

# Wave Equation Numerical Resolution: a Comprehensive Mechanized Proof of a C Program

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# Scientific Computing

**PDE** (Partial Differential Equation)

⇒ weather forecast, numerical simulation, control, ...

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Example: **numerical scheme** over a regular grid.

Goal: **formally prove the C implementation of a numerical scheme.**

# One-Dimensional Wave Equation

Goal: finding a solution to the equation

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

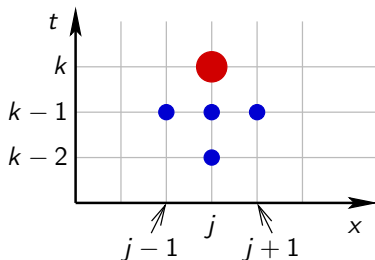
given the initial position  $u_0(x)$  and the initial speed  $u_1(x)$ .

Applications: rope oscillations, sound propagation, radar, oil exploration.

# Numerical Scheme

Discretization:  $u_j^k \approx u(j\Delta x, k\Delta t)$ .

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



Second-order centered finite difference scheme:

$u_j^k$  depends on  $u_{j-1}^{k-1}$ ,  $u_j^{k-1}$ ,  $u_{j+1}^{k-1}$ , and  $u_j^{k-2}$ .

# C Program

- Features: dynamic allocation, floating-point computations.
- Main loop:

```
/* 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.;
}
```

# Verification

Goal: ensure that computed values are accurate approximations of the mathematical solution.



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Issues:

- **Method error:**

Is the numerical scheme an accurate enough approximation of the exact solution?

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How much do they perturb the results?

# Verification

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Issues:

- **Method error:**  
Is the numerical scheme an accurate enough approximation of the exact solution?
- **Round-off errors:**  
Floating-point computations introduce additional errors.  
How much do they perturb the results?
- **Coding errors:**  
Does the C program match the numerical scheme?  
Is the program free of runtime errors?

# Available Methods and Tools

- **Scientific computing:**  
abundant literature, comprehensive and correct overall.
- **Floating-point arithmetic:**  
standard IEEE-754, literature, tools (Gappa).
- **Formal proofs:**  
tools (Coq), libraries ( $\mathbb{R}$ , FP numbers, etc).
- **Program specification verification:**  
tools (Frama-C, Jessie, Why).

# Outline

- 1 Introduction
- 2 Tools
- 3 Method Error
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# Process and Tools

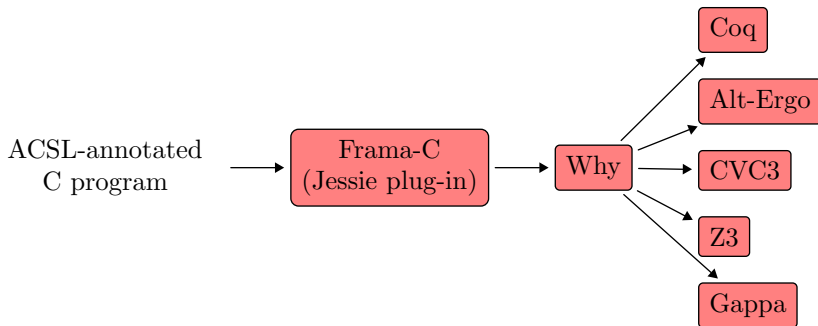
To prove a program:

- annotate it with its **specification**,
- compute its **weakest preconditions**,
- prove the resulting **theorem statements**.

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# Frama-C/Jessie/Why

- Input: a C program with **ACSL** comments.
- Output: a set of theorem statements.
- Purpose: proving the theorems is sufficient to ensure that the program complies with its specification.

```
/*@ requires
  @   ni >= 2 && nk >= 2 && l != 0 &&
  @   dt > 0. && \exact(dt) > 0. &&
  @   ...;
  @
  @ 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) {
```

# SMT Solvers

- Automated theorem provers.
- Especially useful for statements related to coding errors: memory allocations, out-of-bound array accesses, etc.
- Based on Satisfiability Modulo Theories: linear integer/rational arithmetic, arrays, bit vectors, etc.
- Prominent solvers: Alt-Ergo, CVC3, Z3.

# Gappa

- Automated theorem prover.
- Dedicated to FP-related properties:  
no overflow, bounded round-off errors, etc.
- Based on interval arithmetic and rewriting.
- Usable inside a Coq proof.

# Coq

- Interactive proof assistant.
- Higher-order logic.
- Useful for anything that exceeds automated theorem provers.

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# Method Error: What to Bound?

Goal: prove that the exact solution  $u$  and the discrete approximation  $u_j^k$  are close when  $(\Delta x, \Delta t) \rightarrow 0$ .

**Convergence error:**  $e_j^k = \bar{u}_j^k - u_j^k$   
with  $\bar{u}_j^k$  the value of  $u$  at grid point  $(j, k)$ .

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with  $\bar{u}_j^k$  the value of  $u$  at grid point  $(j, k)$ .

**Averaged convergence error:**  $\|e^{k_{\Delta t}(t)}\|_{\Delta x}$   
for all the grid points at time  $k_{\Delta t}(t) = \lfloor \frac{t}{\Delta t} \rfloor \Delta t$ .

**Convergence** of this numerical scheme is a well-known mathematical result:

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

## Proof Sketch: 1/3 Consistency

The discrete approximation  $u_j^k$  is a solution of the numerical scheme (by definition).

**Truncation error:** how close is  $\bar{u}_j^k$  from being a solution of 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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**Consistency:** the truncation error is bounded.

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

Proved in Coq thanks to Taylor expansions and lots of computations.

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**Stability:**  $u_j^k$  does not diverge when  $k \rightarrow \infty$ .

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**Discrete energy:**

$$E^{k+\frac{1}{2}} = \frac{1}{2} \left\| \frac{u^{k+1} - u^k}{\Delta t} \right\|_{\Delta x}^2 + \frac{1}{2} \langle u^k, u^{k+1} \rangle_A$$

kinetic energy

potential energy

with  $\langle v, w \rangle_A = \langle A(v), w \rangle_{\Delta x}$  and  $A(v)_j = -c^2 \frac{v_{j+1} - 2v_j + v_{j-1}}{\Delta x^2}$ .

# Proof Sketch: 2/3 Stability

**Stability:**  $u_j^k$  does not diverge when  $k \rightarrow \infty$ .

**Discrete energy:**

$$E^{k+\frac{1}{2}} = \underbrace{\frac{1}{2} \left\| \frac{u^{k+1} - u^k}{\Delta t} \right\|_{\Delta x}^2}_{\text{kinetic energy}} + \underbrace{\frac{1}{2} \langle u^k, u^{k+1} \rangle_A}_{\text{potential energy}}$$

with  $\langle v, w \rangle_A = \langle A(v), w \rangle_{\Delta x}$  and  $A(v)_j = -c^2 \frac{v_{j+1} - 2v_j + v_{j-1}}{\Delta x^2}$ .

Note: **physical approach** specific to this PDE.

## Proof Sketch: 3/3 Convergence

The convergence error  $e_j^k = \bar{u}_j^k - u_j^k$  is a solution of the numerical scheme when the source term  $s_j^k$  is replaced by the truncation error  $\varepsilon_j^{k+1}$  (and a few other changes).

# Proof Sketch: 3/3 Convergence

The convergence error  $e_j^k = \bar{u}_j^k - u_j^k$  is a solution of the numerical scheme when the source term  $s_j^k$  is replaced by the truncation error  $\varepsilon_j^{k+1}$  (and a few other changes).

- 1  $\varepsilon_j^{k+1}$  is bounded on average, by consistency.
- 2  $e_j^k$  does not diverge, by stability.
- 3 Thus  $u_j^k$  converges to  $\bar{u}_j^k$  when  $(\Delta x, \Delta t) \rightarrow 0$ .

# Convergence

$$\left\| e_h^{k_{\Delta t}(t)} \right\|_{\Delta x} = O \left( \begin{array}{l} t \in [0, t_{\max}] \\ (\Delta x, \Delta t) \rightarrow 0 \\ 0 < \Delta x \wedge 0 < \Delta t \wedge \\ c \frac{\Delta t}{\Delta x} \leq 1 - \xi \end{array} \right. (\Delta x^2 + \Delta t^2).$$

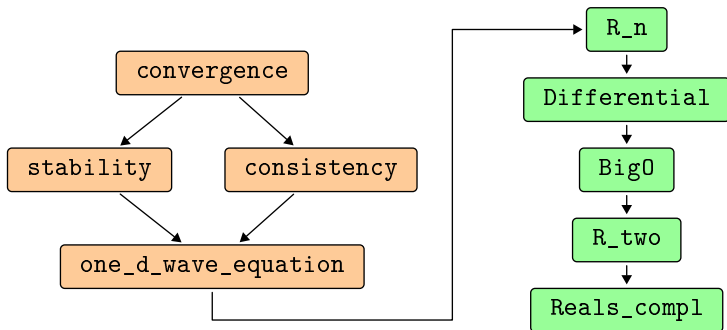
# Convergence

$$\left\| e_h^{k_{\Delta t}(t)} \right\|_{\Delta x} = O \left( \begin{array}{l} t \in [0, t_{\max}] \\ (\Delta x, \Delta t) \rightarrow 0 \\ 0 < \Delta x \wedge 0 < \Delta t \wedge \\ c \frac{\Delta t}{\Delta x} \leq 1 - \xi \end{array} (\Delta x^2 + \Delta t^2) \right).$$

Note: the definition of the big  $O$  is much more detailed than in traditional pen-and-paper proofs.



# Method Error: Conclusion



4500 lines of Coq

≈ as long as a detailed pen-and-paper proof.

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# Round-off Errors

Main loop:

```
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;
```

Operations are performed with **floating-point** arithmetic;  
it introduces **round-off errors** which propagate along computations.

Example:  $a*dp = a \times dp \times (1 + \varepsilon)$  with  $|\varepsilon| \leq 2^{-53}$   
assuming that  $a \times dp$  does not underflow.

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Example:  $a*dp = a \times dp \times (1 + \varepsilon)$  with  $|\varepsilon| \leq 2^{-53}$   
assuming that  $a \times dp$  does not underflow.

Naive **forward error analysis** gives

$$|p_i^k - u_i^k| \leq O(2^k 2^{-53}).$$

Note: if that was optimal, the numerical scheme would be useless.

# Local Round-off Errors

Main loop:

```
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;
```

Local round-off error:

$$\varepsilon_i^{k+1} = p_i^{k+1} - \left( 2p_i^k - p_i^{k-1} + \left( c \frac{\Delta t}{\Delta x} \right)^2 (p_{i+1}^k - 2p_i^k + p_{i-1}^k) \right).$$

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Assuming that all the computed values  $p_i^k$  are less than 2 (the values  $u_i^k$  are less than 1), then Gappa gives

$$|\varepsilon_i^k| \leq 85 \times 2^{-52}.$$

# Round-off Propagation

The **global** error  $p_i^k - u_i^k$  depends on the following local errors:

$$\begin{array}{ccccccc}
 & & & & \varepsilon_i^k & & \\
 & & & & \varepsilon_i^{k-1} & & \\
 & & \varepsilon_{i-1}^{k-1} & & \varepsilon_i^{k-1} & & \varepsilon_{i+1}^{k-1} \\
 & & \varepsilon_{i-2}^{k-2} & & \varepsilon_{i-1}^{k-2} & & \varepsilon_i^{k-2} & & \varepsilon_{i+1}^{k-2} & & \varepsilon_{i+2}^{k-2} \\
 & \dots & & & \vdots & & & & \dots & & \\
 \varepsilon_{i-k}^0 & & \dots & & \varepsilon_i^0 & & \dots & & \varepsilon_{i+k}^0
 \end{array}$$





# Round-off Error

- $p_i^k - u_i^k = \sum_{l=0}^k \sum_{j=-l}^l \lambda_j^l \varepsilon_{i+j}^{k-l}$ .
- $\lambda$  is solution of the numerical scheme: **stability**  $\Rightarrow$  bounded.

# Round-off Error

- $p_i^k - u_i^k = \sum_{l=0}^k \sum_{j=-l}^l \lambda_j^l \varepsilon_{i+j}^{k-l}$ .
- $\lambda$  is solution of the numerical scheme: **stability**  $\Rightarrow$  bounded.

Round-off error:  $O(k^2 2^{-53})$ .

$$|p_i^k - u_i^k| \leq 85 \times 2^{-53} \times (k+1) \times (k+2).$$

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# Annotations: Mathematical Definitions

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

  @ logic real psol_1(real x, real t);
  @ axiom psol_1_def:
  @   \forall real x; \forall real t;
  @   \forall real eps; 0 < 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;

  @ logic real p0(real x);
  @ axiom wave_eq_0: \forall real x; 0 <= x <= 1 ==> psol(x, 0) == p0(x);
  @ ...
  @ } */
```

# Annotations: Mathematical Definitions

```
/*@ axiomatic dirichlet_maths {  
  @ logic real psol(real x, real t); Exact solution  $u$   
  
  @ logic real psol_1(real x, real t);  
  @ axiom psol_1_def:  
  @   \forall real x; \forall real t;  
  @   \forall real eps; 0 < 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;  
  
  @ logic real p0(real x);  
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  @ ...  
  @ } */
```

# Annotations: Mathematical Definitions

```
/*@ axiomatic dirichlet_maths {
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```

Definition of  $\frac{\partial u}{\partial t}$

```
  @ logic real psol_1(real x, real t);
  @ axiom psol_1_def:
  @   \forall real x; \forall real t;
  @   \forall real eps; 0 < 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;
```

```
  @ logic real p0(real x);
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  @ logic real p0(real x);  
  @ axiom wave_eq_0: \forall real x; 0 <= x <= 1 ==> psol(x, 0) == p0(x);  
  @ ...  
  @ } */
```

Initial condition

# Annotations: Relation Between Mathematics and Program

```
/*@ 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);
```



# Annotations: Program Behavior

```
/*@ loop invariant
   @ 1 <= k <= nk &&
   @ analytic_error(p, ni, ni, k, a, dt);
   @ loop variant nk - k; */
for (k=1; k<nk; k++) {
  p[0][k+1] = 0.;
  /*@ 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++) {
    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;
  }
  p[ni][k+1] = 0.;
  /*@ assert analytic_error(p, ni, ni, k + 1, a, dt); */
}
```

# Verification: Proof Obligations

gWhy: a verification conditions viewer

Proof obligations	Alt-Ergo 0.93	Z3 3.2 (SS)	CVC3 2.4.1 (SS)	Gappa 0.15.1	Statistics
▶ User goals	●	●	●	●	0/4
▶ Function forward_prop default behavior	●	●	●	●	24/44
▼ Function forward_prop Safety	●	●	●	●	94/105
1. check FP overflow	●	●	●	●	
2. check FP overflow	●	●	●	●	
3. check FP overflow	●	●	●	●	
4. check FP overflow	●	●	●	●	
5. check FP overflow	●	●	●	●	
6. check FP overflow	●	●	●	●	
7. check FP overflow	●	●	●	●	
8. check arithmetic overflow	●	●	●	●	
9. check arithmetic overflow	●	●	●	●	
10. check arithmetic overflow	●	●	●	●	
11. check arithmetic overflow	●	●	●	●	
12. precondition for user call	●	●	●	●	
13. precondition for user call	●	●	●	●	
14. pointer dereferencing	●	●	●	●	
15. pointer dereferencing	●	●	●	●	
16. pointer dereferencing	●	●	●	●	
17. pointer dereferencing	●	●	●	●	
18. check FP overflow	●	●	●	●	
19. check FP overflow	●	●	●	●	
20. precondition for user call	●	●	●	●	
21. pointer dereferencing	●	●	●	●	
22. pointer dereferencing	●	●	●	●	
23. pointer dereferencing	●	●	●	●	
24. pointer dereferencing	●	●	●	●	
25. check arithmetic overflow	●	●	●	●	
26. check arithmetic overflow	●	●	●	●	
27. variant decreases	●	●	●	●	
28. variant decreases	●	●	●	●	
29. pointer dereferencing	●	●	●	●	
30. pointer dereferencing	●	●	●	●	
31. pointer dereferencing	●	●	●	●	
32. pointer dereferencing	●	●	●	●	
33. pointer dereferencing	●	●	●	●	
34. pointer dereferencing	●	●	●	●	
35. check arithmetic overflow	●	●	●	●	
36. check arithmetic overflow	●	●	●	●	
37. pointer dereferencing	●	●	●	●	

```

forward_prop_safety_po_3
ni_0: int32
nk: int32
dt: double
v: double
l: double
HI: (integer_of_int32(ni_0) >= 2 and
integer_of_int32(nk) >= 2 and
double_value(l) <= 0.0 and
double_value(dt) > 0. and
double_exact(dt) > 0. and
double_exact(v) = c and
double_exact(v) = double_value(v) and
0x1.p-1000 <= double_exact(dt) and
integer_of_int32(ni_0) <= 2147483646 and
integer_of_int32(nk) <= 759650) and
real_of_int(integer_of_int32(nk)) * double_exact(dt) <= T_max and
abs_real((double_exact(dt) - double_value(dt)) / double_value(dt) <= 0x1.p-51 and
0x1.p-500 <= double_exact(dt) * real_of_int(integer_of_int32(ni_0)) * c and
double_exact(dt) * real_of_int(integer_of_int32(ni_0)) * c <= 1.0 -
0x1.p-50 and
sqrt_real(1 /
real_of_int((integer_of_int32(ni_0) * integer_of_int32(ni_0)) +
double_exact(dt) * double_exact(dt))) < alpha_conv)
result: double
HI0: double_value(result) = 1. and
double_exact(result) = 1. and double_model(result) = 1.
HI1: no_overflow_double(nearest_even, real_of_int(integer_of_int32(ni_0)))
result0: double
HI2: double_of_real_post(nearest_even, real_of_int(integer_of_int32(ni_0)),
result0)
no_overflow_double(nearest_even, double_value(result) / double_value(result0))

double xs, double l) {
/* Output variable. */
double **p;

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

dx = 1./ni;
/*@ assert
0 < dx > 0.66 dx <= 0.5 66
0 < \abs(\exact(dx) - dx) / dx <= 0x1.p-53;
0 */

/* Compute the constant coefficient of the stiffness matrix. */
a1 = dt/dx**v;
a = a1*a1;
/*@ assert
0 < a <= 1 66
0 < < \exact(a) <= 1 66

```

# Verification: Automation and Formal Proof

## Verification conditions:

- behavior: what the program is supposed to perform,
- safety: the condition for it to terminate without error.

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
<b>Automatic</b>	<b>23</b>	<b>94</b>	<b>117</b>
<b>Coq</b>	<b>21</b>	<b>11</b>	<b>32</b>
Total	44	105	149

# Outline

- 1 Introduction
- 2 Tools
- 3 Method Error
- 4 Round-off Error
- 5 Verification
- 6 Conclusion**

# Conclusion

Development: <http://fost.saclay.inria.fr/>

- 60 lines of C code,
- 180 lines of ACSL annotations,
- 15000 lines of Coq definitions, theorems, and proofs.

# Conclusion

Development: <http://fost.saclay.inria.fr/>

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What was verified?

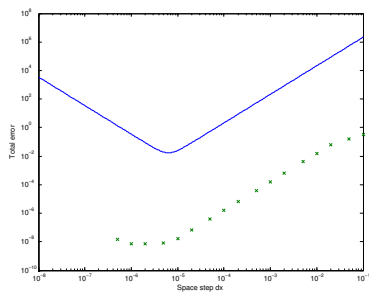
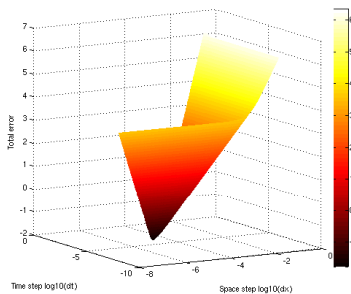
- The C program terminates without any runtime error.
- The method error is the expected one.
- The round-off error is small enough.

# Benefits from Formal Proofs

- Confidence, confidence, confidence.

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- Confidence, confidence, confidence.
- One can extract the constants hidden inside the big  $O$  from the formal proofs:





# Perspectives

- Prove Lax equivalence for several schemes:  
consistency  $\Rightarrow$  (stability  $\Leftrightarrow$  convergence).
- Do not rely on energy-based proofs,  
e.g. use Fourier transforms.

# Questions?

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