actual differential operators.

Note that this has forced us to introduce a small axiom. Indeed, our definition of Taylor approximation depends on differential operators that are total functions, while Coq standard library defines only partial operators. So we have assumed the existence of some total operators that are equal to the partial ones whenever applied to differentiable functions. The axiom states absolutely nothing about the result of these operators for nondifferentiable functions, so no inconsistencies are introduced this way. This is just a specific instance of Hilbert ε operator [44].

4.2 Consistency

The consistency of a numerical scheme expresses the fact that, for $\mathbf{\Delta x}$ small enough, the continuous solution taken at the points of the grid almost solves the numerical scheme. More precisely, we formally prove that when the continuous solution of the wave equation (1)–(4) is sufficiently regular of order 4 uniformly on $[x_{\min}, x_{\max}] \times [0, t_{\max}]$, the numerical scheme (9)–(12) is consistent with the continuous problem at order (2, 2) uniformly on interval $[0, t_{\max}]$ (see definition (21) in Section 2.3). This is obtained using the properties of Taylor approximations. This involves long and complex expressions but the proof is straightforward.

The key idea is to always manipulate uniform Taylor approximations that will be valid for all points of all grids when the discretization steps goes down to zero.

For instance, to take into account the initialization phase corresponding to Equation (10), we have to derive a uniform Taylor approximation of order 1 for the following continuous function (for any v sufficiently regular of order 3)

$$((x,t),(\Delta x,\Delta t)) \quad \mapsto \quad \frac{v(x,t+\Delta t)-v(x,t)}{\Delta t} \; - \; \frac{\Delta t}{2} c^2 \frac{v(x+\Delta x,t)-2v(x,t)+v(x-\Delta x,t)}{\Delta x^2}.$$

Note that the expression of this function involves both $x+\Delta x$ and $x-\Delta x$, meaning that we need a Taylor approximation which is valid for both positive and negative growths. The proof would have been impossible if we had required $0 < \Delta x$ (as a space grid step) in the definition of the Taylor approximation.

Note that in contrast with the case of an infinite string [12], we do not need here a lower bound for $c\frac{\Delta t}{\Delta x}$.

4.3 Stability

The stability of a numerical scheme expresses that the growth of the discrete solution is somehow bounded in terms of the input data (here, the Cauchy data $u_{0\mathrm{h}}$ and $u_{1\mathrm{h}}$, and the source term s_{h}). For the proof of the round-off error (see Section 5), we need a statement of the same form as definition (22) of Section 2.3. Therefore, we formally prove that, under the CFL(ξ) condition (15), the numerical scheme (9)–(12) is stable uniformly on interval $[0, t_{\max}]$.

But, as we choose to prove the convergence of the numerical scheme by using an energetic technique[10], it is more convenient to formulate the stability in terms of the discrete energy. More precisely, we also formally prove that under the CFL(ξ) condition (15), the discrete energy (14) satisfies the following overestimation,

$$\sqrt{E_{\mathrm{h}}(c)(p_{\mathrm{h}})^{k+\frac{1}{2}}} \leq \sqrt{E_{\mathrm{h}}(c)(p_{\mathrm{h}})^{\frac{1}{2}}} + \frac{\sqrt{2}}{2\sqrt{2\xi-\xi^2}} \cdot \Delta t \cdot \sum_{k'=1}^{k} \left\| \left(i \mapsto s_i^{k'} \right) \right\|_{\Delta x}$$

for all $t \in [0, t_{\max}]$ and with $k = \left\lfloor \frac{t}{\Delta t} \right\rfloor - 1$.

The formal proof closely follows the mathematical pen-and-paper proof. Firstly, the evolution of the discrete energy between two consecutive time steps is shown to be proportional to the source term. In particular, the energy is constant when the source is inactive. Then, we obtain the following underestimation of the discrete energy,

$$\forall k, \quad \frac{1}{2}\left(1-\left(c\frac{\Delta t}{\Delta x}\right)^2\right) \left\| \left(i \mapsto \frac{p_i^{k+1}-p_i^k}{\Delta t} \right) \right\|_{\Delta x} \leq E_{\mathrm{h}}(c)(p_{\mathrm{h}})^{k+\frac{1}{2}}.$$

Therefore, the non-negativity of the discrete energy is directly related to the CFL(ξ) condition.

Note that this stability result is valid for any input data $u_{0\mathrm{h}}$, $u_{1\mathrm{h}}$, and s_{h}.

[10] The popular alternative, using the Fourier transform, would have required huge additional Coq developments.

4.4 Convergence

The convergence of a numerical scheme expresses the fact that the discrete solution gets closer to the continuous solution as the discretization steps go down to zero. More precisely, we formally prove that when the continuous solution of the wave equation (1)–(4) is sufficiently regular of order 4 uniformly on $[x_{\min}, x_{\max}] \times [0, t_{\max}]$, and under the CFL($\xi$) condition (15), the numerical scheme (9)–(12) is convergent of order (2, 2) uniformly on interval $[0, t_{\max}]$ (see definition (20) in Section 2.3).

Again, the formal proof closely follows the mathematical pen-and-paper proof. Firstly, we prove that the convergence error e_{h} is itself the discrete solution of a numerical scheme of the same form but with different input data[11]. In particular, the source term (on the right-hand side) is here the truncation error ε_{h} associated with the initial numerical scheme for p_{h}. Then, the previous stability result holds, and we have an overestimation of the square root of the discrete energy associated with the convergence error $E_{\mathrm{h}}(c)(e_{\mathrm{h}})$ that involves a sum of the corresponding source terms, *i.e.* the truncation error. Finally, the consistency result also makes this sum a big O of $\Delta x^2 + \Delta t^2$, and a few more technical steps conclude the proof. Note that several lemmas are necessary to properly take care of the two initialization steps of the numerical scheme.

The Coq proof of the method error is about 5000-line long. About half of it is dedicated to the wave equation and the other half is re-usable (definition and properties of the dot product, the big O, Taylor expansions...). We formally proved without any axiom that the numerical scheme is convergent of order 2, which is the known mathematical result.

An interesting aspect of the formal proof in Coq is that we were able to extract the constants α and C appearing in the big O for the convergence result in order to obtain their precise values. The mathematical expressions are given in Section 6.

5 Round-off Error

As each operation is done with IEEE-754 floating-point numbers, round-off errors will occur and may endanger the accuracy of the final results. On this program, naive forward error analysis gives an error bound that is proportional to $2^k 2^{-53}$ for the computation of a p_i^k. If this bound was sensible, it would cause the numerical scheme to compute only noise after a few steps. Fortunately, round-off error actually compensate themselves. To take into account the compensations and hence prove a usable error bound, we need a precise statement of the round-off error [11] to exhibit the cancellations made by the numerical scheme.

5.1 Local round-off errors

Let δ_i^k be the (signed) floating-point error made in the two lines computing p_i^k (lines 26–27 in Listing 1). Floating-point values as computed by the program will be underlined to distinguish them from the discrete values of previous sections: $\underline{a}$, $\underline{p}_i^k$. They match the expressions `a` and `p[i][k]` in the annotations, while a and p_i^k are represented by `\exact(a)` and `\exact(p[i][k])`.

The δ_i^k are defined as follow:

$$\delta_i^{k+1} = \underline{p}_i^{k+1} - (2\underline{p}_i^k - \underline{p}_i^{k-1} + a \times (\underline{p}_{i+1}^k - 2\underline{p}_i^k + \underline{p}_{i-1}^k)).$$

Note that the program explained in Section 2.4 gives us that

$$\underline{p}_i^{k+1} = \mathrm{fl}\left(2\underline{p}_i^k - \underline{p}_i^{k-1} + \underline{a} \times (\underline{p}_{i+1}^k - 2\underline{p}_i^k + \underline{p}_{i-1}^k)\right)$$

where $\mathrm{fl}(\cdot)$ means that all the arithmetic operations that appear between the parentheses are actually performed by floating-point arithmetic, hence a bit off.

[11] Of course, there is no associated continuous problem.

In order to get a bound on δ_i^k, we need to have the range of $\underline{p}_i^k$. For this bound to be usable in our correctness proof, we need the range to be $[-2, 2]$. We have proved this fact by an induction using the bounds on the method error and the round-off error of all the $\underline{p}^k$ and $\underline{p}^{k-1}$.

To prove the bound on δ_i^k, we perform forward error analysis and then use interval arithmetic to bound each intermediate error. We formally prove that $|\delta_i^{k+1}| \leq 78 \times 2^{-52}$ for a reasonable error bound for a, that is to say $|\underline{a} - a| \leq 2^{-49}$. The whole proof was done automatically by calling Gappa from Coq (see Section 3.3 and [14]).

5.2 Convolution of round-off errors

Note that the global floating-point error $\Delta_i^k = \underline{p}_i^k - p_i^k$ depends not only on δ_i^k, but also on all the δ_{i+j}^{k-l} for $0 < l \leq k$ and $-l \leq j \leq l$. Indeed round-off errors propagate along floating-point computations. Their contributions to Δ_i^k, which are independent and linear (due to the structure of the numerical scheme), can be computed by performing a convolution with a function $\lambda : (\mathbb{Z} \times \mathbb{Z}) \to \mathbb{R}$. This function λ represents the results of the numerical scheme when fed with a single unit value:

$$\lambda_0^0 = 1 \qquad \forall i \neq 0,\ \lambda_i^0 = 0$$
$$\lambda_{-1}^1 = \lambda_1^1 = a \qquad \lambda_0^1 = 2(1-a) \qquad \forall i \notin \{-1, 0, 1\},\ \lambda_i^1 = 0$$
$$\lambda_i^k = a \times (\lambda_{i-1}^{k-1} + \lambda_{i+1}^{k-1}) + 2(1-a) \times \lambda_i^{k-1} - \lambda_i^{k-2}$$

Theorem 1.

$$\Delta_i^k = \underline{p}_i^k - p_i^k = \sum_{l=0}^{k} \sum_{j=-l}^{l} \lambda_j^l \ \delta_{i+j}^{k-l}.$$

Details of the proof can be found in [11], but this point of view using convolution is new. The proof mainly amounts to performing numerous tedious transformations of summations until both sides are proved equal.

The previous proof assumes that the double summation is correct for all (i', k') such that $k' < k$. This would be correct if there was an unbounded set of i where p_i^k is computed. This is no longer the case for a finite string. Indeed, at the ends of the range ($i = 0$ or n_i), p_i^k and $\underline{p}_i^k$ are equal to 0, so Δ_i^k has to be 0 too.

The solution is to define the successive antisymmetric extension in space (as is done for d'Alembert's formula in Section 2.1) and to use it instead of δ. This ensures that both Δ_0^k and $\Delta_{n_i}^k$ are equal to 0. It does not have any consequence on the values of Δ_i^k for $0 < i < n_i$.

5.3 Bound on the global round-off error

The analytic expression of Δ_i^k can be used to obtain a bound on the round-off error. We will need two lemmas for this purpose.

Lemma 1. $\displaystyle\sum_{i=-\infty}^{+\infty} \lambda_i^k = k + 1.$

Proof. We have:
$\displaystyle\sum_{i=-\infty}^{+\infty} \lambda_i^{k+1} = 2\check{a} \sum_{i=-\infty}^{+\infty} \lambda_i^k + 2(1-\check{a}) \sum_{i=-\infty}^{+\infty} \lambda_i^k - \sum_{i=-\infty}^{+\infty} \lambda_i^{k-1} = 2 \sum_{i=-\infty}^{+\infty} \lambda_i^k - \sum_{i=-\infty}^{+\infty} \lambda_i^{k-1}.$

The sum by line verifies a simple linear recurrence. As $\sum \lambda_i^0 = 1$ and $\sum \lambda_i^1 = 2$, we have $\sum \lambda_i^k = k + 1$. □

Lemma 2. $\lambda_i^k \geq 0$.

Proof. The demonstration was found out by M. Kauers and V. Pillwein.

If we denote by P the Jacobi polynomial, we have

$$\lambda_n^j = \sum_{k=j}^{n} \binom{2k}{j+k}\binom{n+k+1}{2k+1}(-1)^{j+k}a^k = a^j \sum_{k=0}^{n-j} P_k^{(2j,0)}(1-2a)$$

Now the conjecture follows directly from the inequality of Askey and Gasper [3], which asserts that $\sum_{k=0}^{n} P_k^{(r,0)}(x) > 0$ for $r > -1$ and $-1 < x \leq 1$ (see Theorem 7.4.2 in The Red Book [2]). □

This assertion is not formally proved. This is a technical detail compared to the rest of our work, that is not worth the immense Coq development it would require: keen results on integrals but also definitions and results about the Legendre, Laguerre, Chebychef and Jacobi polynomials. After admitting this result, we can now prove the property about round-off errors.

Theorem 2.

$$\left|\Delta_i^k\right| = \left|\underline{p}_i^k - p_i^k\right| \leq 78 \times 2^{-53} \times (k+1) \times (k+2).$$

Proof. According to Theorem 1, Δ_i^k is equal to $\sum_{l=0}^{k}\sum_{j=-l}^{l} \lambda_j^l\ \delta_{i+j}^{k-l}$. We know that for all j and l, $|\delta_j^l| \leq 78 \times 2^{-52}$ and that $\sum \lambda_i^l = l+1$. Since the λ_i^k are nonnegative, the error is easily bounded by $78 \times 2^{-52} \times \sum_{l=0}^{k} l + 1$. □

Except for Lemma 2, all the proofs described in this section have been done and machined-checked using Coq.

6 Total Error

Let $\mathcal{E}_\mathrm{h}$ be the total error. It is the sum of the method error (or convergence error) e_h of Sections 2.3 and 4.4, and of the round-off error Δ_h of Section 5.

From Theorem 2, we can estimate[12] the following upper bound for the spatial norm of the round-off error when $\Delta x \leq 1$ and $\Delta t \leq t_{\max}/2$: for all $t \in [0, t_{\max}]$,

$$\begin{aligned}
\left\|\left(i \mapsto \Delta_i^{k_{\Delta t}(t)}\right)\right\|_{\Delta x} &= \sqrt{\sum_{i=0}^{n_i}\left(\Delta_i^{k_{\Delta t}(t)}\right)^2 \Delta x} \\
&\leq \sqrt{(n_i+1)\Delta x} \times 78 \times 2^{-53} \times \left(\frac{t_{\max}}{\Delta t}+1\right) \times \left(\frac{t_{\max}}{\Delta t}+2\right) \\
&\leq \sqrt{x_{\max}-x_{\min}+1} \times 78 \times 2^{-53} \times 3 \times \frac{t_{\max}^2}{\Delta t^2}.
\end{aligned}$$

Thus, from the triangular inequality for the spatial norm, we obtain the following estimation of the total error:

$$\forall t \in [0, t_{\max}],\ \forall \mathbf{\Delta x},\quad \|\mathbf{\Delta x}\| \leq \min(\alpha_e, \alpha_\Delta) \Rightarrow \left\|\left(i \mapsto \mathcal{E}_i^{k_{\Delta t}(t)}\right)\right\|_{\Delta x} \leq C_e(\Delta x^2 + \Delta t^2) + \frac{C_\Delta}{\Delta t^2}$$

where the convergence constants α_e and C_e were extracted from the Coq proof (see Section 4.4) and are given in terms of the constants for the Taylor approximation of the exact solution at degree 3 (α_3 and C_3), and at degree 4 (α_4 and C_4) by

$$\begin{aligned}
\alpha_e &= \min(1, t_{\max}, \alpha_3, \alpha_4), \\
C_e &= 2\mu t_{\max}\sqrt{x_{\max}-x_{\min}}\left(\frac{C'}{\sqrt{2}} + \mu(t_{\max}+1)C''\right)
\end{aligned}$$

[12] When $\frac{t_{\max}}{\Delta t} \geq 2$, we have $\left(\frac{t_{\max}}{\Delta t}+1\right)\left(\frac{t_{\max}}{\Delta t}+2\right) \leq 3\frac{t_{\max}^2}{\Delta t^2}$.

with $\mu = \frac{\sqrt{2}}{\sqrt{2\xi - \xi^2}}$, $C' = \max(1, C_3 + c^2 C_4 + 1)$, and $C'' = \max(C', 2(1+c^2)C_4)$, and where the round-off constants α_Δ and C_Δ, as explained above, are given by

$$\begin{aligned} \alpha_\Delta &= \min(1, t_{\max}/2), \\ C_\Delta &= 234 \times 2^{-53} \times t_{\max}^2 \sqrt{x_{\max} - x_{\min} + 1}. \end{aligned}$$

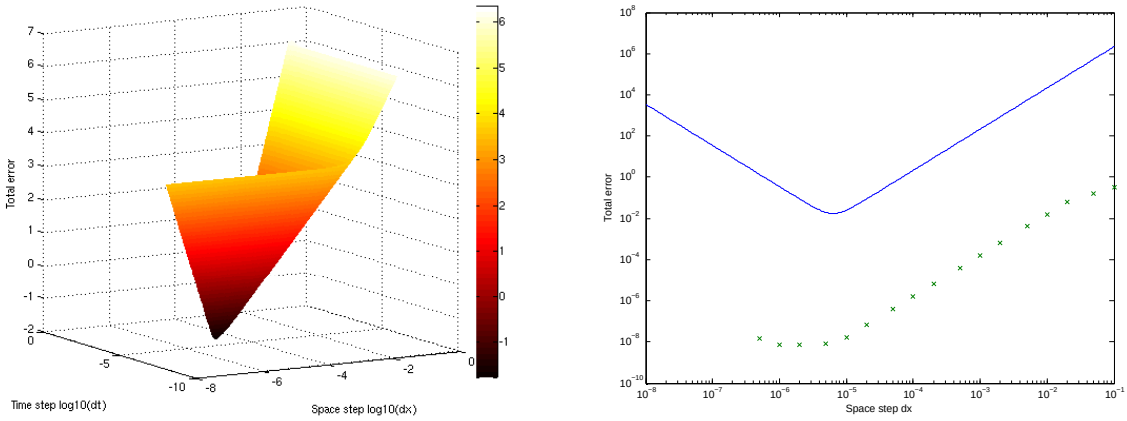


Figure 3: Upper bound for the total error in log-scale. Left: for Δx and Δt satisfying the CFL condition. The lighter area (in yellow) represents the higher values above 10^4, whereas the darker area represents the lower values below 10^{-1}. Right: for an optimal CFL condition with $\Delta t = \frac{1-\xi}{c}\Delta x$. The green crosses represent the effective total error computed by the C program for a few values of the space step.

To give an idea of the relative importance of both errors, we consider the academic case where the space domain is the interval $[0, 1]$, the velocity of waves is $c = 1$, and there is no initial velocity ($u_1(x) = 0$) nor source term ($s(x,t) = 0$). We suppose that the initial position is given by $u_0(x) = \chi\left(\frac{2(x-x_0)}{l}\right)$ where $x_0 = 0.5$, $l = 0.25$, and χ is the C^4 function defined on $[-1, 1]$ by $\chi(z) = (\cos(\frac{\pi}{2}z))^5$, and with null continuation on the real axis. For this function, we may take $\alpha_3 = \alpha_4 = \sqrt{2}/2$, $C_3 = 5120\sqrt{2}$, and $C_4 = 409600/3$. The corresponding solution presents two hump-shaped signals that propagate in each direction along the string, see Figure 1.

The upper bound on the total error is represented in Figure 3. Note that everything is in logarithmic scale. Of course, decreasing the size of the grid step decreases the method error, but in the same time, it increases the round-off error. Hence, the existence of a minimum for the upper bound on the total error (about 0.02 in our test case), corresponding to optimal grid step sizes. Fortunately, the effective total error usually happens to be much smaller than this upper bound (by about a factor of 10^6 in our example).

Even if the effective total error on this example is off by several orders of magnitude with respect to the theoretical bound, this experiment is still reassuring. First, the left side of Figure 3 shows that the optimal choice (the darker part) for choosing Δx and Δt is reached near the limit of the CFL condition. This property matches common knowledge from numerical analysis. Second, the right side shows that both the effective error and the theoretical error have the same asymptotic behavior. So the theorems we have verified in this work are not intrinsically easier than the best ones one could state. It is just that the constants of the formulas extracted from the proofs (which we did not tune for this specific purpose) are not optimal for this example.

7 Mechanization of Proofs

In Sections 4 and 5, we have mostly described a formalization of the method and round-off errors introduced when solving the wave equation problem with the given numerical scheme. We do not yet know whether this formalization actually matches the program described in Section 2.4 and Appendix A. In addition, the program might contain programing errors like out-of-bound accesses, which would possibly be left unattended while comparing the program and its formalization.

To palliate this issue, we will start from the source code, let Frama-C/Why generate proof obligations, put them in relation with the results from the formalization, and let Coq check that the whole aggregate is consistent (as far as the tools can be trusted). Note that the tools have no idea what the code is actually supposed to compute. So the default proof obligations they generate will only ensure that the program does not crash but not that it computes an approximation to the continuous solution. As a consequence, we have annotated the program to guide them toward sufficient proof obligations.

7.1 Program annotations

The full annotations are given in Appendix A. We give here hints about how to specify this program.

There are two axiomatics. The first one corresponds to the mathematics: the exact solution of the wave equation and its properties. It defines the needed values (the exact solution p, and its initialization p_0). We here assume that s and p_1 are zero functions. It also defines the derivatives of p ($psol_1$, first derivative for the first variable of p, and $psol_{11}$, second derivative for the first variable, and $psol_2$ and $psol_{22}$ for the second variable) as functions such that their value is the limit of $\frac{f(x+\Delta x)-f(x)}{\Delta x}$ when $\Delta x \to 0$. As the ACSL annotations are only first order, these definitions are quite cumbersome: each derivative needs 5 lines to be defined.

We also put as axioms the fact that the solution has the expected properties (1–4). The last property needed on the exact solution is its regularity. We require it to be near its Taylor approximations of degrees 3 and 4 on the whole interval $[x_{\min}, x_{\max}]$. For instance, the following annotation states the property for degree 3.

```
0  @ axiom psol_suff_regular_3:
   @   0 < alpha_3 && 0 < C_3 &&
   @   \forall real x; \forall real t; \forall real dx; \forall real dt;
   @   0 <= x <= 1 ==> \sqrt(dx * dx + dt * dt) <= alpha_3 ==>
   @   \abs(psol(x + dx, t + dt) - psol_Taylor_3(x, t, dx, dt)) <=
5  @     C_3 * \abs(\pow(\sqrt(dx * dx + dt * dt), 3));
```

The second axiomatic corresponds to the properties and loop invariant needed by the program. For example, we require the matrix to be separated: it means that a line of the matrix should not mix with another line (or a modification could alter another point of the matrix). We also state the existence of the loop invariant analytic_error that is needed for the applying the results of Section 5.

The initializations functions are specified, but not stated. This corresponds firstly to the function array2d_alloc that initializes the matrix and p_zero that produces an approximation of the p_0 function. Our program verification is modular: our proofs are generic with respect to p_0 and its implementation.

The preconditions of the main functions are the following ones:

- n_i and n_k must be greater than one, but small enough so that $n_i + 1$ and $n_k + 1$ do not overflow.
- the grid sizes $\mathbf{\Delta x}$ must fulfill some mathematical conditions that are required for the convergence of the scheme.
- the floating-point values computed for the grid sizes must be near their mathematical values.

- the constant propagation velocity must be reasonable: it should be between 2^{-1000} and 2^{1000} in order to prevent overflows.

There are two postconditions, corresponding to the method and round-off errors. See Sections 4 and 5 for more details.

7.2 Automation and manual proofs

Given the program code, the Why tool generates 149 verification conditions that have to be proved. While possible, proving all of them in Coq would be rather tedious. Moreover, it would lead to a rather fragile construct: any later modification to the code, however small it is, would cause different proof obligations to be generated, which would then require additional human interaction to adapt the Coq proofs. We prefer to have automated provers (SMT solvers and Gappa) discharge as many of them as possible, so that only the most intricate ones are left to be proven in Coq. The following table shows how many goals are discharged automatically and how many are left to the user.[13]

Prover	Proved Behavior VC	Proved Safety VC	Total
Alt-Ergo	18	80	98
CVC3	18	89	107
Gappa	2	20	22
Z3	21	63	84
Automatically proved	**23**	**94**	**117**
Coq	**21**	**11**	**32**
Total	44	105	149

On safety goals (matrix access, loop variant decrease, overflow), automatic provers are helpful: they prove about 90 % of the goals. On behavior goals (loop invariant, assertion, postcondition), automatic provers succeed for half of the goals. As our loop invariant involves an uninterpreted predicate, the automatic provers cannot prove all the behavior goals (they would have been too complicated anyway). That is why we resort to an interactive higher-order theorem prover, namely Coq.

Coq proofs are split into two sets: first, the mathematical proof of convergence and second, the proofs of bounded round-off errors and absence of runtime errors. Appendix C displays the layout of the Coq formalization.

The following tabular gives the compilation times of the Coq files on a 3-GHz dual core machine.

Type of proofs	Nb spec lines	Nb lines	Compilation time
Convergence	991	5 275	42 s
Round-off + runtime errors	7 737	13 175	32 min

Note that most proof statements regarding round-off and runtime errors are automatically generated (7 321 lines out of 7 737) by the Frama-C/Jessie/Why framework.

The compilation time may seem prohibitive; it is mainly due to calls to the omega decision procedure for Presburger arithmetic. The difficulty does not lie in the arithmetic statement itself, but rather in a large number of useless hypotheses. In order to reduce the compilation time, we could manually massage the hypotheses to speed up the procedure, but this would defeat the point of using an automatic tactic.

8 Conclusion

One of the goals of this work is to favor the use of formal methods in numerical analysis. It may seem to be just wishful thinking, but it is actually seen as needed by some applied mathematicians.

[13] Note that verification conditions might be discharged by one or several automated provers.

This work shows a tight synergy between them and logicians. Three domains are intertwined here: applied mathematics for an initial proof that could be enriched and detailed upon request, computer arithmetic for smart bounds on round-off errors, and formal methods for machine-checking it. This may be the reason why such proofs are scarce as this kind of collaboration is uncommon.

We succeeded in verifying a C program that implements a numerical scheme for the resolution of the one-dimensional acoustic wave equation. This is comprised of three sets of proofs. First we formalized the wave equation and proved the convergence of a scheme for its numerical resolution. Second we proved that the C program behaves safely: no out-of-bound array accesses and no overflow during floating-point computations. Third we proved that the round-off errors are not causing the numerical results to go astray. This is the first verification of this kind of program that covers all its aspects, both mathematics and implementation.

An unexpected side effect of having performed this formal verification in Coq is our ability to extract the constants hidden inside the proofs. That way, we are able to explicitly bound the total error rather than just having the usual $O(\Delta x^2 + \Delta t^2)$ bound. In particular, we can compare the magnitudes of the method error and round-off error and then decide how to scale the discretization grid.

Each proof came with its own hurdles. For ensuring the correct behavior of the program, the most tedious point was to prove that setting a result value did not cause other values to change, that is, that all the lines of the matrix are properly separated. In particular, verifying the loop invariant requires checking that, except for the new value, the properties of the memory are preserved. An unexpectedly tedious part was to check that the program actually complies with our mathematical model for the numerical scheme.

Another difficulty lies in the mathematical proof itself. We based our work on proofs found in books, courses, and articles. It appears that pen-and-paper proofs are sometimes sketchy: they may be fuzzy about the needed hypotheses, especially when switching quantifiers. We have also learned that filling the gaps may cause us to go back to the drawing board and to change the basic blocks of our formalization to make them more generic (*e.g.* devising a big O that needs to be uniform and also generic with respect to a property P).

For this exploratory work, we considered the simple three-point scheme for the one-dimensional wave equation. Further works involve scaling to higher-dimension. The one-dimensional case showed us that summations and finite support functions play a much more important role in the development than we first expected. We are therefore moving to the SSReflect interface and libraries for Coq [9], so as to simplify the manipulations of these objects in the higher-dimensional case.

Another perspective is to generalize our approach to other higher-order numerical schemes for the same equation, and to other PDEs. However, the proofs of Section 4 are entangled with particulars of the presented problem, and would therefore have to be redone for other problems. So a more fruitful approach would be to prove once and for all the Lax equivalence theorem that states that consistency implies the equivalence between convergence and stability. This would considerably reduce the amount of work needed for tackling other schemes and equations.

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A Source Code

```
0
/*@ axiomatic dirichlet_maths {
  @
  @ logic real c;
  @ logic real p0(real x);
5 @ logic real psol(real x, real t);

  @ axiom c_pos: 0 < c;

  @ logic real psol_1(real x, real t);
10 @ axiom psol_1_def:
  @   \forall real x; \forall real t;
  @   \forall real eps; \exists real C; 0 < C && \forall real dx;
  @   \abs(dx) < C ==>
  @   \abs((psol(x + dx, t) - psol(x, t)) / dx - psol_1(x, t)) < eps;
15
  @ logic real psol_11(real x, real t);
  @ axiom psol_11_def:
  @   \forall real x; \forall real t;
  @   \forall real eps; \exists real C; 0 < C && \forall real dx;
20 @   \abs(dx) < C ==>
  @   \abs((psol_1(x + dx, t) - psol_1(x, t)) / dx - psol_11(x, t)) < eps;

  @ logic real psol_2(real x, real t);
  @ axiom psol_2_def:
25 @   \forall real x; \forall real t;
  @   \forall real eps; \exists real C; 0 < C && \forall real dt;
  @   \abs(dt) < C ==>
  @   \abs((psol(x, t + dt) - psol(x, t)) / dt - psol_2(x, t)) < eps;

30 @ logic real psol_22(real x, real t);
  @ axiom psol_22_def:
  @   \forall real x; \forall real t;
  @   \forall real eps; \exists real C; 0 < C && \forall real dt;
  @   \abs(dt) < C ==>
35 @   \abs((psol_2(x, t + dt) - psol_2(x, t)) / dt - psol_22(x, t)) < eps;

  @ axiom wave_eq_0: \forall real x; 0 <= x <= 1 ==> psol(x, 0) == p0(x);
  @ axiom wave_eq_1: \forall real x; 0 <= x <= 1 ==> psol_2(x, 0) == 0;
  @ axiom wave_eq_2:
40 @   \forall real x; \forall real t;
  @   0 <= x <= 1 ==> psol_22(x, t) - c * c * psol_11(x, t) == 0;
  @ axiom wave_eq_dirichlet_1: \forall real t; psol(0, t) == 0;
  @ axiom wave_eq_dirichlet_2: \forall real t; psol(1, t) == 0;

45 @ logic real psol_Taylor_3(real x, real t, real dx, real dt);
  @ logic real psol_Taylor_4(real x, real t, real dx, real dt);

  @ logic real alpha_3; logic real C_3;
  @ logic real alpha_4; logic real C_4;
50
  @ axiom psol_suff_regular_3:
  @   0 < alpha_3 && 0 < C_3 &&
  @   \forall real x; \forall real t; \forall real dx; \forall real dt;
  @   0 <= x <= 1 ==> \sqrt(dx * dx + dt * dt) <= alpha_3 ==>
55 @   \abs(psol(x + dx, t + dt) - psol_Taylor_3(x, t, dx, dt)) <=
  @     C_3 * \abs(\pow(\sqrt(dx * dx + dt * dt), 3));

  @ axiom psol_suff_regular_4:
  @   0 < alpha_4 && 0 < C_4 &&
60 @   \forall real x; \forall real t; \forall real dx; \forall real dt;
  @   0 <= x <= 1 ==> \sqrt(dx * dx + dt * dt) <= alpha_4 ==>
  @   \abs(psol(x + dx, t + dt) - psol_Taylor_4(x, t, dx, dt)) <=
  @     C_4 * \abs(\pow(\sqrt(dx * dx + dt * dt), 4));
```

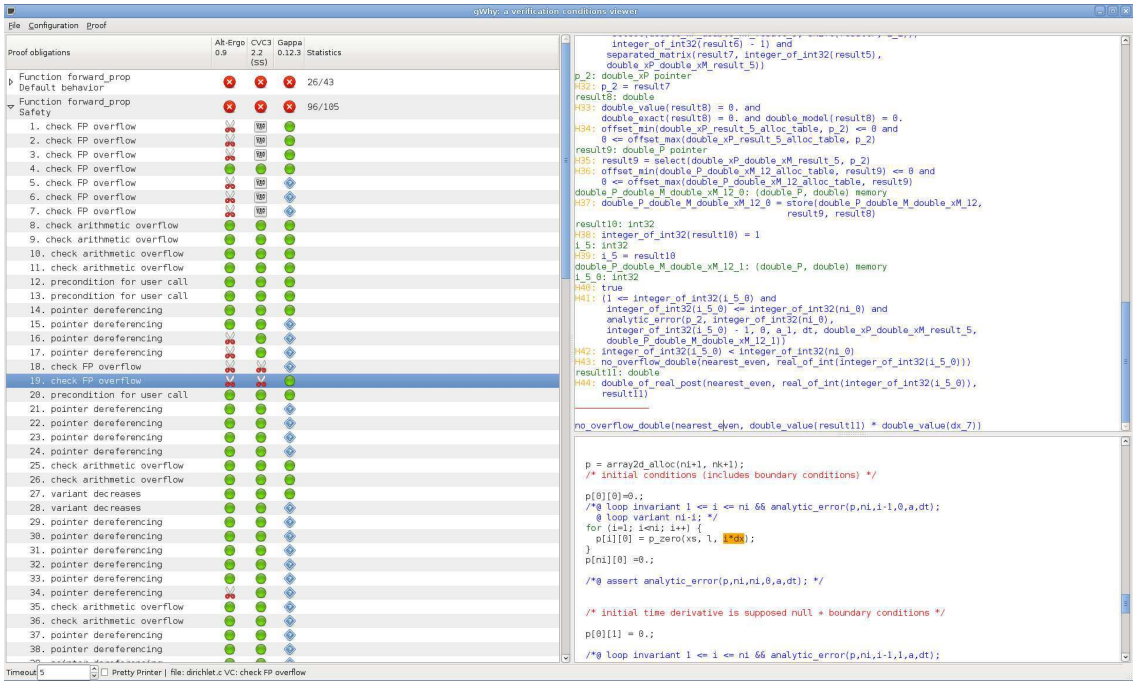
```
  @ axiom psol_le:
  @   \forall real x; \forall real t;
  @   0 <= x <= 1 ==> 0 <= t ==> \abs(psol(x, t)) <= 1;

  @ logic real T_max;
  @ axiom T_max_pos: 0 < T_max;

  @ logic real C_conv; logic real alpha_conv;
  @ lemma alpha_conv_pos: 0 < alpha_conv;
  @
  @ } */


/*@ axiomatic dirichlet_prog {
  @
  @  predicate analytic_error{L}
  @    (double **p, integer ni, integer i, integer k, double a, double dt)
  @    reads p[..][..];
  @
  @  lemma analytic_error_le{L}:
  @    \forall double **p; \forall integer ni; \forall integer i;
  @    \forall integer nk; \forall integer k;
  @    \forall double a; \forall double dt;
  @    0 < ni ==> 0 <= i <= ni ==> 0 <= k ==>
  @    0 < \exact(dt) ==>
  @    analytic_error(p, ni, i, k, a, dt) ==>
  @    \sqrt(1. / (ni * ni) + \exact(dt) * \exact(dt)) < alpha_conv ==>
  @    k <= nk ==> nk <= 7598581 ==> nk * \exact(dt) <= T_max ==>
  @    \exact(dt) * ni * c <= 1 - 0x1.p-50 ==>
  @    \forall integer i1; \forall integer k1;
  @    0 <= i1 <= ni ==> 0 <= k1 < k ==>
  @    \abs(p[i1][k1]) <= 2;
  @
  @  predicate separated_matrix{L}(double **p, integer leni) =
  @    \forall integer i; \forall integer j;
  @    0 <= i < leni ==> 0 <= j < leni ==> i != j ==>
  @    \base_addr(p[i]) != \base_addr(p[j]);
  @
  @ logic real sqr_norm_dx_conv_err{L}
  @   (double **p, real dx, real dt, integer ni, integer i, integer k)
  @   reads p[..][..];
  @ logic real sqr(real x) = x * x;
  @ lemma sqr_norm_dx_conv_err_0{L}:
  @   \forall double **p; \forall real dx; \forall real dt;
  @   \forall integer ni; \forall integer k;
  @   sqr_norm_dx_conv_err(p, dx, dt, ni, 0, k) == 0;
  @ lemma sqr_norm_dx_conv_err_succ{L}:
  @   \forall double **p; \forall real dx; \forall real dt;
  @   \forall integer ni; \forall integer i; \forall integer k;
  @   0 <= i ==>
  @   sqr_norm_dx_conv_err(p, dx, dt, ni, i + 1, k) ==
  @     sqr_norm_dx_conv_err(p, dx, dt, ni, i, k) +
  @     dx * sqr(psol(1. * i / ni, k * dt) - \exact(p[i][k]));
  @ logic real norm_dx_conv_err{L}
  @   (double **p, real dt, integer ni, integer k) =
  @   \sqrt(sqr_norm_dx_conv_err(p, 1. / ni, dt, ni, ni, k));
  @
  @ } */


/*@ requires leni >= 1 && lenj >= 1;
  @ ensures
  @   \valid_range(\result, 0, leni - 1) &&
  @   (\forall integer i; 0 <= i < leni ==>
  @    \valid_range(\result[i], 0, lenj - 1)) &&
  @   separated_matrix(\result, leni);
  @ */
```

```
double **array2d_alloc(int leni, int lenj);


/*@ requires (l != 0);
  @ ensures
  @   \round_error(\result) <= 14 * 0x1.p-52 &&
  @   \exact(\result) == p0(\exact(x));
  @ */
double p_zero(double xs, double l, double x);


/*@ requires
  @   ni >= 2 && nk >= 2 && l != 0 &&
  @   dt > 0. && \exact(dt) > 0. &&
  @   \exact(v) == c && \exact(v) == v &&
  @   0x1.p-1000 <= \exact(dt) &&
  @   ni <= 2147483646 && nk <= 7598581 &&
  @   nk * \exact(dt) <= T_max &&
  @   \abs(\exact(dt) - dt) / dt <= 0x1.p-51 &&
  @   0x1.p-500 <= \exact(dt) * ni * c <= 1 - 0x1.p-50 &&
  @   \sqrt(1. / (ni * ni) + \exact(dt) * \exact(dt)) < alpha_conv;
  @
  @ ensures
  @   \forall integer i; \forall integer k;
  @   0 <= i <= ni ==> 0 <= k <= nk ==>
  @   \round_error(\result[i][k]) <= 78. / 2 * 0x1.p-52 * (k + 1) * (k + 2);
  @
  @ ensures
  @   \forall integer k; 0 <= k <= nk ==>
  @   norm_dx_conv_err(\result, \exact(dt), ni, k) <=
  @     C_conv * (1. / (ni * ni) + \exact(dt) * \exact(dt));
  @ */
double **forward_prop(int ni, int nk, double dt, double v,
                      double xs, double l) {

  /* Output variable. */
  double **p;

  /* Local variables. */
  int i, k;
  double a1, a, dp, dx;

  dx = 1./ni;
  /*@ assert
    @   dx > 0. && dx <= 0.5 &&
    @   \abs(\exact(dx) - dx) / dx <= 0x1.p-53;
    @ */

  /* Compute the constant coefficient of the stiffness matrix. */
  a1 = dt/dx*v;
  a = a1*a1;
  /*@ assert
    @   0 <= a <= 1 &&
    @   0 < \exact(a) <= 1 &&
    @   \round_error(a) <= 0x1.p-49;
    @ */

  /* Allocate space-time variable for the discrete solution. */
  p = array2d_alloc(ni+1, nk+1);

  /* First initial condition and boundary conditions. */
  /* Left boundary. */
  p[0][0] = 0.;
  /* Time iteration -1 = space loop. */
  /*@ loop invariant
    @   1 <= i <= ni &&
    @   analytic_error(p, ni, i - 1, 0, a, dt);
```

```
    @ loop variant ni - i; */
  for (i=1; i<ni; i++) {
    p[i][0] = p_zero(xs, l, i*dx);
  }
  /* Right boundary. */
  p[ni][0] = 0.;
  /*@ assert analytic_error(p, ni, ni, 0, a, dt); */

  /* Second initial condition (with p_one=0) and boundary conditions. */
  /* Left boundary. */
  p[0][1] = 0.;
  /* Time iteration 0 = space loop. */
  /*@ loop invariant
    @   1 <= i <= ni &&
    @   analytic_error(p, ni, i - 1, 1, a, dt);
    @ loop variant ni - i; */
  for (i=1; i<ni; i++) {
    /*@ assert \abs(p[i-1][0]) <= 2; */
    /*@ assert \abs(p[i][0]) <= 2; */
    /*@ assert \abs(p[i+1][0]) <= 2; */
    dp = p[i+1][0] - 2.*p[i][0] + p[i-1][0];
    p[i][1] = p[i][0] + 0.5*a*dp;
  }
  /* Right boundary. */
  p[ni][1] = 0.;
  /*@ assert analytic_error(p, ni, ni, 1, a, dt); */

  /* Evolution problem and boundary conditions. */
  /* Propagation = time loop. */
  /*@ loop invariant
    @   1 <= k <= nk &&
    @   analytic_error(p, ni, ni, k, a, dt);
    @ loop variant nk - k; */
  for (k=1; k<nk; k++) {
    /* Left boundary. */
    p[0][k+1] = 0.;
    /* Time iteration k = space loop. */
    /*@ loop invariant
      @   1 <= i <= ni &&
      @   analytic_error(p, ni, i - 1, k + 1, a, dt);
      @ loop variant ni - i; */
    for (i=1; i<ni; i++) {
      /*@ assert \abs(p[i-1][k]) <= 2; */
      /*@ assert \abs(p[i][k]) <= 2; */
      /*@ assert \abs(p[i+1][k]) <= 2; */
      /*@ assert \abs(p[i][k-1]) <= 2; */
      dp = p[i+1][k] - 2.*p[i][k] + p[i-1][k];
      p[i][k+1] = 2.*p[i][k] - p[i][k-1] + a*dp;
    }
    /* Right boundary. */
    p[ni][k+1] = 0.;
    /*@ assert analytic_error(p, ni, ni, k + 1, a, dt); */
  }

  return p;

}
```

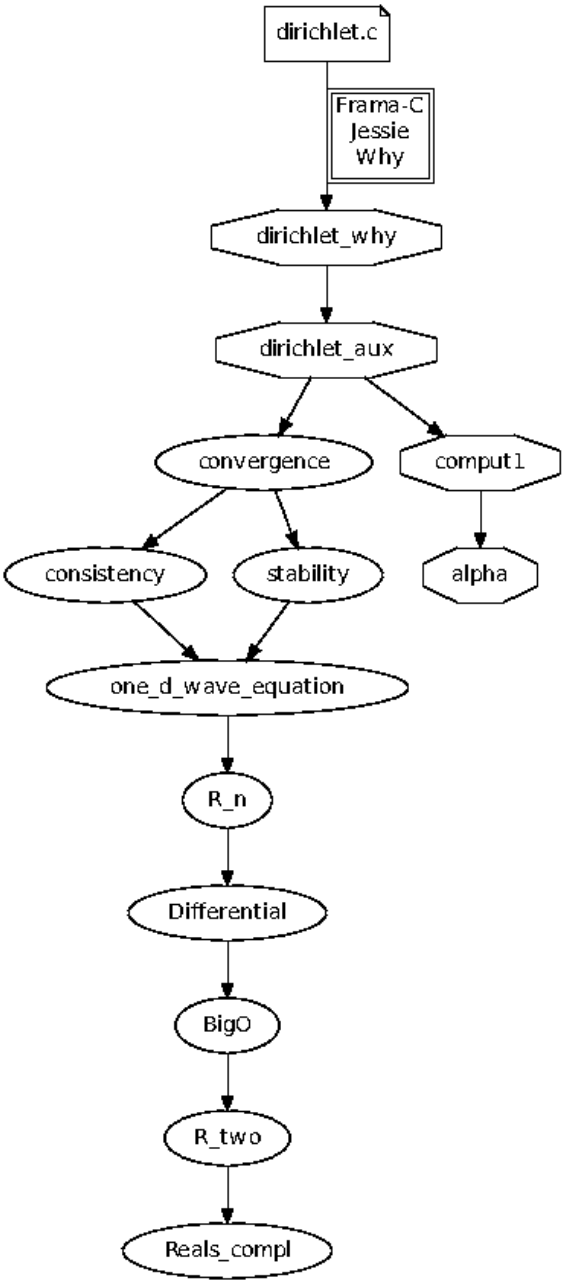
B Screenshot

This is a screenshot of gWhy: we have the list of all the verification conditions and if they are proved by the various automatic tools.



C Dependency Graph

In the following graph, the ellipse nodes are Coq files formalizing the wave equation and the convergence of its numerical scheme. The octagon nodes are Coq files that deal with proof obligations generated from the `dirichlet.c` program file, that is, propagation of round-off errors and error-free execution. Arrows represent dependencies between the Coq files.



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