Interactive Theorem Proving 2010

Formal Proof of a Wave Equation Resolution Scheme: the Method Error

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DE RECHERCHE
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Motivations

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PDE (Partial Differential Equation) \Rightarrow weather forecast \Rightarrow nuclear simulation \Rightarrow optimal control \Rightarrow ...
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 \Rightarrow mathematical proofs of the convergence of the numerical scheme (we compute something close to the PDE solution if the grids size decreases)

Let us machine-check this kind of proof! (in Coq)

Outline

- Wave equation resolution scheme?
- Pormal proof: basic blocks
 - Dot product
 - Big O
- 3 Formal proof: convergence
- 4 Conclusion & perspectives

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Wave Equation?

Looking for $u: \mathbb{R}^2 \to \mathbb{R}$ regular enough such that:

$$\frac{\partial^2 u(x,t)}{\partial t^2} - c^2 \frac{\partial^2 u(x,t)}{\partial x^2} = s(x,t)$$

with given values for the initial position $u_0(x)$ and the initial velocity $u_1(x)$.

⇒ rope oscillation, sound, radar, oil prospection...

Scheme?

We want $u_j^k \approx u(j\Delta x, k\Delta t)$.

$$\frac{u_j^k - 2u_j^{k-1} + u_j^{k-2}}{\Delta t^2} - c^2 \frac{u_{j+1}^{k-1} - 2u_j^{k-1} + u_{j-1}^{k-1}}{\Delta x^2} = s_j^{k-1}$$

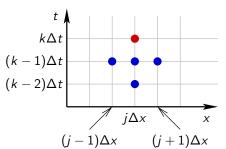
And other horrible formulas to initialize u_j^0 and u_j^1 .

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Three-point scheme: u_j^k depends on u_{j-1}^{k-1} , u_j^{k-1} , u_{j+1}^{k-1} and u_j^{k-2} .

So what?

We measure that u and u_j^k are close when $(\Delta x, \Delta t) \to 0$.

We define $e_j^k \stackrel{\text{def}}{=} \bar{u}_j^k - u_j^k$: convergence error where \bar{u}_j^k is the value of u at the (j,k) point of the grid.

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We want to bound $\left\|e_h^{k_{\Delta t}(t)}\right\|_{\Delta x}$: the average of the convergence error on all points of the grid at a given time $k_{\Delta t}(t) = \left\lfloor \frac{t}{\Delta t} \right\rfloor \Delta t$.

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We want to prove:

$$\left\|e_h^{k_{\Delta t}(t)}\right\|_{\Delta x} = O_{[0,t_{\max}]}(\Delta x^2 + \Delta t^2)$$

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We only consider functions having a finite support:

$$\{f: \mathbb{Z} \to \mathbb{R} \mid \exists a, b \in \mathbb{Z}, \forall i \in \mathbb{Z}, f(i) \neq 0 \Rightarrow a \leq i \leq b\}.$$

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We have an uninterpreted $\langle .,. \rangle$ such that

$$\forall f \ g \ a \ b, (\forall i, (f(i) \neq 0 \lor g(i) \neq 0) \Rightarrow a \leq i \leq b) \Rightarrow \langle f, g \rangle = \sum_{i=a}^{b} f(i)g(i)$$

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Hence $||f|| \stackrel{\text{def}}{=} \sqrt{\langle f, f \rangle}$.

Hence a predicate FS (finite support) with lemmas and a dedicated tactic.

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Big O = big pain

Usually, the big O uses one variable and $f(\mathbf{x}) = O_{\|\mathbf{x}\| \to 0}(g(\mathbf{x}))$ means

$$\exists \alpha, C > 0, \quad \forall \mathbf{x} \in \mathbb{R}^n, \quad \|\mathbf{x}\| \le \alpha \Rightarrow |f(\mathbf{x})| \le C \cdot |g(\mathbf{x})|.$$

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$$\forall \mathbf{x}, \exists \alpha, C > 0, \quad \forall \Delta \mathbf{x} \in \mathbb{R}^2, \quad \|\Delta \mathbf{x}\| \le \alpha \Rightarrow |f(\mathbf{x}, \Delta \mathbf{x})| \le C \cdot |g(\Delta \mathbf{x})|$$

does not work.

Uniform big O

We used a uniform big O:

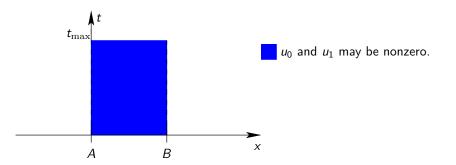
$$\exists \alpha, C > 0, \quad \forall \mathbf{x}, \Delta \mathbf{x}, \quad \|\Delta \mathbf{x}\| \leq \alpha \Rightarrow |f(\mathbf{x}, \Delta \mathbf{x})| \leq C \cdot |g(\Delta \mathbf{x})|.$$

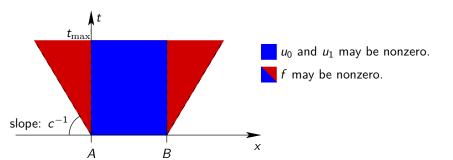
where variables ${\bf x}$ and ${\bf \Delta x}$ are restricted to subsets of \mathbb{R}^2 . (for example such that $\Delta t>0$)

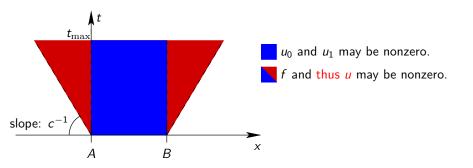
 \Rightarrow Taylor expansions

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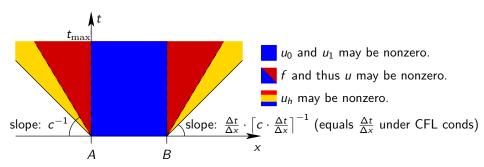




One axiom about the exact solution of the PDE:

$$x \notin [A - c \cdot t, B + c \cdot t] \quad \Rightarrow \quad u(x, t) = 0$$

(mathematically proved using d'Alembert's formula)



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Proof idea 1/3: consistency

The truncation error is defined as how much the exact solution solves the numerical scheme:

$$\varepsilon_j^{k-1} = \frac{\bar{u}_j^k - 2\bar{u}_j^{k-1} + \bar{u}_j^{k-2}}{\Delta t^2} - c^2 \frac{\bar{u}_{j+1}^{k-1} - 2\bar{u}_j^{k-1} + \bar{u}_{j-1}^{k-1}}{\Delta x^2} - s_j^{k-1}$$

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The consistency is the boundedness of the truncation error:

$$\left\| \varepsilon_h^{k_{\Delta t}(t)} \right\|_{\Delta x} = O_{[0,t_{\max}]}(\Delta x^2 + \Delta t^2)$$

By Taylor series and many computations.

Proof idea 2/3: stability

We define a discrete energy by

$$E_h(c)(u_h)^{k+\frac{1}{2}} \stackrel{\text{def}}{=} \frac{1}{2} \left\| \frac{u_h^{k+1} - u_h^k}{\Delta t} \right\|_{\Delta x}^2 + \frac{1}{2} \left\langle u_h^k, u_h^{k+1} \right\rangle_{A_h(c)}$$

kinetic energy

potential energy

$$\langle v_h, w_h \rangle_{A_h(c)} \stackrel{\mathsf{def}}{=} \langle A_h(c) \, v_h, w_h \rangle_{\Delta x} \; \mathsf{and} \; (A_h(c) \, v_h)_j \stackrel{\mathsf{def}}{=} - c^2 \tfrac{v_{j+1} - 2v_j + v_{j-1}}{\Delta x^2}.$$

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$$\langle v_h, w_h \rangle_{A_h(c)} \stackrel{\mathsf{def}}{=} \langle A_h(c) \, v_h, w_h \rangle_{\Delta_X} \; \mathsf{and} \; (A_h(c) \, v_h)_j \stackrel{\mathsf{def}}{=} - c^2 \tfrac{v_{j+1} - 2v_j + v_{j-1}}{\Delta_X^2}.$$

Note that this energy is constant if f = 0.

We prove an overestimation and an underestimation of this energy.

 $\Rightarrow u_h$ does not diverge.

Proof idea 3/3: convergence

The convergence error is solution of the same discrete scheme with inputs

$$u_{0,j} = 0,$$
 $u_{1,j} = \frac{e_j^1}{\Delta t},$ and $s_j^k = \varepsilon_j^{k+1}.$

+ proofs about the initializations.

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All these proofs require the existence of ζ and ξ in]0,1[with $\zeta \leq 1-\xi$ and we require that $\zeta \leq \frac{c\Delta t}{\Delta x} \leq 1-\xi$ (CFL conditions).

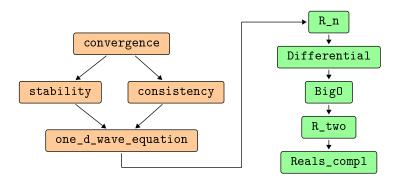
Convergence

We proved that:

$$\left\|e_h^{k_{\Delta t}(t)}\right\|_{\Delta x} = O_{\begin{subarray}{l} t \in [0, t_{\max}] \\ (\Delta x, \Delta t) \to 0 \\ 0 < \Delta x \land 0 < \Delta t \land \\ \zeta \le c \frac{\Delta t}{\Delta x} \le 1 - \xi \end{subarray}} (\Delta x^2 + \Delta t^2).$$

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4500 lines of Coq (half dedicated, half re-usable) \approx as long as a detailed paper proof

• synergy applied mathematicians / logicians

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- filling the gaps of pen&paper proofs

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- 1 axiom: finite support of the exact solution $(+1 \ \varepsilon \ \text{operator})$

• re-use the proofs with reflections (the rope has two ends).

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- link this to the C program
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- link this to the C program
 ⇒ full proof of the program (with already done floating-point proof)
- extract the C and α of the big O (done)
- prove Lax equivalence for as many schemes as possible: consistency ⇒ (stability ⇔ convergence)
- other schemes for the same PDE
- other PDEs
- ODEs

Thank you for your attention



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