Automatic pre- and postconditions for partial differential equations

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Abstract. Based on a simple automata-theoretic and algebraic framework, we study equational reasoning for Initial Value Problems (IVPs) of polynomial Partial Differential Equations (PDEs). In order to represent IVPs in their full generality, we introduce *stratified* systems, where function definitions can be decomposed into distinct subsystems, focusing on different subsets of independent variables. Under a certain coherence condition, for such stratified systems we prove existence and uniqueness of formal power series solutions, which conservatively extend the classical analytic ones. We then give a — in a precise sense, complete — algorithm to compute weakest preconditions and strongest postconditions for such systems. To some extent, this result reduces equational reasoning on PDE initial value (and boundary) problems to algebraic reasoning. We illustrate some experiments conducted with a proof-of-concept implementation of the method.

1 Introduction

Techniques for reasoning on ordinary differential equations (ODEs) are at the heart of current formal methods and tools for continuous and hybrid systems, which form an active research area, see e.g. [28,29,19,13,14,4,8] and references therein. Although examples of hybrid systems whose continuous dynamics is described by *partial* differential equations (PDEs) abound, formal techniques for reasoning on PDEs have comparably received much less attention. Existing proposals mostly focus on specific types of equations, such as the Hamilton-Jacobi equations [10,20]. The present paper, building on [5], is meant as a contribution to developing formal methods for reasoning on PDEs. Our approach is *formal*, in the sense of being entirely based on simple coalgebra (automata theory) and algebra (polynomials), rather than on calculus like most of the previous proposals. Nevertheless, the resulting notion of PDE solution can be used to reason on the classical analytic one, in a sense made precise below.

In [5] we have shown that, subject to a certain coherence condition, a system Σ of polynomial PDEs, given an arbitrary initial data specification, admits a unique solution in the set of commutative formal power series (CFPSs; Section 2). Most important, this solution can be expressed operationally, in terms of the transition function of a suitable automaton. This lays the basis for mechanical checking of equations: that is, check that a given (polynomial) expression involving the PDE variables becomes identically 0 when the solution is plugged into it. The corresponding procedure is similar in spirit to an on-the-fly bisimulation checking algorithm. Pragmatically, these CFPS solutions

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conservatively extend classical ones: if an analytic solution of Σ in the classical sense exists, then its Taylor expansion from 0, seen as a formal power series, coincides with the unique CFPS solution.

In the present paper, we make two substantial steps forward. First, we introduce *stratified systems*, by which one can represent fairly complicated initial value problems — and, through changes of coordinates, also boundary problems. Second and most crucial, we give a (relatively) complete algorithm to automatically compute *pre-* and *postconditions* of a given system. In particular, this allows one to automatically compute *all* valid polynomial equations that fit a user-specified format (e.g., all conservation laws up to a given degree), rather than just checking the validity of given ones.

More in detail, in a stratified system we have distinct sets of equations (subsystems): in each of them, a distinct subset of the independent variables is fixed to zero. This way, in a system with, say, two independent variables x and y, the solution, $f(x,y)$, can be made dependent on constraints involving not only $f(x,y)$ and its derivatives, but also $f(x,0)$ and its x-derivatives, and $f(0,y)$ and its y-derivatives. This is how initial value problems are formulated in their generality. Under a syntactic acyclicity condition among subsystems, we prove existence and uniqueness of solutions for stratified systems and an automata-theoretic representation of the corresponding Taylor coefficients (Section 3).

This result lays the basis of an algorithm to automatically compute both weakest *preconditions* (= sets of initial data specifications) and strongest *postconditions* (= valid polynomial equations). The method is complete, subject to certain assumptions (Section 4). This way one can, for example, automatically *discover* all polynomial equations up to a given degree, valid under a given set of initial data specifications. Or vice-versa, compute the largest set of initial data specifications for given equations to be valid. The original IVP is therefore reduced to a purely algebraic system, which can be used for equational reasoning and, in some cases, to find explicit solutions. Concepts from algebraic geometry are used to prove the termination and correctness of this algorithm. Using a proof-of-concept implementation (Section 5), we illustrate this algorithm on well-known examples drawn from mathematical physics. Relations with other works, in particular on ODEs [2,3], is discussed in the concluding section (Section 6). Proofs and additional technical material omitted from the main body of the paper are reported in a separate Appendix (Appendix A).

2 Background

We review some notation and terminology from the theory of formal power series and from the formal theory of PDEs, including the main result of [5].

Commutative formal power series and polynomials Assume a finite set $X = \{x_1,...,x_n\}$ of *independent variables* is given. The set X, ranged over by $t,x,...$, will be kept fixed for the rest of the paper. Let $X^{\otimes}$, ranged over by $\tau,\xi,...$, be the set of *monomials*[1] that can be formed from the elements of X, in other words, the commutative monoid freely generated by X. Let us fix any total order $\mathbf{x} = (x_1,...,x_n)$ of the

[1] In general, we shall adopt for monomials the same notation we use for strings, as the context is sufficient to disambiguate. In particular, we overload the symbol ε to denote both the empty string and the unit monomial. When $X = \emptyset$, $X^{\otimes} \stackrel{\triangle}{=} \{\varepsilon\}$.

variables in X. Given a vector $\boldsymbol{\alpha} = (\alpha_1, ..., \alpha_n)$ of nonnegative integers (a *multi-index*), we let $\mathbf{x}^{\boldsymbol{\alpha}}$ denote the monomial $x_1^{\alpha_1} \cdots x_n^{\alpha_n}$. For $\xi = \mathbf{x}^{\boldsymbol{\alpha}}$ and $\tau = \mathbf{x}^{\boldsymbol{\beta}}$, we let $\xi \leq \tau$ if for each $i = 1, ..., n$, $\alpha_i \leq \beta_i$. A *commutative formal power series* (CFPS) with indeterminates in X and coefficients in $\mathbb{R}$ is a total function $f : X^{\otimes} \to \mathbb{R}$. The set of such CFPSs will be denoted by $\mathbb{R}[\![X]\!]$. We will sometimes use the suggestive notation $\sum_{\boldsymbol{\alpha} \in \mathbb{N}^n} f(\mathbf{x}^{\boldsymbol{\alpha}}) \cdot \mathbf{x}^{\boldsymbol{\alpha}}$ to denote a CFPS f. By slight abuse of notation, for each $\mu \in \mathbb{R}$, we will denote the CFPS that maps ε to μ and anything else to 0 simply as μ; while x_i will denote the i-th identity, the CFPS that maps x_i to 1 and anything else to 0. The definitions the sum $f + g$, (convolution) product $f \cdot g$, inverse f^{-1} (if $f(\varepsilon) \neq 0$) and partial derivative $\frac{\partial f}{\partial x}$ operations on CFPS are standard, and enjoy the usual algebraic properties (we also review these operations in Appendix A.1). In particular sum and product make $\mathbb{R}[\![X]\!]$ a ring with 0 and 1 as identities.

If the *support* of f, $\mathrm{supp}(f) \stackrel{\triangle}{=} \{\tau : f(\tau) \neq 0\}$, is finite, we will call f a *polynomial*. The set of polynomials, denoted by $\mathbb{R}[X]$, is closed under the above defined operations of sum, product (which make it a ring) and partial derivative, but in general not inverse. It is important to note that, when confining to polynomials, sum, product and partial derivative are well defined even in case the cardinality of the set of indeterminates X is infinite.

Partial differential equations The definitions in this paragraph are standard, or slight variations of the standard ones as found in the formal theory of PDEs, cf. [21,17,5] and references therein. A finite, nonempty set U of *dependent variables*, disjoint from X and ranged over by $u, v, ...$, is given. We let $\mathcal{D} \stackrel{\triangle}{=} \{u_\tau : u \in U, \tau \in X^{\otimes}\}$ be the set of the *derivatives*. Informally, a symbol $u \in U$ represents a function, and u_τ its partial derivative $\frac{\partial u}{\partial \tau}$; here u_ε will be identified with u. We let $\mathcal{P} \stackrel{\triangle}{=} \mathbb{R}[X \cup \mathcal{D}]$, ranged over by $E, F, ...$, denote the set of *(differential) polynomials* with coefficients in $\mathbb{R}$ and indeterminates in $X \cup \mathcal{D}$. Considered as formal objects, differential polynomials are just finite-support CFPSs, as per previous paragraph. As such, they inherit the operations of sum, product and partial derivative, along with the corresponding properties. Syntactically, we shall write polynomials as expressions of the form $\sum_{\gamma \in M} \lambda_\gamma \cdot \gamma$, for $0 \neq \lambda_\gamma \in \mathbb{R}$ and $M \subseteq_{\mathrm{fin}} (X \cup \mathcal{D})^{\otimes}$. Note that this notation is consistent with the sum and product operations defined on polynomials. For example, $E = v_z u_{xy} + v_y^2 + u + 5x$ is a polynomial[2]. For an independent variable $x \in X$, the *total derivative* of $E \in \mathcal{P}$ w.r.t. x is just the derivative of E w.r.t x, taking into account that $\frac{\partial u_\tau}{\partial x} = u_{x\tau}$ and the chain rule. Formally, the operator $D_x : \mathcal{P} \to \mathcal{P}$ is defined by (note $\sum$ below has only finitely many nonzero terms)

$$D_x E \stackrel{\triangle}{=} \frac{\partial E}{\partial x} + \sum_{u,\tau} u_{x\tau} \cdot \frac{\partial E}{\partial u_\tau}$$

where $\frac{\partial E}{\partial a}$ denotes the partial derivative of polynomial E along $a \in X \cup \mathcal{D}$. $D_x(\cdot)$ inherits differentiation rules for sum and product that are the analog of those for partial derivatives $\partial(\cdot)/\partial x$ (see (13)).As an example, for the polynomial E above, we have $D_x E = v_{xz} u_{xy} + v_z u_{xxy} + 2 v_y v_{xy} + u_x + 5$. In particular, $D_x u_\tau = u_{x\tau}$ and $D_x x^k = k x^{k-1}$. Just as

[2] Real arithmetic expressions will be used as a meta-notation for polynomials: e.g. $(u + u_x + 1) \cdot (x + u_y)$ denotes the polynomial $xu + uu_y + xu_x + u_x u_y + x + u_y$.

partial derivatives, total derivatives commute with each other, that is $D_x D_y F = D_y D_x F$. This suggests to extend the notation to monomials: for any monomial $\tau = x_1 \cdots x_m$, we let $D_\tau F$ be $D_{x_1} \cdots D_{x_m} F$, where the order of the derivatives is irrelevant. We formally introduce systems of PDEs below, along with the key notions of *parametric* and *principal* derivatives. Informally, parametric derivatives play a role similar to the lower order derivatives in ODEs initial value problems: just like in ODEs, once we fix their values at the origin, the solution of the system should be uniquely determined. On the other hand, equations for principal derivatives depend on the parametric ones, just like higher order derivatives in ODEs depend on the lower order ones.

Definition 1 (system of PDEs). *A* system of PDEs *is a nonempty set* Σ *of equations (pairs) of the form* $u_\tau = E$*, with* $E \in \mathcal{P}$*. The set of derivatives* u_τ *that appear as left-hand sides of equations in* Σ *is denoted by* $\mathrm{dom}(\Sigma)$*. Based on* Σ*, the set* $\mathcal{D}$ *is partitioned into the sets of* principal *and* parametric *derivatives, defined as follows.*

$$\mathcal{P}\mathrm{r}(\Sigma) \stackrel{\triangle}{=} \{u_{\tau\xi} : u_\tau \in \mathrm{dom}(\Sigma) \text{ and } \xi \in X^{\otimes}\} \qquad \mathcal{P}\mathrm{a}(\Sigma) \stackrel{\triangle}{=} \mathcal{D} \setminus \mathcal{P}\mathrm{r}(\Sigma)\,.$$

We let $\mathcal{P}_0(\Sigma) \stackrel{\triangle}{=} \mathbb{R}[X \cup \mathcal{P}\mathrm{a}(\Sigma)]$ *be the set of* Σ-normal forms.

Example 1 (Heat equation). The Heat equation in one spatial dimension, $u_t(t,x) = u_{xx}(t,x)$, corresponds to $X = \{t,x\}$, $U = \{u\}$ and $\Sigma = \{u_t = u_{xx}\}$. Here we have $\mathcal{P}\mathrm{r}(\Sigma) = \{u_{t\tau} : \tau \in X^{\otimes}\}$ and $\mathcal{P}\mathrm{a}(\Sigma) = \{u_{x^j} : j \geq 0\}$. See Figure 1, left.

Note that we do *not* insist that each derivative occurs at most once as left-hand side in Σ. The *infinite prolongation* of a system Σ, denoted Σ^∞, is the system of PDEs of the form $u_{\xi\tau} = D_\xi F$, where $u_\tau = F$ is in Σ and $\xi \in X^{\otimes}$. Of course, $\Sigma^\infty \supseteq \Sigma$. Moreover, Σ and Σ^∞ induce the *same* sets of principal and parametric derivatives.

We can now introduce the concept of *solution* of PDEs, which is based on a PDE's analog of initial value problems (IVPs). We say a function $\psi : \mathcal{P} \to \mathbb{R}[\![X]\!]$ is a *homomorphism* if it is a ring homomorphism — preserves sum, product and their identities as expected — and additionally: preserves derivatives, that is $\psi(D_x E) = \frac{\partial}{\partial x}\psi(E)$, and maps each $x_i \in X$ to the i-th identity CFPS. For any function $\psi : U \to \mathbb{R}[\![X]\!]$, its homomorphic extension $\mathcal{P} \to \mathbb{R}[\![X]\!]$ is defined as expected and, by slight abuse of notation, still denoted by "ψ". In the definition below, it is useful to bear in mind that, informally, for any $f \in \mathbb{R}[\![X]\!]$, $f(\varepsilon)$ is the formal counterpart of $f(0)$, and that for each parametric derivative $u_\tau \in \mathcal{P}\mathrm{a}(\Sigma)$, the initial data value $\rho(u_\tau)$ is the formal counterpart of $\frac{\partial u}{\partial \tau}(0)$.

Definition 2 (initial value problem). *Let* Σ *be a system of PDEs. An* initial data specification *is a mapping* $\rho : \mathcal{P}\mathrm{a}(\Sigma) \to \mathbb{R}$*. An* initial value problem (IVP) *is a pair* $\mathbf{iP} = (\Sigma, \rho)$.

A solution *of* $\mathbf{iP}$ *is a homomorphism* $\psi : \mathcal{P} \to \mathbb{R}[\![X]\!]$ *such that: (a) the initial value conditions are satisfied, that is* $\psi(u_\tau)(\varepsilon) = \rho(u_\tau)$ *for each* $u_\tau \in \mathcal{P}\mathrm{a}(\Sigma)$*; and (b) all equations are satisfied, that is* $\psi(u_\tau) = \psi(F)$ *for each* $u_\tau = F$ *in* Σ^∞.

For Σ to have a solution, a few syntactic conditions must be imposed, whose purpose is to avoid inconsistencies in the equational theory generated by Σ. A *ranking* is a total order $\prec$ of $\mathcal{D}$ such that: (a) $u_\tau \prec u_{x\tau}$, and (b) $u_\tau \prec v_\xi$ implies $u_{x\tau} \prec v_{x\xi}$, for each $x \in X$, $\tau, \xi \in X^{\otimes}$ and $u, v \in U$. Dickson's lemma [11] implies that $\mathcal{D}$ with $\prec$ is a well-order, and in particular that there is no infinite descending chain in it. The system Σ is $\prec$-*normal* if, for each equation $u_\tau = E$ in Σ, $u_\tau \succ v_\xi$, for each v_ξ appearing in E. An easy but important consequence of condition (b) above is that if Σ is normal then also its prolongation Σ^∞ is normal.

Now, consider the equational theory over $\mathcal{P}$ induced by the equations in Σ^∞. More precisely, write $E \to_\Sigma F$ if F is the polynomial that is obtained from E by replacing one occurrence of u_τ with G, for some equation $u_\tau = G \in \Sigma^\infty$. Note, in particular, that $E \in \mathcal{P}$ cannot be rewritten if and only if $E \in \mathcal{P}_0(\Sigma)$. We let $=_\Sigma$ denote the reflexive, symmetric and transitive closure of $\to_\Sigma$. The following definition formalizes the key concepts of consistency and coherence of Σ. Basically, as shown in [5], under the natural requirement of normality, consistency is a necessary and sufficient condition for Σ to admit a unique solution under *arbitrary* initial conditions.

Definition 3 (coherence). *Let Σ be a system of PDEs.*

- Σ *is* consistent *if for each $E \in \mathcal{P}$ there is a unique $F \in \mathcal{P}_0(\Sigma)$ such that $E =_\Sigma F$.*
- *Let $\prec$ be a ranking. A system Σ is* $\prec$-coherent *if it is $\prec$-normal and consistent.*

As an example, the Heat equation in Example 1 is obviously consistent, as it features just one equation. Moreover, it is $\prec$-coherent w.r.t. the ranking $u_\tau \prec u_\xi$ iff $\tau \prec_{\mathrm{lex}} \xi$, where $\prec_{\mathrm{lex}}$ is the lexicographic monomial order induced by $t > x$. For any consistent system, we can define a *normal form function*

$$S_\Sigma : \mathcal{P} \to \mathcal{P}_0(\Sigma)$$

by letting $S_\Sigma E \stackrel{\triangle}{=} F$, for the unique $F \in \mathcal{P}_0(\Sigma)$ such that $E \to_\Sigma^* F$. The term $S_\Sigma E$ will be often abbreviated as SE, if Σ is understood from the context. Deciding if a (finite) system Σ is coherent, for a suitable ranking $\prec$, is of course a nontrivial problem. Since $\prec$ is a well-order, there are no infinite sequences of rewrites $E_1 \to_\Sigma E_2 \to_\Sigma E_3 \to_\Sigma \cdots$: therefore it is possible to rewrite any E into some $F \in \mathcal{P}_0(\Sigma)$ in a finite number of steps. Proving coherence reduces then to proving $\to_\Sigma$ confluent. For our purposes, it is enough to know that completing a given system of equations to make it coherent, or deciding that this is impossible, can be achieved by one of many existing computer algebra algorithms, like those in [21,17]; see the discussion and the references in [5]. In many cases arising from applications, say mathematical physics, transforming the system into a coherent form for an appropriate ranking can be accomplished manually, without much difficulty: see the examples in Section 5.

We can now characterize explicitly the solutions of a coherent Σ. Informally, for any fixed ρ, the CFPS associated with $E \in \mathcal{P}$ takes each monomial $\tau \in X^\otimes$ to the real obtained by evaluating the τ-derivative of E under ρ, once this derivative is written in normal form. Formally, the characterization is based on a transition function, $\delta_\Sigma : \mathcal{P} \times X \to \mathcal{P}_0(\Sigma)$, defined as

$$\delta_\Sigma(E,x) \stackrel{\triangle}{=} S_\Sigma D_x E\,. \tag{1}$$

It can be shown (see [5]) that δ_Σ satisfies the following commutation property: $\delta_\Sigma(\delta_\Sigma(E,x),y) = \delta_\Sigma(\delta_\Sigma(E,y),x)$ for all $x,y \in X$. This justifies the notation $\delta_\Sigma(E,\tau)$ for $\tau \in X^\otimes$, with $\delta_\Sigma(E,\varepsilon) \stackrel{\triangle}{=} S_\Sigma E$. Next, an initial data specification $\rho : \mathcal{P}\mathrm{a}(\Sigma) \to \mathbb{R}$ can be extended homomorphically to a function $\mathcal{P}_0(\Sigma) \to \mathbb{R}$, interpreting $+$ and $\cdot$ as the usual sum and product over $\mathbb{R}$, and letting $\rho(x) \stackrel{\triangle}{=} 0$ for each independent variable $x \in X$. The following theorem of existence and uniqueness of solutions is the main result of [5]. (for the sake of completeness, the proof is also reproduced in Appendix A.2). Below, recall that for $\boldsymbol{\alpha} = (\alpha_1, ..., \alpha_n) \in \mathbb{N}^n$, $\boldsymbol{\alpha}! = \alpha_1! \cdots \alpha_n!$.

Theorem 1 (existence and uniqueness of solution, [5]). *Let Σ be finite and coherent. For any initial data specification ρ, there is a unique solution $\phi_{\mathbf{iP}} : \mathcal{P} \to \mathbb{R}[\![X]\!]$ of the IVP $\mathbf{iP} = (\Sigma, \rho)$. Moreover, $\phi_{\mathbf{iP}}$ satisfies the following formula, for each $E \in \mathcal{P}$ and $\tau = \mathbf{x}^{\boldsymbol{\alpha}} \in X^{\otimes}$.*

$$\phi_{\mathbf{iP}}(E)(\tau) = \frac{\rho(\delta_\Sigma(E, \tau))}{\boldsymbol{\alpha}!}\,. \tag{2}$$

We remark that our concept of solution of a PDE IVP conservatively extends the classical solution concept, in the following sense: if a classical solution exists that is analytic around the origin, then its Taylor expansion, seen as a formal power series, coincides with the CFPS solution (Appendix A.4).

3 Stratified systems

Consider the Heat equation of Example 1. Suppose we want to specify that the temperature at time $t = 0$ varies along the x-line according to, say, $u(0,x) = \exp(-x) = \sum_{j \geq 0} \frac{(-1)^j}{j!} x^j$. With the pure PDE formalism introduced so far, the only way to specify $u(0,x)$ is by explicitly giving the values of all its derivatives at the origin, via the initial data ρ. That is, by specifying the parametric derivatives of u: $\rho(u_{x^j}) = (\frac{\partial^j}{\partial x^j} u(0,x))_{|x=0} \stackrel{\triangle}{=} (-1)^j$, for each $j \geq 0$. Such a ρ is an infinite object which does not obviously lend itself to equational and algorithmic manipulations. It would be more natural, instead, to specify $u(0,x)$ simply via a subsystem $\Sigma_0 = \{u_x = -u\}$ (plus the single initial condition $\rho(u) = 1$), somehow prescribing that this equation applies when fixing $t = 0$, so that the resulting function only depends on x. More generally, a pure PDE system Σ alone cannot express general IVPs, where one wants to specify constraints on the functions obtained by keeping the value of certain independent variables fixed. This limitation is overcome by stratified systems, introduced below.

We first introduce *subsystems*. Let us fix once and for all a nonempty set of dependent variables U, and a finite set of independent variables X. For $Y \subseteq X$, a Y-subsystem defines, informally, functions where variables outside Y have been zeroed. In particular, derivatives can be taken only along variables in Y. We need now some standard notation on partial orders. For a partial order $\preceq$ defined over some universe set A and for $B \subseteq A$, we will let $\uparrow_{\preceq} (B) \stackrel{\triangle}{=} \{a \in A : a \succeq b \text{ for some } b \in B\}$ denote the upward closure of B w.r.t $\preceq$; similarly, we will let $\downarrow_{\preceq} (B)$ denote the downward closure of B. Moreover, we will let $\min_{\preceq}(B) \stackrel{\triangle}{=} \{b \in B : \text{ whenever } b' \in B \text{ and } b' \preceq b \text{ then } b' = b\}$ denote the set of $\preceq$-minimal element of B. Additionally, we define the following partial order $\leq_Y$ on the set of derivatives $\mathcal{D}$, depending on $Y \subseteq X$: $u_\tau \leq_Y u_{\tau'}$ if and only if $\tau' = \tau\xi$ for some $\xi \in Y^{\otimes}$. In the definition of subsystem given below, the intuition is that the $\leq_Y$-minimal derivatives, the set U_Γ, act as the dependent variables of a new system of PDEs with independent variables in Y and derivatives in $\mathcal{D}_\Gamma$.

Fig. 1. u-derivatives arranged according to the partial order: $u_\tau \le u_\xi$ iff $\tau \le \xi$. In the Hasse diagrams, derivatives corresponds to line intersections, with elements in some $\mathrm{dom}(\Sigma)$ marked by a black dot. **Left**: system Σ of Example 1, where dark-shaded region = $\mathcal{P}\mathrm{r}(\Sigma)$, white region = $\mathcal{P}\mathrm{a}(\Sigma)$. **Right**: stratified system $H = \{\Gamma_1, \Gamma_2\}$ of Example 2, where dark-shaded region = $\mathcal{P}\mathrm{r}(\Gamma_1)$, light-shaded region = $\mathcal{P}\mathrm{r}(\Gamma_2)$, white region = $\mathcal{P}\mathrm{a}(H)$.

Definition 4 (subsystem). *Let Σ a set of equations and $Y \subseteq X$. For $\Gamma = (\Sigma, Y)$, we define the following subsets of $\mathcal{D}$.*

$$U_\Gamma \stackrel{\triangle}{=} \min_{\le_Y}(\downarrow_{\le_Y} \{u_\tau : u_\tau \textit{ occurs in } \Sigma\}) \qquad \mathcal{D}_\Gamma \stackrel{\triangle}{=} \uparrow_{\le_Y} (U_\Gamma)$$
$$\mathcal{P}\mathrm{r}(\Gamma) \stackrel{\triangle}{=} \uparrow_{\le_Y} (\mathrm{dom}(\Sigma)) \qquad \mathcal{P}\mathrm{a}(\Gamma) \stackrel{\triangle}{=} \mathcal{D}_\Gamma \setminus \mathcal{P}\mathrm{r}(\Gamma)\,.$$

*We let $\mathcal{P}_\Gamma \stackrel{\triangle}{=} \mathbb{R}[Y \cup \mathcal{D}_\Gamma]$. We say $\Gamma = (\Sigma, Y)$ is a Y-*subsystem *if U_Γ is finite, and for each polynomial E appearing in Σ, $E \in \mathcal{P}_\Gamma$. We call Γ a* main *subsystem if $Y = X$ and $U_\Gamma = U$. Finally, $\Gamma^\infty \stackrel{\triangle}{=} \{u_{\tau\xi} = D_\xi G : u_\tau = G \in \Sigma \textit{ and } \xi \in Y^\otimes\}$.*

Stratified systems can encode initial value problems in their general form. A precedence relation among subsystems, $\Gamma_i \prec \Gamma_j$, formalizes that equations in Γ_j depends on parametric variables that are defined (are principal) in Γ_i.

Definition 5 (stratified system). *A* stratified system *is a finite set of subsystems $H = \{\Gamma_1, \ldots, \Gamma_m\}$ ($m \ge 1$, $\Gamma_i = (\Sigma_i, X_i)$, $\Sigma_i \neq \emptyset$, $X_i \subseteq X$) such that:*

(a) for some $1 \le j \le m$, Γ_j is a main subsystem; we will conventionally take $j = 1$;
(b) for any $i \neq j$, $\mathcal{P}\mathrm{r}(\Gamma_i) \cap \mathcal{P}\mathrm{r}(\Gamma_j) = \emptyset$;
(c) the binary relation over $\{1, \ldots, m\}$ defined as $i \prec j$ iff $\mathcal{P}\mathrm{r}(\Gamma_i) \cap \mathcal{P}\mathrm{a}(\Gamma_j) \neq \emptyset$, is acyclic.

The parametric derivatives and normal forms of H are $\mathcal{P}\mathrm{a}(H) \stackrel{\triangle}{=} \mathcal{D} \setminus (\cup_{i=1}^m \mathcal{P}\mathrm{r}(\Gamma_i))$ and $\mathcal{P}_0(H) \stackrel{\triangle}{=} \mathbb{R}[\mathcal{P}\mathrm{a}(H)]$, respectively. H is coherent *if all of its subsystems are coherent w.r.t. one and the same ranking on $\mathcal{D}$.*

Note that each H features a unique main subsystem.

Example 2 (Heat equation with initial temperature). Consider the Heat equation of Example 1, with an initial temperature exponentially decaying from the origin, $u_x(0,x) = -u(0,x)$. The corresponding stratified system is $H = \{\Gamma_1, \Gamma_2\} = \{(\Sigma_1, X_1), (\Sigma_2, X_2)\}$ with $\Sigma_1 = \{u_t = u_{xx}\}$, $X_1 = X = \{t, x\}$ and $\Sigma_2 = \{u_x = -u\}$, $X_2 = \{x\}$. We have (see Fig. 1, right):

$$U_{\Gamma_1} = \{u\} \quad \mathcal{D}_{\Gamma_1} = \{u_\tau : \tau \in X^\otimes\} \quad \mathcal{P}\mathrm{r}(\Gamma_1) = \{u_{t\tau} : \tau \in X^\otimes\} \quad \mathcal{P}\mathrm{a}(\Gamma_1) = \{u_{x^j} : j \ge 0\}$$
$$U_{\Gamma_2} = \{u\} \quad \mathcal{D}_{\Gamma_2} = \{u_{x^j} : j \ge 0\} \quad \mathcal{P}\mathrm{r}(\Gamma_2) = \{u_{x^j} : j \ge 1\} \quad \mathcal{P}\mathrm{a}(\Gamma_2) = \{u\}\,.$$

Note that $\mathcal{D}_{\Gamma_1} = \mathcal{D}$, so Γ_1 is the main subsystem, and that $\mathcal{P}\mathrm{a}(H) = \{u\}$. Clearly, $2 \prec 1$, as $\mathcal{P}\mathrm{r}(\Gamma_2) \cap \mathcal{P}\mathrm{a}(\Gamma_1) \neq \emptyset$; on the other hand, $1 \not\prec 2$, as $\mathcal{P}\mathrm{r}(\Gamma_1) \cap \mathcal{P}\mathrm{a}(\Gamma_2) = \emptyset$; so the relation $\prec$ is acyclic. Finally, fixing the lexicographic order induced by $t > x$, H is trivially seen to be coherent.

In order to define solutions of stratified systems, let us introduce some additional notation about CFPSs. For a CFPS $f \in \mathbb{R}[\![X]\!]$ and $Y \subseteq X$, we can consider the CFPS $f_{|Y^{\otimes}} \in \mathbb{R}[\![Y]\!]$. For an intuitive explanation of this concept, assume e.g. f represents $f(x_1, x_2)$ and $Y = \{x_2\}$: recalling that we take the origin as the expansion point, $f_{|Y^{\otimes}}$ represents $f(0, x_2)$, that is, f where the variables not in Y have been replaced by 0. Formally, for $\psi : \mathcal{P} \to \mathbb{R}[\![X]\!]$ and a subsystem $\Gamma = (\Sigma, Y)$, we let $\psi_\Gamma : \mathcal{P}_\Gamma \to \mathbb{R}[\![Y]\!]$ be defined as: $\psi_\Gamma(E) \stackrel{\triangle}{=} \psi(E)_{|Y^{\otimes}}$ for each $E \in \mathcal{P}_\Gamma$.

Definition 6 (solutions of H). *Let H be a stratified system.*

1. *A* solution *of H is a homomorphism $\psi : \mathcal{P} \to \mathbb{R}[\![X]\!]$ such that for each $\Gamma_i \in H$, $\psi_{\Gamma_i} : \mathcal{P}_{\Gamma_i} \to \mathbb{R}[\![X_i]\!]$ respects all the equations in Γ_i^∞.*
2. *Let $\rho : \mathcal{P}\mathrm{a}(H) \to \mathbb{R}$ be an initial data specification and $\Gamma_0 = (\Sigma_0, X_0) \stackrel{\triangle}{=} (\{u_\tau = \rho(u_\tau) : u_\tau \in \mathcal{P}\mathrm{a}(H)\}, \emptyset)$. A* solution of the initial value problem $\mathbf{iP} = (H, \rho)$ *is solution of the stratified system $H \cup \{\Gamma_0\}$.*

We can linearly order the subsystems of H according to a total order compatible with $\prec$ and then lift inductively existence and uniqueness (Theorem 1) to H.

Theorem 2 (existence and uniqueness for H). *Let H be a coherent stratified system. For any initial data specification ρ for H, there is a unique solution of* $\mathbf{iP} = (H, \rho)$.

We illustrate the idea behind the proof of Theorem 2 on the Heat equation of Example 2.

Example 3 (Example 2, cont.). Let us fix any initial data specification $\rho(u) = u_0 \in \mathbb{R}$ for H. As prescribed by Def. 6(2), we consider the extended system $\overline{H} \stackrel{\triangle}{=} H \cup \{\Gamma_0\}$, where $\Gamma_0 = (\{u = u_0\}, \emptyset)$. Note that $U_{\Gamma_0} = \mathcal{D}_{\Gamma_0} = \mathcal{P}\mathrm{r}(\Gamma_0) = \{u\}$ and $\mathcal{P}\mathrm{a}(\Gamma_0) = \emptyset$. Now we build a sequence of IVPs $\mathbf{iP}_i$, and corresponding solutions $\psi_i : \mathcal{P}_{\Gamma_i} \to \mathbb{R}[\![X_i]\!]$, for the subsystems Γ_i's in $\overline{H}$. The construction proceeds inductively on a linear order compatible with $\prec$, that is: $0 \prec 2 \prec 1$. The definition of each initial data specification $\rho_i : \mathcal{P}\mathrm{a}(\Gamma_i) \to \mathbb{R}$ relies on the solutions ψ_j for $j \prec i$. The existence of such solutions is guaranteed by Theorem 1. In particular:

– $\mathbf{iP}_0 = (\{u = u_0\}, \rho_0)$, with $\rho_0(u) \stackrel{\triangle}{=} \emptyset$ (empty function), has solution[3] $\psi_0 : \mathcal{P}_{\Gamma_0}(= \mathbb{R}[u]) \to \mathbb{R}[\![\emptyset]\!]$;
– $\mathbf{iP}_2 = (\{u_x = -u\}, \rho_2)$, with $\rho_2(u) \stackrel{\triangle}{=} \psi_0(u)(\varepsilon)$, has solution $\psi_2 : \mathcal{P}_{\Gamma_2}(= \mathbb{R}[x, u]) \to \mathbb{R}[\![x]\!]$;
– $\mathbf{iP}_1 = (\{u_t = u_{xx}\}, \rho_1)$, with $\rho_1(u_{x^k}) \stackrel{\triangle}{=} \psi_2(u_{x^k})(\varepsilon)$ $(k \geq 0)$, has solution $\psi_1 : \mathcal{P}_{\Gamma_1}(= \mathcal{P}) \to \mathbb{R}[\![t, x]\!]$.

[3] Specifically, $\psi_0(E)(\varepsilon) = E(u_0)$ for each $E \in \mathbb{R}[u]$.

It can be shown — and this is the nontrivial part of Theorem 2 — that the solution of the main subsystem, ψ_1, is a solution of $\overline{H}$ (Def. 6(1)), and in particular: $(\psi_1)_{\Gamma_i} = \psi_i$ for each i. Hence ψ_1 is the (unique) solution of (H,ρ).

In view of the subsequent algorithmic developments, the next step is to obtain a formula for the Taylor coefficients of the solutions of H, in analogy with the formula (2) for pure systems. This formula will be based on the transition function of the main subsystem, δ_{Σ_1}. However, a pivotal role will now be also played by a reduction function $S_H : \mathcal{P} \to \mathcal{P}_0(H)$, introduced below: it will allow one to rewrite any $E \in \mathcal{P}$ to a normal form in $\mathcal{P}_0(H)$, where it can be evaluated for any given initial data specification ρ for H. Below, $\to_{\Sigma_i}$ (resp. $\to_X$) denotes the rewrite relation over $\mathcal{P}$ induced by the equations in Γ_i^∞ (resp. $\{x = 0 : x \in X\}$).

Definition 7 (reduction S_H). *Let $H = \{\Gamma_1, ..., \Gamma_m\}$ be a coherent stratified system. Let $\to_H \subseteq \mathcal{P} \times \mathcal{P}$ be $\to_H \stackrel{\triangle}{=} \to_{\Sigma_1} \cup \cdots \cup \to_{\Sigma_m} \cup \to_X$. For each $E \in \mathcal{P}$, we let $S_H E$ denote an arbitrarily fixed $F \in \mathcal{P}_0(H)$ such that $E \to_H^* F$.*

Note that $S_H E$ is well defined due to normality[4] of H. Let ϕ be a solution of an IVP (H,ρ). We remark that in general it is not true that $\phi(E) = \phi(S_H E)$ (trivially, $S_H x = 0$, but $\phi(x) \neq 0$). It *is* true, however, that $\phi(E)(\varepsilon) = \phi(S_H E)(\varepsilon)$; moreover $\phi(S_H E)(\varepsilon) = \rho(S_H E)$. This fact is quite intuitive, recalling the informal interpretation of $f(\varepsilon)$ as $f(0)$ for a CFPS f. For instance, in the Heat equation system of Example 2, one would have $u_t(0,0) = u_{xx}(0,0) = u(0,0)(= \rho(u))$, where the first and second equality follow from applying Σ_1 and Σ_2 (twice), respectively. Formally, we have the following formula, giving the Taylor coefficients of $\phi(E)$. This is also key to the algorithm in the next section.

Corollary 1 (Taylor coefficients). *Let H be a coherent stratified system. Denote by δ_{Σ_1} the transition function of the main subsystem of H. For any initial data specification ρ for H, the unique solution ϕ of (H,ρ) enjoys the following, for every $E \in \mathcal{P}$ and $\tau = \mathbf{x}^{\boldsymbol{\alpha}} \in X^{\otimes}$.*

$$\phi(E)(\tau) = \frac{\rho(S_H(\delta_{\Sigma_1}(E,\tau)))}{\boldsymbol{\alpha}!}\,. \tag{3}$$

Example 4 (Example 2, cont.). Consider any initial data specification $\rho(u) = u_0 \in \mathbb{R}$ for H, let ψ be the solution of (H,ρ) and $f = \psi(u)$. We compute the first few coefficients of f by applying (3) with $E = u$. Let us first compute a few $S_H(\delta_{\Sigma_1}(u,\tau))$ s. Recall that the definition of $=_{\Sigma_i}$ is based on Γ_i^∞ ($i = 1,2$).

$$\begin{array}{lll} S_H(\delta_{\Sigma_1}(u,\varepsilon)) = S_H u = u, & S_H(\delta_{\Sigma_1}(u,t)) = S_H u_{xx} = S_H(-u_x) = u, & S_H(\delta_{\Sigma_1}(u,x)) = S_H u_x = -u \\ S_H(\delta_{\Sigma_1}(u,tt)) = S_H u_{x^4} = u, & S_H(\delta_{\Sigma_1}(u,tx)) = S_H u_{x^3} = -u, & S_H(\delta_{\Sigma_1}(u,xx)) = S_H u_{xx} = u\,. \end{array}$$

In general, one can check that for $\tau = (t,x)^{\boldsymbol{\alpha}}$, $\boldsymbol{\alpha} = (\alpha_1,\alpha_2) \in \mathbb{N}^2$, $S_H(\delta_{\Sigma_1}(u,\tau)) = (-1)^{\alpha_2} u$. Hence, by (3), we have the CFPS: $f = u_0 + u_0 t - u_0 x + (u_0/2)t^2 - u_0 tx + (u_0/2)x^2 \cdots = \sum_{\tau = \mathbf{x}^{\boldsymbol{\alpha}}} (-1)^{\alpha_2}(u_0/\boldsymbol{\alpha}!)\tau$.

[4] In fact, more is true: $\to_H$ is terminating and confluent, so there is a unique H-normal form F s.t. $E \to_H^* F$. See Appendix A.3. Therefore the arbitrariness in Def. 7 is only apparent.

4 Algorithms for pre- and postconditions

We will first recall some terminology and some basic facts from algebraic geometry, then introduce pre- and postconditions and finally the POST algorithm to compute them.

Preliminaries From now on, we will restrict our attention to the following subclass of systems.

Definition 8 (FP systems). *A stratified system H is* finite-parameter *(FP) if $\mathcal{P}a(H)$ is finite.*

For instance, in Example 2 the system H is FP, while $H' \stackrel{\triangle}{=} \{\Gamma_1\}$ is not. In concrete applications, one would expect that most systems are FP. Let us now recall some additional notation and terminology about polynomials. According to (3), the calculation of the Taylor coefficients of a solution of a FP IVP $\mathbf{iP} = (H,\rho)$ involves evaluating expressions in $\mathcal{P}_0(H) = \mathbb{R}[\mathcal{P}a(H)]$. As $k \stackrel{\triangle}{=} |\mathcal{P}a(H)| < +\infty$, elements of $\mathcal{P}_0(H)$ can be treated as usual multivariate polynomials in a *finite* number of indeterminates. In particular, we can identify initial data specifications ρ for H with points in $\mathbb{R}^k$. Accordingly, for polynomials $E \in \mathcal{P}_0(H)$ and initial data specification $\rho \in \mathbb{R}^k$, it is notationally convenient to write $\rho(E)$ as $E(\rho)$, that is the value in $\mathbb{R}$ obtained by evaluating the polynomial E at the point $\rho \in \mathbb{R}^k$.

In what follows, we shall rely on a few basic notions from algebraic geometry, which we quickly review below (a more detailed review can be found in Appendix A.2). See [11, Ch.2–4] for a comprehensive treatment. An *ideal* $J \subseteq \mathcal{P}_0(H)$ is a nonempty set of polynomials closed under addition, and under multiplication by polynomials in $\mathcal{P}_0(H)$. For $P \subseteq \mathcal{P}_0(H)$, $\langle\, P \,\rangle \stackrel{\triangle}{=} \{\sum_{i=1}^m F_i \cdot E_i \,:\, m \geq 0, F_i \in \mathcal{P}_0(H), E_i \in P\}$ denotes the smallest ideal which includes P, and $\mathbf{V}(P) \subseteq \mathbb{R}^k$ the *(affine) variety* induced by P: $\mathbf{V}(P) \stackrel{\triangle}{=} \{\rho \in \mathbb{R}^k \,:\, E(\rho) = 0 \text{ for each } E \in P\} \subseteq \mathbb{R}^k$. For $W \subseteq \mathbb{R}^k$, $\mathbf{I}(W) \stackrel{\triangle}{=} \{E \in \mathcal{P}_0(H) : E(\rho) = 0 \text{ for each } \rho \in V\}$ is the ideal induced by W. We will use a few basic facts about ideals and varieties: (a) both $\mathbf{I}(\cdot)$ and $\mathbf{V}(\cdot)$ are inclusion reversing: $P_1 \subseteq P_2$ implies $\mathbf{V}(P_1) \supseteq \mathbf{V}(P_2)$ and $W_1 \subseteq W_2$ implies $\mathbf{I}(W_1) \supseteq \mathbf{I}(W_2)$; (b) any ascending chain of ideals $I_0 \subseteq I_1 \subseteq \cdots \subseteq \mathcal{P}_0(H)$ stabilizes in a finite number of steps (Hilbert's basis theorem); (c) for finite $P \subseteq \mathcal{P}_0(H)$, the problem of deciding if $E \in \langle\, P \,\rangle$ is decidable, by computing a Gröbner basis (a set of generators with special properties) of $\langle\, P \,\rangle$.

Preconditions and postconditions. Let H be a coherent, FP system and let $k \stackrel{\triangle}{=} |\mathcal{P}a(H)|$. Informally, computing the *preconditions* of a given set $Q \subseteq \mathcal{P}$ means finding all the initial data specifications $\rho \in \mathbb{R}^k$ under which all the polynomials in Q represent valid equations for the system H — that is, they become identically zero when one plugs the solution of (H,ρ) into them. Dually, computing the *postconditions* of a given set of initial data specifications $W \subseteq \mathbb{R}^k$ means finding the set $Q \subseteq \mathcal{P}$ of all polynomial equations that are valid under all initial data $\rho \in W$. Here, we shall confine ourselves to *algebraic* sets W, that is $W = \mathbf{V}(P)$ for some $P \subseteq \mathcal{P}_0(H)$ — think of P as a set of constraints on the initial data. Formally, we have the following definition. Recall that for any $\rho \in \mathbb{R}^k$, we let $\phi_{(H,\rho)} : \mathcal{P} \to \mathbb{R}[\![X]\!]$ denote the unique solution of the IVP (H,ρ).

Definition 9 (pre- and postconditions). *Let H be coherent and* FP. *Let P and Q be sets of polynomials such that $P \subseteq \mathcal{P}_0(H)$ and $Q \subseteq \mathcal{P}$. We define the sets of* weakest preconditions $\mathrm{wp}_H(Q) \subseteq \mathbb{R}^k$ *and of the* strongest postconditions $\mathrm{sp}_H(P) \subseteq \mathcal{P}$ *as follows.*

$$\mathrm{wp}_H(Q) \stackrel{\triangle}{=} \{\rho \in \mathbb{R}^k : \phi_{(H,\rho)}(E) = 0 \textit{ for each } E \in Q\}$$
$$\mathrm{sp}_H(P) \stackrel{\triangle}{=} \{E \in \mathcal{P} : \phi_{(H,\rho)}(E) = 0 \textit{ for each } \rho \in \mathbf{V}(P)\}\,.$$

Any subset of $\mathrm{wp}_H(Q)$ will be called an (algebraic) precondition for Q, and any subset of $\mathrm{sp}_H(P)$ a postcondition for $\mathbf{V}(P)$. We focus here on computing strongest postconditions, which, as we shall see, can be used to compute preconditions as well. Actually, it is computationally convenient to introduce a *relativized* version of this problem.

Problem 1 (relativized strongest postcondition) *Let H be coherent,* FP. *Given user-specified sets $P \subseteq_{\mathrm{fin}} \mathcal{P}_0(H)$ and $R \subseteq \mathcal{P}$, find a finite characterization of* $\mathrm{sp}_H(P) \cap R$.

By ‘finding a finite characterization’, we mean effectively computing a finite set of generators, of an appropriate algebraic type, for the set in question (see next paragraph). Following a well-established tradition in the field of continuous and hybrid system, the set R will be represented by means of a polynomial template.

The POST **algorithm** We first introduce *polynomial templates* [28], that is, polynomials in $\mathrm{Lin}(\mathbf{a})[X \cup \mathcal{D}]$, where $\mathrm{Lin}(\mathbf{a})$ are (formal) linear combinations of the parameters in $\mathbf{a} = (a_1, \ldots, a_s)$ (for fixed $s \geq 1$) with real coefficients. For instance, $\ell = 5a_1 + 42a_2 - 3a_3$ is one such expression[5]. In other words, a polynomial template has the form $\pi = \sum_i \ell_i \gamma_i$ for distinct monomials $\gamma_i \in (X \cup \mathcal{D})^{\otimes}$, and ℓ_i linear expressions in the parameters a_i s. For example, the following is a template: $\pi = (5a_1 + (3/4)a_3)u_x v^2 x y^2 + (7a_1 + (1/5)a_2)uv_{xy} + (a_2 + 42a_3)$. A *parameter evaluation* is a vector $v = (v_1, \ldots, v_s) \in \mathbb{R}^s$; we denote by $\pi[v] \in \mathcal{P}$ the polynomial obtained from π by replacing each occurrence of a_i with v_i in the linear expressions of π and evaluating them. For $V \subseteq \mathbb{R}^s$, $\pi[V] \stackrel{\triangle}{=} \{\pi[v] : v \in V\} \subseteq \mathcal{P}$.

For a user specified template π with s parametes, our goal is to solve Problem 1 with $R = \pi[\mathbb{R}^s]$. In other words, for a given $P \subseteq \mathcal{P}_0(H)$ that describes an algebraic variety of initial data specifications, we want to compute

$$\mathrm{sp}_H(P) \cap \pi[\mathbb{R}^s]\,. \tag{4}$$

Informally, we will achieve this by building a sequence of vector spaces $\mathbb{R}^s \supseteq V_0 \supseteq V_1 \supseteq \cdots$, such that $\pi[V_i]$ contains polynomials whose derivatives up to order i vanish on all points in $\mathbf{V}(P)$. This sequence converges to a vector space, say V_m, such that $\pi[V_m]$ contain polynomials whose derivatives of *every* order vanish on $\mathbf{V}(P)$. On account of Corollary 1, equation (3), such polynomials belong to $\mathrm{sp}_H(P)$. A nontrivial point in this scheme is being able to detect convergence of the sequence of vector spaces V_i.

Formally, we first extend δ_{Σ_1} and S_H to templates as expected: for $\pi = \sum_i \ell_i \gamma_i$, $\delta_{\Sigma_1}(\pi, x) \stackrel{\triangle}{=} \sum_i \ell_i \delta_{\Sigma_1}(\gamma_i, x)$ and $S_H \pi \stackrel{\triangle}{=} \sum_i \ell_i S_H \gamma_i$, seen as a polynomials in $\mathrm{Lin}(\mathbf{a})[X \cup \mathcal{D}]$ and $\mathrm{Lin}(\mathbf{a})[\mathcal{P}\mathrm{a}(H)]$, respectively. We shall make use of the following substitution properties of templates, which hold true in coherent systems (Lemma A.15 in Appendix A.5). For each $x \in X$ and $v \in \mathbb{R}^s$:

$$\delta_{\Sigma_1}(\pi[v], x) = \delta_{\Sigma_1}(\pi, x)[v] \qquad\qquad S_H(\pi[v]) = (S_H \pi)[v]\,. \tag{5}$$

[5] Linear expressions with a constant term, such as $2 + 5a_1 + 42a_2 - 3a_3$ are not allowed.

We are now set to introduce the POST algorithm. Given $P \subseteq \mathcal{P}_0(H)$ and a template π, fix P_0 s.t. $I_0 \stackrel{\triangle}{=} \langle\, P_0 \,\rangle \subseteq \mathbf{I}(\mathbf{V}(P))$ ($P_0 = P$ is a possible choice). The algorithm consists in generating two sequences of sets, $V_i \subseteq \mathbb{R}^s$ and $J_i \subseteq \mathcal{P}_0(H)$, for $i \geq 0$. The idea is that, at step i, V_i collects those $v \in \mathbb{R}^s$ such that $S_H(\pi[v])$, and its derivatives up to order i, vanish on $\mathbf{V}(P)$, that is belong to $\mathbf{I}(\mathbf{V}(P))$. As $\mathbf{I}(\mathbf{V}(P))$ may be hard to compute, it is convenient to permit replacing it with some $\langle\, P_0 \,\rangle \subseteq \mathbf{I}(\mathbf{V}(P))$. The J_i's are used to detect stabilization. We use π_τ as an abbreviation of $\delta_{\Sigma_1}(\pi,\tau)$.

$$V_i \stackrel{\triangle}{=} \bigcap_{\tau : |\tau| \leq i} \{v \in \mathbb{R}^s : (S_H\pi_\tau)[v] \in I_0\} \tag{6}$$

$$J_i \stackrel{\triangle}{=} \Big\langle \bigcup_{\tau : |\tau| \leq i} (S_H\pi_\tau)[V_i] \Big\rangle . \tag{7}$$

Consider the least m such that *both* $V_m = V_{m+1}$ and $J_m = J_{m+1}$: we let $\mathrm{POST}_H(P_0,\pi) \stackrel{\triangle}{=} (V_m, J_m)$. Note that m is well defined. Indeed, $V_0 \supseteq V_1 \supseteq \cdots$ forms a descending chain of finite-dimensional vector spaces in $\mathbb{R}^s$, which must stabilize at some m'; then $J_{m'} \subseteq J_{m'+1} \subseteq \cdots$ forms an ascending chain of ideals in $\mathcal{P}_0(H)$, which must stabilize at some $m \geq m'$. We remark that neither of the two conditions $V_{m+1} = V_m$ or $J_m = J_{m+1}$ taken alone does imply stabilization, in general. The next theorem states correctness and relative completeness of POST. Part (a) says that the set of polynomials $\pi[V_m]$ is a post-condition of P and, in case $\langle\, P_0 \,\rangle = \mathbf{I}(\mathbf{V}(P))$, coincides with the strongest postcondition relative to π, that is (4). Part (b) says that J_m represents the weakest precondition of $\pi[V_m]$: this can be useful to look for preconditions in general, but will not be discussed here.

Theorem 3 (relative completeness of POST). *Let H be coherent and FP. Let $P \subseteq \mathcal{P}_0(H)$ and π be a template. Fix P_0 s.t. $I_0 \stackrel{\triangle}{=} \langle\, P_0 \,\rangle \subseteq \mathbf{I}(\mathbf{V}(P))$. Let $\mathrm{POST}_H(P_0,\pi) = (V_m, J_m)$.*

(a) $\pi[V_m] \subseteq \mathrm{sp}_H(P) \cap \pi[\mathbb{R}^s]$*, with equality if* $I_0 = \mathbf{I}(\mathbf{V}(P))$*;*
(b) $\mathbf{V}(J_m) = \mathrm{wp}_H(\pi[V_m])$.

Proof. In the proof we shall make use of the following stabilization property of the sequence of the (V_i, J_i)s (Lemma A.16 in the Appendix A.5).

$\mathrm{POST}_H(P_0,\pi) = (V_m, J_m)$ implies that for each $j \geq 1$, $V_m = V_{m+j}$ and $J_m = J_{m+j}$. (8)

Let us consider part (a) of the theorem. Fix any $v \in V_m$, we must prove that $\pi[v] \in \mathrm{sp}_H(P)$, that is $\phi_{(H,\rho)}(\pi[v]) = 0$ for each $\rho \in \mathbf{V}(P)$. By Corollary 1, our task reduces to showing that, for each τ, $(S_H(\pi[v]_\tau))(\rho) = (S_H\pi_\tau)[v](\rho) = 0$ (here we have used (5)), for each $\rho \in \mathbf{V}(P)$. That is, for each τ, $(S_H\pi_\tau)[v] \in \mathbf{I}(\mathbf{V}(P))$. The latter is implied by $(S_H\pi_\tau)[v] \in I_0 \subseteq \mathbf{I}(\mathbf{V}(P))$. By definition (6), this holds for each τ such that $v \in V_{|\tau|}$. Hence for each τ, as $v \in V_0 \supseteq \cdots \supseteq V_m = V_{m+1} = \cdots$ (by (8)). Assume now that $I_0 = \mathbf{I}(\mathbf{V}(P))$ and consider $v \in \mathbb{R}^s$ such that $\pi[v] \in \mathrm{sp}_H(P)$: we show that $v \in V_m$. Our task is showing that for each τ with $|\tau| \leq m$, $(S_H\pi_\tau)[v] \in \mathbf{I}(\mathbf{V}(P))$. The latter means precisely that $(S_H\pi_\tau)[v](\rho) = 0$ for each $\rho \in \mathbf{V}(P)$. But this holds by definition of $\pi[v] \in \mathrm{sp}_H(P)$

and Corollary 1: indeed, for each τ, $(S_H(\pi[v]_\tau))(\rho) = (S_H\pi_\tau)[v](\rho) = 0$ (here we have used (5)), for each $\rho \in \mathbf{V}(P)$.

Let us consider part (b). First, consider any $\rho \in \mathrm{wp}_H(\pi[V_m])$. By definition and Corollary 1 (and using (5)), this is equivalent to $(S_H\pi_\tau)[v](\rho) = 0$ for each $v \in V_m$ and τ. By definition of ideal J_m, this implies $F(\rho) = 0$ for each $F \in J_m$, that is $\rho \in \mathbf{V}(J_m)$. On the other hand, consider any $\rho \in \mathbf{V}(J_m)$ and any $v \in V_m$. Clearly $\rho \in \mathbb{R}^k$. Then proving that $\rho \in \mathrm{wp}_H(\pi[V_m])$, that is $\phi_{(H,\rho)}(\pi[v]) = 0$, is equivalent, via Corollary 1 (and again (5)), to showing that $(S_H\pi_\tau)[v](\rho) = 0$, for each τ. Consider any such τ: for $k \geq m$ large enough, by definition of J_k and the fact that $V_m = V_k$, we have $J_k \supseteq (S_H\pi_\tau)[V_m]$, hence $J_m = J_k \supseteq (S_H\pi_\tau)[V_m]$ (by (8)), therefore $(S_H\pi_\tau)[v](\rho) = 0$, as required.

The vector spaces V_i s in (6) can be effectively represented by the successive linear constraints imposed by (6) on the template parameters $\mathbf{a} = (a_1, ..., a_s)$. In turn, this permits computing finite sets of generators for the ideals J_i s in (7). This is illustrated with an example below. For a set of linear expressions $L \subseteq \mathrm{Lin}(\mathbf{a})$, we let $\mathrm{span}(L) \stackrel{\triangle}{=} \{v \in \mathbb{R}^s : \ell[v] = 0 \text{ for each } \ell \in L\} \subseteq \mathbb{R}^s$ be the vector space of parameter evaluations that annihilate all expressions in L.

Example 5 (Example 2, cont.). Fix $P = P_0 = \emptyset$, hence $\mathbf{V}(P) = \mathbb{R}$ (here $k = |\{u\}| = 1$ and we impose no constraints on the initial data) and $I_0 = \mathbf{I}(\mathbf{V}(P)) = \{0\}$. We seek for linear relations between u and u_x, considering the template $\pi \stackrel{\triangle}{=} a_1u + a_2u_x$. We compute $\textsc{Post}_H(P_0, \pi) = (V_m, J_m)$ as follows. Below we reuse the equalities for $S_H(\delta_{\Sigma_1}(u, \tau))$ computed in Example 4.

- $(i = 0)$. $S_H\pi = (a_1 - a_2)u$. Therefore $V_0 = \mathrm{span}(\{a_1 - a_2\}) = \{(\lambda, \lambda) : \lambda \in \mathbb{R}\}$ and $J_0 = \{0\}$.
- $(i = 1)$. $S_H\pi_x = S_H(a_1u_x + a_2u_{xx}) = (a_2 - a_1)u$ and $S_H\pi_t = S_H(a_1u_{xx} + a_2u_{x^3}) = (a_1 - a_2)u$. Therefore $V_1 = \mathrm{span}(\{a_2 - a_1, a_1 - a_2\}) = V_0$ and similarly $J_1 = J_0$.

Hence the algorithm stabilizes already at $m = 0$, returning $V_0 = \{(\lambda, \lambda) : \lambda \in \mathbb{R}\}$ and $J_0 = \{0\}$. This means that the valid instances of π are of the form $\lambda(u + u_x)$, for all $\lambda \in \mathbb{R}$. Or, equivalently, that $u_x = -u$ is a valid equation, under any initial data specification.

Suppose $\textsc{Post}_H(P_0, \pi) = (V_m, J_m)$. Given a parameter evaluation $v \in \mathbb{R}^s$, checking if $\pi[v] \in \pi[V_m]$ is equivalent to checking if $v \in V_m$: this can be effectively done knowing a basis B_m of the vector space V_m. In practice, it is more convenient to succinctly represent the whole set $\pi[V_m]$ returned by $\textsc{Post}_H$ in terms of a new *result template* π' with $s' \leq s$ parameters, such that $\pi'[\mathbb{R}^{s'}] = \pi[V_m]$. In the example above, $\pi' = a_1(u + u_x)$. The result template π' can in fact be computed directly from π, by propagating, via substitutions, the linear constraints on $\mathbf{a}$ arising from (6) as they are generated (further details in Appendix A.6).

5 Examples

We have put a proof-of-concept implementation of the $\textsc{Post}$ algorithm of Section 4 at work on some IVPs drawn from mathematical physics. We illustrate two cases below[6].

[6] Additional examples, concerning boundary problems and conservation laws, are reported in Appendix A.7. Code and examples are available at `https://github.com/micheleatunifi/`

Burgers' equation We consider the inviscid case of the Burgers' equation [1,7], with a linear initial condition at $t = 0$ (for b, c arbitrary real constants).

$$u_t = -u \cdot u_x \qquad\qquad u(0,x) = bx + c\,.$$

We fix $X = \{t,x\}$ and $U = \{u,b,c\}$. The above IVP is encoded by the stratified system $H = \{\Gamma_1, \Gamma_2\}$, where

$$\Gamma_1 = (\{u_t = -uu_x\} \cup \Sigma_{aux1},\ \{t,x\}) \qquad \Gamma_2 = (\{u_x = b\} \cup \Sigma_{aux2},\ \{x\})\,.$$

$\Sigma_{aux1} = \{b_t = 0, c_t = 0, c_x = 0\}$ and $\Sigma_{aux2} = \{b_x = 0\}$ just encode that b, c are constants. As $\mathcal{P}\mathrm{a}(H) = \{u,b,c\}$, the system is FP. Moreover, H, with the lexicographic order induced by $u > b > c$ and $t > x$, is coherent. We fix the set of possible initial data specifications to $\mathbf{V}(P)$ where $P = \{u - c\}$: this just ensures that $u(0,0) = c$. In order to discover interesting postconditions of P, we consider a complete polynomial template of total degree 3 over the indeterminates $Z \stackrel{\triangle}{=} \{t,x\} \cup \mathcal{P}\mathrm{a}(H)$, $\pi = \sum_{\gamma_i \in Z^{\otimes}, |\gamma_i| \le 3} a_i \gamma_i$, which consists of $s = 56$ terms. Letting $P_0 = P$, we run $\textsc{Post}_H(P, \pi)$, which halts at the iteration $m = 5$, returning (V_5, J_5). This took about 6s in our experiment. The algorithm returns V_5 in the form of a 1-parameter result template π', such that $\pi'[\mathbb{R}] = \pi[V_5]$: the set of all instances of π' forms a valid postcondition of P. In this case Theorem 3(a) implies that $\pi'[\mathbb{R}] = \mathrm{sp}_H(P) \cap \pi[\mathbb{R}^s]$. Specifically, we find, for a_1 a template parameter:

$$\pi' = a_1 \cdot (ctu + u - b - cx)\,.$$

In other words, up to the multiplicative constant a_1, $ctu + u = b + cx$ is the only equation of degree ≤ 3 satisfied by the solutions of H, for initial data specifications $\rho \in \mathbf{V}(P)$. This equation can be easily solved algebraically for u — note that we are actually manipulating CFPSs— and yields the unique solution of the IVP:

$$u = \frac{cx + b}{ct + 1}\ .$$

Conservation laws Conservation laws may provide important qualitative insights about a system and are also crucial in applications. The following definition of conservation laws is standard and rephrased from [18, Ch.4,Sect.3] in our notation. Given a stratified system H, a (polynomial) *conservation law* for H is a n-tuple $\mathbf{C} = (C_1, \ldots, C_n) \in \mathcal{P}^n$ whose divergence

$$\nabla \mathbf{C} \stackrel{\triangle}{=} D_{x_1} C_1 + \cdots + D_{x_n} C_n \tag{9}$$

becomes identically 0 after plugging into it any solution of H: formally, $\nabla \mathbf{C} \in \mathrm{sp}_H(\emptyset)$. This can be generalized to $\nabla \mathbf{C} \in \mathrm{sp}_H(P)$, for any given $P \subseteq \mathcal{P}_0(H)$ defining a set of initial data specifications. The literature on conservation laws typically confines to the the special case with no initial conditions, that is $H = \{(\Sigma, X)\}$ and $P = \emptyset$. Here we will call such laws *pure* for Σ. In this context, when $n = 1$ and $X = \{t\}$, $\nabla \mathbf{C} = 0$ expresses a first integral of motion of the system. For $n = 2$ and $X = \{t,x\}$, $\Psi \stackrel{\triangle}{=} C_1$ is called a *density* and $\Phi \stackrel{\triangle}{=} C_2$ is called a *flux*, and $\nabla \mathbf{C} = 0$ becomes $D_t \Psi = -D_x \Phi$. When any analytic solution $u(t,x)$ of the IVP is plugged into Ψ and Φ, it is seen that for any

`PDEPY/blob/master/PDE.py`. Execution times reported here are for a Python Anaconda distribution running under Windows 10 on a Surface Pro laptop.

interval $[a,b]$

$$\frac{d}{dt}\int_a^b \Psi\, dx = \Phi_{|x=a} - \Phi_{|x=b}$$

(see [18, Ch.4,Prop.4.20]). In other words, the spatial integral of the density — think of this as a mass — varies over time only depending on the flux at the boundaries of the domain. If the interval $[a,b]$ can be chosen in such a way that the neat flux is zero, $\Phi_{|x=a} = \Phi_{|x=b}$, which is often the case in applications, then there is no variation at all, that is $\int_a^b \Psi\, dx$ is a conserved quantity of the system.

Since an equation $\nabla \mathbf{C} = 0$ is a particular postcondition of the system, in principle we can apply POST to the systematic search of polynomial conservation laws for a given IVP. We demonstrate this application on the following IVP for the wave equation in one spatial dimension:

$$u_{tt} = u_{xx} \qquad u_t(0,x) = 0 \qquad u(0,x) = A\sin(x) + B\cos(x) \tag{10}$$

for arbitrary real constants A, B. More specifically, the one above is a Cauchy problem. This problem is coded up as an FP, coherent stratified system $H = \{(\Sigma_1, \{t,x\}), (\Sigma_2, \{x\})\}$, where the auxiliary variables v, w represent generic sinusoids $A\sin(x) + B\cos(x)$ and $A\cos(x) + B\sin(x)$, respectively:

$$\Sigma_1 = \{u_{tt} = u_{xx}, v_t = 0, w_t = 0\} \qquad \Sigma_2 = \{u_t = 0, u_x = w, v_x = -w, w_x = v\}.$$

For this example we fix, somewhat arbitrarily, the subset $T = \{t, x, u, u_t, u_x, v\} \subseteq \mathcal{D}$, and look for all polynomial conservation laws of degree ≤ 2 that can be built out of T. To this end, we first build π_1 and π_2, two complete polynomial templates of degree 2 with indeterminates in T, based on two disjoint sets of template parameters. Then let $\pi \stackrel{\triangle}{=} D_t\pi_1 + D_x\pi_2$ represent a template for divergences. As there are no constraints on the initial data ($P = \emptyset$), we run $\text{POST}_H(\emptyset, \pi)$, obtaining an output (V, J), after 7 iterations and about 13s. By theorem Theorem 3(a), $\pi[V] \subseteq \text{sp}_H(\emptyset)$, and since $\pi[V] = (D_t\pi_1 + D_x\pi_2)[V] = D_t(\pi_1[V]) + D_x(\pi_2[V]) = \{D_t\pi_1[v] + D_x\pi_2[v] : v \in V\}$, we have found the set of all polynomial conservation laws of H of the desired type. From V and π_1, π_2, we can also recover explicitly the vector space of conserved density-flux pairs (Ψ, Φ):

$$(\pi_1, \pi_2)[V] \stackrel{\triangle}{=} \{(\pi_1[v], \pi_2[v]) : v \in V\}.$$

A basis for $(\pi_1, \pi_2)[V]$ can be easily built out of the result template returned by POST. Below we report the density-flux pairs of just two nontrivial conservation laws in the basis we computed[7].

$$\Psi_1 = \tfrac{1}{2}u_x^2 + \tfrac{1}{2}u_t^2\,,\ \Phi_1 = -u_x u_t \qquad \Psi_2 = u_x u_t\,,\ \Phi_2 = -u_x^2 + v^2/2\,.$$

The spatial integral of Ψ_1 has the meaning of total energy (potential + kinetic), that of Ψ_2 of wave linear momentum — cf. [18, Ch.4,Ex.4.36]. Importantly, the found conservation laws, $(\pi_1, \pi_2)[V]$, are not necessarily valid for different IVPs of the wave equation. In particular, while $(\pi_1, \pi_2)[V]$ includes *all* pure conservation laws of the considered type, this inclusion is in general strict. For instance, only the leftmost law above is pure for the wave equation. Indeed, if we change the first initial condition in (10) to

[7] Full list in Appendix A.7.

e.g. $u_t(0,x) = C\exp(-x^2)$ (C arbitrary constant), and repeat the experiment, we end up with a different set of laws, not including the rightmost law above.

6 Conclusion and related work

We have put forward a framework for equational reasoning on PDE IVPs, based on simple algebra and coalgebra. In particular, we have obtained an algorithm to compute pre- and postconditions of such problems, which is complete relatively to a given template. To the best of our knowledge, no such completeness result for equational reasoning on PDE IVPs exists in the literature.

The present paper is broadly related to recent and ongoing work in the field of formal tools for ODEs, such us the theory of differential equivalences by Cardelli et al., see [8] and references therein. More specifically, our development here conceptually parallels and extends our previous work on polynomial ODEs, in particular [2,3]. The POST algorithm has a similar structure to the algorithm by the same name in [3]. Technically, though, the case of PDEs is remarkably more challenging, for the following reasons. (a) In PDEs, both the existence of solutions and the transition structure itself depend on coherence. In ODEs, (analytic) solutions always exist in the polynomial case, coherence is trivial and the resulting transition structure is quite simple. (b) In PDE IVPs and the related stratified systems, a prominent role is played by the acyclicity of their structure, which is again trivial in ODEs. (c) In PDEs, differential polynomials live in the infinite-indeterminates space $\mathcal{P}$, which requires reduction to $\mathcal{P}_0(H)$ via S_H, and, for the POST algorithm, a finiteness assumption on parametric derivatives; in ODEs, $\mathcal{P} = \mathcal{P}_0(\Sigma)$ has always finitely many indeterminates.

Our work is related to the field of Differential Algebra (DA), see [6,17,23,21,26] and references therein. In particular, Boulier et al.'s RosenfeldGröbner algorithm [6], computes the ideal of the differential and polynomial consequences of a system Σ. This ideal, for pure systems and no constraints on the initial data, is related to our strongest postcondition; however, how to encode general IVPs, pre- and postconditions in their format is far from trivial, if possible at all. More generally, while DA techniques can be used to reduce systems to a coherent form, which is required by our approach, they do not seem to be concerned with IVPs or boundary problems as such. The only exceptions we are aware of are [24,25], which focus on linear ODEs.

In the present framework, we can only reason about *classical (analytic)* solutions of PDEs and their IVPs. In practice, *weak* solutions [12, Ch.1], admitting discontinuities representing e.g. shock waves, are often considered in applications. While an extension of our framework to weak solutions is desirable, it is unclear at the present stage if it is feasible at all. We leave this as a matter for future reflections.

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A Proofs and additional technical material

A.1 Operations on formal power series

Let $f,g \in \mathbb{R}[\![X]\!]$, the set of CFPS with indeterminates in X and real coefficients. For each $\xi = \mathbf{x}^{\boldsymbol{\alpha}}$ and $\tau = \mathbf{x}^{\boldsymbol{\beta}}$ with $\xi \leq \tau$, we let τ/ξ denote the monomial $\mathbf{x}^{(\beta_1-\alpha_1,\ldots,\beta_n-\alpha_n)}$. We have the following definitions of sum and product. For each $\tau \in X^{\otimes}$:

$$(f+g)(\tau) \stackrel{\triangle}{=} f(\tau)+g(\tau) \qquad\qquad (f\cdot g)(\tau) \stackrel{\triangle}{=} \sum_{\xi\leq\tau} f(\xi)\cdot g(\tau/\xi)\,. \tag{11}$$

These operations correspond to the usual sum and product of functions, when (convergent) CFPSs are interpreted as analytic functions. These operations enjoy associativity, commutativity and distributivity, which make $\mathbb{R}[\![X]\!]$ a ring. Moreover, if $f(\varepsilon) \neq 0$ there exists a unique CFPS $f^{-1} \in \mathbb{R}[\![X]\!]$ that is a multiplicative inverse of f, that is $f\cdot f^{-1} = 1$.

The partial derivative of f along $x_i \in X$, $\frac{\partial f}{\partial x_i}$, is defined as as follows, for each $\tau = \mathbf{x}^{(\alpha_1,\ldots,\alpha_n)} \in X^{\otimes}$:

$$\frac{\partial f}{\partial x_i}(\tau) \stackrel{\triangle}{=} (\alpha_i+1) f(x_i\tau)\,. \tag{12}$$

Finally, the following familiar rules of differentiation are satisfied:

$$\frac{\partial(f+g)}{\partial x} = \frac{\partial f}{\partial x} + \frac{\partial g}{\partial x} \qquad\qquad \frac{\partial(f\cdot g)}{\partial x} = \frac{\partial f}{\partial x}\cdot g + f\cdot\frac{\partial g}{\partial x}\,. \tag{13}$$

A.2 Proofs of Section 2

We give here a self-contained proof of Theorem 1. This result is reproduced from [5]. The proof is based on simple coalgebraic concepts, which are recalled below.

Commutative coalgebras Let X be a finite set of *actions* (or *variables*), ranged over by $x,y,\ldots$ and O a nonempty set. We recall that a *(Moore) coalgebra*[8] with actions in X and outputs in O is a triple $C = (\mathcal{S},\delta,o)$ where: $\mathcal{S}$ is a set of *states*, $\delta : \mathcal{S}\times X \to \mathcal{S}$ is a *transition* function, and $o : \mathcal{S} \to O$ is an *output* function (see e.g. [27]). A *bisimulation* in C is a binary relation $R \subseteq \mathcal{S}\times\mathcal{S}$ such that whenever $s\,R\,t$ then: (a) $o(s) = o(t)$, and (b) for each x, $\delta(s,x)\,R\,\delta(t,x)$. It is an (easy) consequence of the general theory of bisimulation that a largest bisimulation over C, called bisimilarity and denoted by $\sim_C$, exists, is the union of all bisimulation relations, and is an equivalence relation over $\mathcal{S}$. Given two coalgebras with actions in X and outputs in O, C_1 and C_2, a *morphism* from C_1 to C_2 is a function $\mu : \mathcal{S}_1 \to \mathcal{S}_2$ that: (1) preserves outputs ($o_1(s) = o_2(\mu(s))$, and (2) preserves transitions ($\mu(\delta_1(s,x)) = \delta_2(\mu(s),x)$), for each state s and action x). It is an easy consequence of this definition that a morphism preserves bisimulation in both directions, that is: $s \sim_{C_1} t$ if and only if $\mu(s) \sim_{C_2} \mu(t)$.

We introduce now the subclass of Moore coalgebras we will focus on. We say a coalgebra C has *commutative actions* (or just that is *commutative*) if for each state s and actions x,y, it holds that $\delta(\delta(s,x),y) \sim_C \delta(\delta(s,y),x)$. We will introduce below an example of commutative coalgebra. In what follows, we let σ range over X^*, and, for any state s, let $s(\sigma)$ be defined inductively as: $s(\varepsilon) \stackrel{\triangle}{=} s$ and $s(x\sigma) \stackrel{\triangle}{=} \delta(s,x)(\sigma)$.

[8] In the paper, we only consider Moore coalgebras. For brevity, we shall omit the qualification "Moore".

Lemma A.1. *Let C be a commutative coalgebra. If $\sigma, \sigma' \in X^*$ are permutation of one another then for any state $s \in S$, $s(\sigma) \sim_C s(\sigma')$.*

We define the coalgebra of CFPSs, C_F

$$C_{\mathrm{F}} \stackrel{\triangle}{=} (\mathbb{R}[\![X]\!], \delta_{\mathrm{F}}, o_{\mathrm{F}})$$

where $\delta_{\mathrm{F}}(f,x) = \frac{\partial f}{\partial x}$ and $o_{\mathrm{F}}(f) = f(\varepsilon)$ (the constant term of f). Bisimilarity in C_{F}, denoted by $\sim_{\mathrm{F}}$, coincides with equality. It is easily seen that for each x, y, $\frac{\partial}{\partial y}\frac{\partial f}{\partial x} = \frac{\partial}{\partial x}\frac{\partial f}{\partial y}$, so that C_{F} is a commutative coalgebra. Now fix any commutative coalgebra $C = (S, \delta, o)$. We define the function $\mu : S \to \mathbb{R}[\![X]\!]$ as follows. For each $\tau = \mathbf{x}^{\boldsymbol{\alpha}}$

$$\mu(s)(\tau) \stackrel{\triangle}{=} \frac{o(s(\tau))}{\boldsymbol{\alpha}!} \tag{14}$$

where $\boldsymbol{\alpha}! \stackrel{\triangle}{=} \alpha_1! \cdots \alpha_n!$. Here, abusing slightly notation, we let $o(s(\tau))$ denote $o(s(\sigma))$, for some string σ obtained by arbitrarily ordering the elements in τ: the specific order does not matter, in view of Lemma A.1 and of condition (a) in the definition of bisimulation.

Lemma A.2. *Let C be a commutative coalgebra and $f = \mu(s)$. For each x, $\frac{\partial f}{\partial x} = \mu(\delta(s,x))$.*

Proof. Let $x = x_i$. For each $\tau = \mathbf{x}^{\boldsymbol{\alpha}}$ in $X^{\otimes}$ we have

$$\begin{aligned}
\frac{\partial f}{\partial x_i}(\tau) &= (\alpha_i + 1) f(x_i \tau) \\
&= (\alpha_i + 1) \frac{o\left(s(x_i \tau)\right)}{\boldsymbol{\alpha}!(\alpha_i + 1)} \\
&= \frac{o\left(\delta(s, x_i)(\tau)\right)}{\boldsymbol{\alpha}!} \\
&= \mu\left(\delta(s, x_i)\right)(\tau)
\end{aligned}$$

where the first and second equality follow from (12) and (14), respectively, and the third one from the definition of $s(x_i\tau)$. This proves the wanted statement.

Based on the above lemma and the fact that $\sim_{\mathrm{F}}$ is equality, we can prove the following corollary, saying that C_{F} is *final* in the class of *commutative* coalgebras.

Corollary A.1 (coinduction and finality of C_{F}). *Let C be a commutative coalgebra. The function μ in* (14) *is the unique coalgebra morphism from C to C_{F}. Moreover, the following* coinduction *principle is valid: $s \sim_C t$ if and only if $\mu(s) = \mu(t)$ in $\mathbb{R}[\![X]\!]$.*

Proof. We have: (1) $o(s) = \mu(s)(\varepsilon)$ by definition of μ, and (2) $\mu(\delta(s,x)) = \delta_{\mathrm{F}}(\mu(s),x)$, by Lemma A.2. This proves that μ is a coalgebra morphism. Next, we prove that $\sim_{\mathrm{F}}$ coincides with equality in $\mathbb{R}[\![X]\!]$. More precisely, we prove that for each τ and for each f,g: $f \sim_{\mathrm{F}} g$ implies $f(\tau) = g(\tau)$. Proceeding by induction on the length of τ, we see that the base case is trivial, while for the induction step $\tau = x_i\tau'$ we have: $f \sim_{\mathrm{F}} g$ implies $\frac{\partial f}{\partial x_i} \sim_{\mathrm{F}} \frac{\partial g}{\partial x_i}$ (bisimilarity), which in turn implies $\frac{\partial f}{\partial x_i}(\tau') = \frac{\partial g}{\partial x_i}(\tau')$ (induction hypothesis);

but by (12), $f(x_i\tau') = (\frac{\partial f}{\partial x_i}(\tau'))/(\alpha_i+1)$ and $g(x_i\tau') = (\frac{\partial g}{\partial x_i}(\tau'))/(\alpha_i+1)$, and this completes the induction step. From the coincidence of $\sim_{\mathrm{F}}$ with equality in $\mathbb{R}[\![X]\!]$, and the fact that any morphism preserves bisimilarity in both directions, the last part of the statement (coinduction) follows immediately. Finally, let ν be any morphism from C to C_{F}. From the definitions of bisimulation and morphism it is easy to see that for each s, $\mu(s) \sim_{\mathrm{F}} \nu(s)$: this implies $\mu(s) = \nu(s)$ by coinduction, and proves uniqueness of μ.

Proof of Theorem 1 In what follows, we fix a coherent, finite Σ. We will first develop an algebraic characterization of $S_\Sigma(\cdot)$. As we will see shortly, this amounts to showing that $\to_\Sigma^*$ corresponds to taking the remainder of multivariate polynomial division by a suitable Gröbner basis derived from Σ.

To this purpose, it is convenient to identify equations $u_\tau = F$ with polynomials $u_\tau - F$, so that Σ and Σ^∞ can be regarded as sets of polynomials, rather than of equations. We define now a concept of saturation of a set of equations w.r.t. a set of derivatives. Consider any finite set $\Sigma' \subseteq \Sigma^\infty$. Define

$$\mathrm{Sat}(\Sigma') \stackrel{\triangle}{=} \{u_\tau - F \in \Sigma^\infty : u_\tau \text{ occurs in } \Sigma'\} \tag{15}$$

and the sequence of finite sets $\mathrm{Sat}^0(\Sigma') \subseteq \mathrm{Sat}^1(\Sigma') \subseteq \cdots$, where: $\mathrm{Sat}^0(\Sigma') \stackrel{\triangle}{=} \Sigma'$ and $\mathrm{Sat}^{i+1}(\Sigma') \stackrel{\triangle}{=} \mathrm{Sat}(\mathrm{Sat}^i(\Sigma'))$. This chain must converge in finitely many steps, that is, there is $k \geq 0$ s.t. $\mathrm{Sat}^{k+j}(\Sigma') = \mathrm{Sat}^k(\Sigma')$ for each $j \geq 0$. If not, one could exploit the normality of Σ to find a descending sequence of derivatives: $u^0_{\tau_0} \succ u^1_{\tau_1} \succ \cdots$, where $u^i_{\tau_i} \stackrel{\triangle}{=} \max\left(\mathrm{dom}(\mathrm{Sat}^{i+1}(\Sigma')) \setminus \mathrm{dom}(\mathrm{Sat}^i(\Sigma'))\right)$, which is impossible. Now, fix any finite set of derivatives $D \subseteq \mathcal{D}$ and let $\Sigma' = \{u_\tau - F \in \Sigma^\infty : u_\tau \text{ occurs in } \Sigma \text{ or } D\}$ in the above construction: we will denote the resulting limit set $\mathrm{Sat}^k(\Sigma')$ as Σ^D, and call it the *saturation of* Σ *w.r.t. to* D. We note that, by construction: (a) Σ^D is finite, (b) $\Sigma^\infty \supseteq \Sigma^D \supseteq \Sigma$, and (c) the set of principal derivatives occurring in Σ^D coincides with $\mathrm{dom}(\Sigma^D)$. Now let D' be the set of all (parametric and principal) derivatives occurring in Σ^D, we let $\mathcal{P}_D(\Sigma) \stackrel{\triangle}{=} \mathbb{R}[X \cup D']$.

Next, we review a few basic notions from algebraic geometry. For a detailed treatment, see [11, Ch.2,3]. Let $\mathcal{R} = \mathbb{R}[Z]$, for any finite set Z of indeterminates. A set $J \subseteq \mathcal{R}$ is an *ideal* if $0 \in J$, J is closed under addition, and for any $E \in J$ and and $F \in \mathcal{R}$, we have $E \cdot F \in J$. For $P \subseteq \mathcal{R}$, we let $\left\langle\, P \,\right\rangle \stackrel{\triangle}{=} \{\sum_{i=1}^m F_i \cdot E_i : m \geq 0, F_i \in \mathcal{P}_D, E_i \in P\}$ denote the smallest ideal in $\mathcal{R}$ which includes P. A *monomial order* $\prec$ is a total order of the monomials in $Z^\otimes$ that is a well-order, that is has no infinite descending chains. Seeing a polynomial E as a linear combination of monomials, its *leading term* $\mathrm{LT}(E) = \lambda\gamma$ ($0 \neq \lambda \in \mathbb{R}$) is the term whose monomial γ is highest in the given monomial order; $\mathrm{LM}(E) = \gamma$ is the corresponding *leading monomial*. A *multivariate division* of a polynomial F by a finite set of polynomials B is defined as follows.

- One step reduction: $F \xrightarrow{\eta,H} G$ iff $H \in B$ and for some term $\lambda\gamma$ of F: $\eta = \frac{\lambda\gamma}{\mathrm{LT}(H)}$ and $G = F - \eta H$.
- Multivariate division of F by B: a sequence $F = F_0 \xrightarrow{\eta_1,H_1} F_1 \xrightarrow{\eta_2,H_2} \cdots \xrightarrow{\eta_k,H_k} F_k$ such that no monomial in the last term F_k is divisible by any leading term in B.

The last term F_k is called a *remainder* of the division. Clearly, one has $F = \sum_{i=1}^{k} \eta_i H_i + F_k$. In general, there may be different division sequences, and remainders are not unique. A *Gröbner basis* for J w.r.t. to a given monomial order is a finite set of polynomials B such that $J = \langle B \rangle$ and the leading monomial of every element in J is divisible by the leading monomial of some element in B. Equivalently, $J = \langle B \rangle$ and the reminder of the multivariate division of every polynomial in $\mathcal{R}$ by B is unique. As a consequence, for every polynomial $E \in \mathcal{R}$ there are unique polynomials E_0 and E_r such that $E = E_0 + E_r$, $E_0 \in J$ and E_r is a remainder of the multinomial division of E by the Gröbner basis B; in particular, no monomial in E_r is divisible by the leading term of any polynomial in B. The unique remainder E_r is denoted by $E \bmod B$.

Lemma A.3. *Let Σ be finite and coherent. Let D be a finite set of derivatives that includes those occurring in Σ. For a suitable monomial order, Σ^D is a Gröbner basis of $\langle \Sigma^D \rangle$ in $\mathcal{P}_D(\Sigma)$. Moreover, for each $F \in \mathcal{P}_D(\Sigma)$, we have $SF = F \bmod \Sigma^D$.*

Proof. Over $(X \cup D)^{\otimes}$, consider the lexicographic monomial order [11, Ch.2] $\prec$ induced by the ranking over D inherited from $\mathcal{D}$, extended by the rules: $x_1 \prec \cdots \prec x_n \prec u_\tau$ for all derivatives $u_\tau \in D$. Clearly Σ^D generates $\langle \Sigma^D \rangle$. We now prove that the multivariate division of any $F \in \mathcal{P}_D(\Sigma)$ by Σ^D gives a unique remainder: this will be sufficient to prove Σ^D is a Gröbner basis. Consider any multivariate division sequence of F by Σ^D, say $F = F_0 \xrightarrow{\eta_1, H_1} F_1 \xrightarrow{\eta_2, H_2} \cdots \xrightarrow{\eta_k, H_k} F_k$, with F_k a remainder. Note that for each $i = 0, \dots, k$, $F_i \in \mathcal{P}_D(\Sigma)$. By definition of remainder, no monomial in F_k is divisible by any leading term in Σ^D. As the set of leading terms of Σ^D is $\mathrm{dom}(\Sigma^D)$, no principal derivative occurs in F_k, that is F_k is a Σ-normal form. Now, it is immediate to check that a one-step reduction is equivalent to a rewrite step of $\to_\Sigma$, that is: $A \to_\Sigma B$ iff[9] there are $\eta, H \in \Sigma^D$ s.t. $A \xrightarrow{\eta, H} B$. As a consequence, the whole division sequence above implies a sequence of rewrites: $F = F_0 \to_\Sigma F_1 \to_\Sigma \cdots \to_\Sigma F_k$. Hence any remainder of a multivariate division of F by Σ^D is a Σ-normal form, $=_\Sigma$-equivalent to F. By consistency of Σ, this normal form is unique: we conclude that the remainder of the division by Σ^D is unique. This completes the prove that Σ^D is a Gröbner basis in $\mathcal{P}_D(\Sigma)$. The same reasoning also shows that SF equals $F \bmod \Sigma^D$.

We also need a distributivity property of $S(\cdot)$ over sum and product of polynomials.

Lemma A.4. *Let Σ be finite and coherent. For any $E, F \in \mathcal{P}$, $S(E+F) = SE + SF$ and $S(E \cdot F) = (SE) \cdot (SF)$.*

Proof. An easy consequence of Lemma A.3. We check the case of product, as the sum is easier. Let D be the set of derivatives occurring in Σ, E, F. By Lemma A.3, we have $E = E_0 + SE$ and $F = F_0 + SF$, for $E_0, F_0 \in \langle \Sigma^D \rangle$, from which we get $E \cdot F = (E_0 F_0 + E_0 SF + F_0 SE) + (SE)(SF) = G_0 + (SE)(SF)$. Note that: (a) $G_0 \in \langle \Sigma^D \rangle$, and (b) $(SE) \cdot (SF)$ is a Σ-normal form, in particular no monomial in it is divisible by the leading terms in Σ^D. By the property of Gröbner bases, this means that $(E \cdot F) \bmod \Sigma^D = (SE) \cdot (SF)$, that is $S(E \cdot F) = (SE) \cdot (SF)$.

[9] Explicitly, $A \xrightarrow{\eta, H} B$ is equivalent to $H = u_\tau - F$, $A = \eta \cdot u_\tau + A'$ and $B = A' + \eta \cdot F$, for some u_τ, F, A'. This is equivalent to $A \to_\Sigma B$.

Lemma A.5. *Let Σ be finite and coherent. For each $x \in X$ and $F \in \mathcal{P}$, $SD_xSF = SD_xF$.*

Proof. This is an application of Lemma A.3 and Lemma A.4. Take a finite D containing all the derivatives in Σ and F. As $F = F_0 + SF$, for $F_0 \in \langle\, \Sigma^D \,\rangle$, by distributivity over sum of $S(\cdot)$ and D_x, we have: $SD_xF = SD_x(F_0 + SF) = SD_xF_0 + SD_xSF$. It will suffice now to check that $SD_xF_0 = 0$. By definition $F_0 = \sum_{u,j} H_{u,j}(u_{\tau_j} - F_j)$, for $H_{u,j} \in \mathcal{P}_D(\Sigma)$ and $u_{\tau_j} - F_j \in \Sigma^D$. Using the distributivity of $S(\cdot)$ and the properties of total derivative D_x, we have $SD_xF_0 = \sum_{u,j} S(D_xH_{u,j})S(u_{\tau_j} - F_j) + S(H_{u,j})S(u_{x\tau_j} - D_xF_j)$. Each summand here is 0, indeed both $u_{\tau_j} - F_j =_\Sigma 0$ and $u_{x\tau_j} - D_xF_j =_\Sigma 0$, as both equations are in Σ^∞.

Next, a result about solutions.

Lemma A.6. *Let Σ be finite and coherent. Let* $\mathbf{iP} = (\Sigma, \rho)$ *and let ψ be a solution of* $\mathbf{iP}$. *For each $E, F \in \mathcal{P}$, $E =_\Sigma F$ implies $\psi(E) = \psi(F)$.*

Proof. By Lemma A.3, for each E, $E = E_0 + SE$, with $E_0 \in \langle\, \Sigma^D \,\rangle$, for a suitable D. As ψ is by definition a homomorphism and a solution, $\psi(E_0) = 0$ and $\psi(E) = \psi(E_0 + SE) = \psi(E_0) + \psi(SE) = \psi(SE)$. Moreover, $E =_\Sigma F$ means $SE = SF$, which is enough to conclude.

With any coherent (w.r.t. some ranking) Σ and initial data specification ρ, $\mathbf{iP} = (\Sigma, \rho)$, we can now associate a coalgebra as follows.

$$C_{\mathbf{iP}} \stackrel{\triangle}{=} (\mathcal{P}, \delta_\Sigma, o_\rho)$$

where δ_Σ is defined in (1) and $o_\rho(E) \stackrel{\triangle}{=} \rho(SE)$. We will denote by $\sim_{\mathbf{iP}}$ bisimilarity in $C_{\mathbf{iP}}$. As a consequence of Lemma A.5, $\delta_\Sigma(\delta_\Sigma(E,x),y) = \delta_\Sigma(\delta_\Sigma(E,y),x)$, so that for any monomial τ, the notation $\delta_\Sigma(E,\tau)$ is well defined. As an example of transition, for the heat equation $\Sigma = \{u_{xx} = au_t\}$, one has $\delta_\Sigma(u_{xx}, t) = au_{tt}$.

As expected, $C_{\mathbf{iP}}$ is a commutative coalgebra. Moreover, each expression is bisimilar to its normal form. This is the content of the following lemma.

Lemma A.7. *Let* $\mathbf{iP} = (\Sigma, \rho)$*, with Σ finite and coherent. Then: (1) $C_{\mathbf{iP}}$ is commutative; and (2) For each $E \in \mathcal{P}$, $E \sim_{\mathbf{iP}} SE$.*

Proof. For what concerns part 1, for each x, y and F, we have

$$\begin{aligned} \delta_\Sigma(\delta_\Sigma(F,x),y) &= SD_xSD_yF \\ &= SD_xD_yF \\ &= SD_yD_xF \\ &= SD_ySD_xF \\ &= \delta_\Sigma(\delta_\Sigma(F,y),x) \end{aligned} \tag{16}$$

where the second equality and fourth follow from Lemma A.5, and the third one is a property of total derivatives.

For what concerns part 2, it is sufficient to show that the relation $R = \{(E, SE) : E \in \mathcal{P}\} \cup Id$, where Id is the identity relation, is a bisimulation. Condition (a) of the definition holds trivially; concerning condition (b), for any x we have that $\delta_\Sigma(E,x) = SD_xE = SD_xSE = \delta_\Sigma(SE,x)$, where the second equality follows again from Lemma A.5.

As a consequence of the previous lemma, part 1, and of Corollary A.1, there exists a unique morphism from $C_{\mathbf{iP}}$ to C_{F}. This morphism is the unique solution of **iP** we are after. We need a lemma, saying that the unique coalgebra morphism ϕ from $C_{\mathbf{iP}}$ to C_{F} is compositional.

Lemma A.8. *Let* $\mathbf{iP} = (\Sigma, \rho)$*, with* Σ *finite and coherent, and let* $\phi_{\mathbf{iP}}$ *be the unique coalgebra morphism from* $C_{\mathbf{iP}}$ *to* C_{F}*. Then* $\phi_{\mathbf{iP}}$ *is a homomorphism over* $\mathcal{P}$*.*

Proof. In this proof we write $\phi_{\mathbf{iP}}$ as ϕ. We have to prove that ϕ preserves the i-th identities $x_i \in X$, partial derivatives, as well as $+$, $\times$ along with their identities, on polynomials. The proof is based on standard coalgebraic techniques. This may involve exhibiting a relation $R \subseteq \mathbb{R}[\![X]\!] \times \mathbb{R}[\![X]\!]$ that is a bisimulation and contains the wanted pair(s), so that the result follows by coinduction (Corollary A.1).

- Identity $x_i \in X$. The relation $R \stackrel{\triangle}{=} \{\, (\phi(x_i), x_i)\, , (1,1)\, , (0,0)\,\}$ is a bisimulation, thus proving that $\phi(x_i) = x_i$.
- Derivative $D_x E$. By Lemma A.6, $\phi(D_x E) = \phi(SD_x E) = \phi(\delta_\Sigma(E,x)) = (\partial/\partial x)\phi(E)$, where the last step follows by definition of coalgebra morphism.
- Sum $+$. Let $R \stackrel{\triangle}{=} \{\, (\phi(F+G)\, , \phi(F)+\phi(G))\, :\, F,G \in \mathcal{P}\,\}$. It can be checked that R is a bisimulation. Clause (a) of the definition of bisimulation requires invoking the definition of morphism and the distributivity of $S(\cdot)$ (Lemma A.4): $\phi(F+G)(\varepsilon) = o_\rho(F+G) = \rho(S(F+G)) = \rho(SF) + \rho(SG) = o_\rho(F) + o_\rho(G) = \phi(F)(\varepsilon) + \phi(G)(\varepsilon)$. Clause (b) of the definition requires using again Lemma A.6.
- Product $\times$. Let us first introduce the technique of bisimulation up to, see e.g. [27]. For any relation $R \subseteq \mathbb{R}[\![X]\!] \times \mathbb{R}[\![X]\!]$, define its $+$-closure $R_+ \subseteq \mathbb{R}[\![X]\!] \times \mathbb{R}[\![X]\!]$ as

  $$R_+ \stackrel{\triangle}{=} \left\{ \left(\sum_{i \in I} f_i, \sum_{i \in I} g_i \right) : I \text{ is a finite set of indices and } (f_i, g_i) \in R \text{ for each } i \in I \right\}.$$

  One says R is a *bisimulation up to* $+$ if whenever $(f,g) \in R$ then: (a) $f(\varepsilon) = g(\varepsilon)$ and (b) for each $x \in X$, $((\partial/\partial x)f\, , (\partial/\partial x)g) \in R_+$. One proves that if R is a bisimulation up to $+$ then $R \subseteq \sim_{\mathrm{F}}$, the largest bisimilarity in $\mathbb{R}[\![X]\!]$ (which coincides with equality). To see this, one simply checks that R_+, which includes R, is a bisimulation: this is almost immediate (of course one exploits here the associativity of $+$ on $\mathbb{R}[\![X]\!]$).

  Now, consider $R \stackrel{\triangle}{=} \{\, (\phi(F \cdot G)\, , \phi(F) \times \phi(G))\, :\, F,G \in \mathcal{P}\,\}$. One checks that R is a bisimulation up to $+$. Indeed, clause (a) of the definition of bisimulation up to is similar to clause (a) of the sum above, and is omitted. Concerning clause (b), considering the derivatives along any $x \in X$, one has:

  $$(\partial/\partial x)\phi(F \cdot G) = \phi\,(D_x F \cdot G) + \phi\,(F \cdot D_x G) \stackrel{\triangle}{=} A$$
  $$(\partial/\partial x)(\phi(F) \cdot \phi(G)) = \phi(D_x F) \times \phi(G) + \phi(F) \times \phi(D_x G) \stackrel{\triangle}{=} B\,.$$

  In deriving both equalities above, one exploits the fact that ϕ is a morphism, hence commutes with derivatives, as well as Lemma A.6. In the first equality, one additionally exploits that ϕ preserves sum, which has been proved in the previous item. Clearly $(A,B) \in R_+$, thus satisfying clause (b) of the the definition of bisimulation up to $+$. This completes the proof for this case.

– Identities $0,1$. The proof follows immediately from the preservation of sum and product. For instance, $\phi(1) = \phi(1 \cdot 1) = \phi(1) \times \phi(1)$. Since $\phi(1)(\varepsilon) = o_\rho(1) = 1$, there exists $\phi(1)^{-1}$ in $\mathbb{R}[\![X]\!]$: multiplying $\phi(1) = \phi(1) \times \phi(1)$ by $\phi(1)^{-1}$, we get the wanted $\phi(1) = 1$.

Proof of Theorem 1. Let $\phi_{\mathbf{iP}}$ denote the unique morphism from $C_{\mathbf{iP}}$ to C_{F}. By virtue of Lemma A.8, $\phi_{\mathbf{iP}}$ is a homomorphism. We prove that $\phi_{\mathbf{iP}}$ is actually the unique solution of **iP**. We first prove that that $\phi_{\mathbf{iP}}$ respects the initial data specification. Let u_τ be parametric. By the definition of coalgebra morphism and of output functions in C_{F} and $C_{\mathbf{iP}}$, we have

$$\begin{aligned} \phi_{\mathbf{iP}}(u_\tau)(\varepsilon) &= o_{\mathrm{F}}(\phi_{\mathbf{iP}}(u_\tau)) = o_\rho(u_\tau) \\ \rho(Su_\tau) &= \quad \rho(u_\tau) \end{aligned}$$

which proves the wanted condition. Next, we have to prove that $\phi_{\mathbf{iP}}$ satisfies the equations in Σ^∞. But for each such equation, say $u_\tau = F$, we have $Su_\tau =_\Sigma SF$ by the definition of $=_\Sigma$, hence $u_\tau \sim_{\mathbf{iP}} F$ by Lemma A.7(2), hence the thesis by coinduction (Corollary A.1). We finally prove uniqueness of the solution. Assume ψ is a solution of **iP**. We prove that ψ is a coalgebra morphism from $C_{\mathbf{iP}}$ to C_{F}, hence $\psi = \phi_{\mathbf{iP}}$ will follow by coinduction (Corollary A.1). Let $E \in \mathcal{P}$. There are two steps in the proof.

– $\psi(E)(\varepsilon) = \rho(SE) = o_\rho(E)$. This follows directly from Lemma A.6, since $\psi(E) = \psi(SE)$.
– For each x, $\frac{\partial \psi(E)}{\partial x} = \psi(\delta_\Sigma(E,x))$. First, we note that $\frac{\partial \psi(E)}{\partial x} = \psi(D_x E)$. This is proven by induction on the size[10] of E: in the base case when $E = u_\tau$, just use the fact that, by the definition of solution, $\frac{\partial \psi(u_\tau)}{\partial x} = \frac{\partial}{\partial x}\frac{\partial \psi(u)}{\partial \tau} = \frac{\partial \psi(u)}{\partial \tau x} = \psi(u_{\tau x}) = \psi(D_x u_\tau)$; in the induction step, use the fact that ψ is an homomorphism over $\mathcal{P}$, and the differentiation rules of D_x and $\frac{\partial}{\partial x}$ for sum and product. Now applying Lemma A.6, we get $\psi(D_x E) = \psi(S D_x E) = \psi(\delta_\Sigma(E,x))$, which is the wanted equality.

Finally, formula (2) is an immediate consequence of the definition of coalgebra $C_{\mathbf{iP}}$ and of the final morphism $\phi_{\mathbf{iP}} = \mu$ in (14).

A.3 Proofs of Section 3

We first state a simple property of solutions of pure IVPs (Σ, ρ).

Lemma A.9. *Let ψ be the solution of a finite, coherent IVP* $\mathbf{iP} = (\Sigma, \rho)$*. For each $E \in \mathcal{P}$ and $\xi = \mathbf{x}^{\boldsymbol{\alpha}}$, $\psi(E)(\xi) = \frac{\psi(D_\xi E)(\varepsilon)}{\boldsymbol{\alpha}!}$.*

Proof. An immediate application of formula (2) and of the definition of δ_Σ in (1). Note in particular that $\psi(D_\xi E)(\varepsilon) = \rho(S_\Sigma D_\xi E) = \rho(\delta_\Sigma(E, \xi))$.

The next lemma basically says that each subsystem $\Gamma_i = (\Sigma_i, X_i)$ in a coherent stratified system can be interpreted as a coherent system in the dependent variables U_{Γ_i} and the independent variables X_i.

[10] That is, $\sum_{\tau \in \mathrm{supp}(E)} |\tau|$.

Lemma A.10. *Let $H = \{\Gamma_1, ..., \Gamma_k\}$ be a coherent stratified system. Then, for each i, (Σ_i, X_i), seen as a pure system of PDEs with dependent variables in U_{Γ_i}, independent variables in X_i and derivatives in $\mathcal{D}_i \stackrel{\triangle}{=} \{\upsilon_\xi : \upsilon \in U_{\Gamma_i}, \xi \in X_i^{\otimes}\}$, is coherent in the sense of Definition 3.*

Proof. By assumption each Σ_i is $\prec$-normal, for one and the same ranking $\prec$ defined on $\mathcal{D}$. The ranking $\prec$ induces a total order $\prec'$ over $\mathcal{D}_i$ defined as: $(u_\tau)_\xi \prec' (v_{\tau'})_{\xi'}$ iff $u_{\tau\xi} \prec v_{\tau'\xi'}$. The total order $\prec'$ is a ranking over $\mathcal{D}_i$: this immediately stems from $\prec$ being a ranking over $\mathcal{D}$. By the same reasoning, Σ_i is $\prec'$-normal when elements of $\mathcal{D}_{\Gamma_i}$ are interpreted as elements of $\mathcal{D}_i$.

We next prove Theorem 2. In fact, it is technically convenient for the subsequent development to prove a slightly more detailed statement, which also provides us with information about the form of the solution.

Theorem A.1 (Theorem 2). *Let H be a coherent stratified system. For any initial data specification* ρ *for H, there is a unique solution* $\phi_{\mathbf{iP}}$ *of* $\mathbf{iP} = (H, \rho)$. *Moreover, for each i,* $(\phi_{\mathbf{iP}})_{\Gamma_i}$ *is also the unique solution of* (Σ_i, ρ_i)*, for some* ρ_i *whose restriction to* $\mathcal{P}\mathrm{a}(H)$ *coincides with* ρ.

Proof. Consider the stratified system $\overline{H} \stackrel{\triangle}{=} H \cup \{\Gamma_0\}$. We will define below a set of initial value problems $\mathbf{iP}_i = (\Gamma_i, \rho_i)$ (Definition 2), $i = 0, ..., k$, where each Γ_i is seen as a pure system of PDEs with independent variables X_i and dependent variables U_{Γ_i}. By Lemma A.10, each Γ_i is coherent, hence $\mathbf{iP}_i$ will have a unique solution ψ_i in the sense of Definition 2 (Theorem 1). Note that, under the identification $\mathcal{D}_i = \mathcal{D}_{\Gamma_i}$, ψ_i induces a function $\mathcal{P}_{\Gamma_i} \to \mathbb{R}[\![X_i]\!]$: this function, still denoted by ψ_i, respects the equations in Σ_i. Similarly, ρ_i induces a function $\mathcal{P}\mathrm{a}(\Gamma_i) \to \mathbb{R}$.

We proceed now to the actual definition of the $\mathbf{iP}_i$s by induction on the relation over subsystem indices $(i \prec j)$, which is by definition acyclic. Note that $\mathcal{P}\mathrm{a}(\overline{H}) = \emptyset$, so that each $u_\tau \in \mathcal{D}$ is principal for exactly one subsystem.

- The base case is when $\mathcal{P}\mathrm{a}(\Gamma_i) = \emptyset$. Then we let $\mathbf{iP}_i \stackrel{\triangle}{=} ((\Sigma_i, X_i), \emptyset)$, where $\emptyset$ denotes here the empty function, and let ψ_i be the corresponding unique solution (Theorem 1).
- Assume $\mathcal{P}\mathrm{a}(\Gamma_i) \neq \emptyset$. Then we let $\mathbf{iP}_i \stackrel{\triangle}{=} ((\Sigma_i, X_i), \rho_i)$, where $\rho_i : \mathcal{P}\mathrm{a}(\Gamma_i) \to \mathbb{R}$ is the initial data specification defined by $\rho_i(u_\tau) \stackrel{\triangle}{=} \psi_j(u_\tau)(\varepsilon)$, for each $u_\tau \in \mathcal{P}\mathrm{a}(\Gamma_i)$; here j is the unique index such that $j \prec i$ and $u_\tau \in \mathcal{P}\mathrm{r}(\Gamma_j)$, and ψ_j is the unique solution of $\mathbf{iP}_j$.

Now we show that $\psi \stackrel{\triangle}{=} \psi_1$ is a solution of $\overline{H}$ (recall that $X_1 = X$ by convention). In fact, we show that for each i, $\psi_{\Gamma_i} = \psi_i$ from which the wanted claim follows. We first show that for each subsystem Γ_i and $u_\tau \in \mathcal{D}_{\Gamma_i}$

$$\psi_{\Gamma_i}(u_\tau)(\varepsilon) = \psi_i(u_\tau)(\varepsilon) . \tag{17}$$

This is obvious if $i = 1$, hence assume $i \neq 1$. We distinguish the case $u_\tau \in \mathcal{P}\mathrm{a}(\Gamma_i)$ from the case $u_\tau \in \mathcal{P}\mathrm{r}(\Gamma_i)$. In the first case, let j be the unique index such that $u_\tau \in \mathcal{P}\mathrm{r}(\Gamma_j)$, so that $j \prec i$. Note that $j \neq 1$: otherwise, one would have $1 \prec i$, which is impossible, due to acyclicity and $i \prec 1$ (as to the latter, note that there must exist $u_{\tau'} \in \mathcal{P}\mathrm{r}(\Gamma_i) \cap \mathcal{P}\mathrm{a}(\Gamma_1)$; in fact $\mathcal{P}\mathrm{r}(\Gamma_i) \neq \emptyset$, as $\Sigma_i \neq \emptyset$). Then the following equalities follow from the definitions of $\psi_{\Gamma_k}, \psi_k, \rho_k$ $(0 \leq k \leq m)$.

$$
\begin{aligned}
\psi_{\Gamma_i}(u_\tau)(\varepsilon) &= \psi_1(u_\tau)(\varepsilon) \\
&= \rho_1(u_\tau) \\
&= \psi_j(u_\tau)(\varepsilon) \\
&= \rho_i(u_\tau) \\
&= \psi_i(u_\tau)(\varepsilon)\,.
\end{aligned}
$$

In the second case, $u_\tau \in \mathcal{P}\mathrm{r}(\Gamma_i)$, we have the following.

$$
\begin{aligned}
\psi_{\Gamma_i}(u_\tau)(\varepsilon) &= \psi_1(u_\tau)(\varepsilon) \\
&= \rho_1(u_\tau) \\
&= \psi_i(u_\tau)(\varepsilon)\,.
\end{aligned}
$$

This proves (17). Now in order to show that $\psi_{\Gamma_i} = \psi_i$, consider the following, for arbitrary $u_\tau \in \mathcal{D}_{\Gamma_i}$ and $\xi \in X_i^{\otimes}$, $\xi = \mathbf{x}^{\boldsymbol{\alpha}}$.

$$
\begin{aligned}
\psi_{\Gamma_i}(u_\tau)(\xi) &= \psi_{\Gamma_i}(u_{\tau\xi})(\varepsilon)/\boldsymbol{\alpha}! && (18)\\
&= \psi_i(u_{\tau\xi})(\varepsilon)/\boldsymbol{\alpha}! && (19)\\
&= \psi_i(u_\tau)(\xi) && (20)
\end{aligned}
$$

where (18) and (20) follow from Lemma A.9 applied to ψ_1 and ψ_i respectively, and (19) from (17).

Next, we prove that ψ is the unique solution. Suppose ϕ is a solution of $\overline{H}$. Then it easily follows by induction on $\prec$ that for each i, ϕ_{Γ_i} is a solution of $\mathbf{iP}_i$ as defined above (under the identification $\mathcal{D}_{\Gamma_1} = \mathcal{D}_i$). By uniqueness (Theorem 1), ϕ_{Γ_i} is the unique solution of $\mathbf{iP}_i$, hence $\phi_{\Gamma_i} = \psi_i$ as defined above. Moreover, clearly $\phi = \phi_{\Gamma_1}$. Hence $\phi = \phi_{\Gamma_1} = \psi_1 = \psi$.

The last part of the statement follows by construction of $\phi_{\mathbf{iP}}$.

In oder to prove Corollary 1, it is convenient to introduce an algebraic characterization of $S_H(\cdot)$, similarly to what we have done for $S(\cdot)$. Again, we identify equations $u_\tau = F$ with polynomials $u_\tau - F$. Let $\Gamma_i = (\Sigma_i, X_i)$ be a subsystem of H. The definition of saturation of Σ_i w.r.t. a finite set $D \subseteq \mathcal{D}$ remains formally the same, provided in the definition of saturation (15) we replace Σ^∞ with Γ_i^∞:

$$
\mathrm{Sat}_i(\Sigma') \stackrel{\triangle}{=} \{u_\tau - F \in \Gamma_i^\infty : u_\tau \text{ occurs in } \Sigma'\}\,. \qquad (21)
$$

Then for $\Sigma_i' = \{u_\tau - F \in \Gamma_i^\infty : u_\tau \text{ occurs in } \Sigma_i \text{ or } D\}$, we denote by Σ_i^D the limit set of the sequence $\mathrm{Sat}_i^j(\Sigma_i')$s $(j \geq 0)$. By construction: (a) Σ_i^D is finite, (b) $\Gamma_i^\infty \supseteq \Sigma_i^D \supseteq \Sigma_i$, and (c) the set of principal derivatives occurring in Σ_i^D coincides with $\mathrm{dom}(\Sigma_i^D)$. We let

$$
\Sigma_H^D \stackrel{\triangle}{=} \cup_{i=1}^k \Sigma_i^D \cup X\,.
$$

Let D' be the set of all derivatives occurring in Σ_H^D, we define $\mathcal{P}_D(H) \stackrel{\triangle}{=} \mathbb{R}[X \cup D']$.

Lemma A.11. *Let H be coherent. Let D be a finite set of derivatives that includes those occurring in H. For a suitable monomial order, Σ_H^D is a Gröbner basis of $\langle \Sigma_H^D \rangle$ in $\mathcal{P}_D(H)$. Moreover, for each $F \in \mathcal{P}_D(H)$, we have $S_H F = F \bmod \Sigma_H^D$.*

Proof. The proof that Σ_H^D is Gröbner basis parallels that given for Σ^D in the proof of Lemma A.3, but there is a difference in the way uniqueness of the remainder is proved. For the same monomial order considered in Lemma A.3, assume we have two division sequences of F by Σ_H^D, yielding remainders F_r and F_r', respectively. This implies, for some polynomials $G_i, G_i' \in \mathcal{P}_D(H)$:

$$\begin{aligned} F &= \sum_{E_i \in \Sigma_H^D} G_i \cdot E_i + F_r \\ &= \sum_{E_i \in \Sigma_H^D} G_i' \cdot E_i + F_r' . \end{aligned}$$

Note that both F_r and F_r' are H-normal forms. Consider now an arbitrary initial data specification ρ and the unique solution ϕ of (H,ρ) (Theorem 2). Note that, by definition of solution, $\phi(E_i)(\varepsilon) = 0$ for each $E_i \in \Sigma_H^D$. Since ϕ is also a homomorphism, the above equations for F imply that $\phi(F_r)(\varepsilon) = \phi(F_r')(\varepsilon)$. But, since ϕ is also a coalgebra morphism, $\phi(F_r)(\varepsilon) = o_\rho(F_r) = \rho(S_H F_r) = \rho(F_r)$, where the last step follows because F_r is a H-normal form. Similarly, $\phi(F_r')(\varepsilon) = \rho(F_r')$. Hence, for arbitrary ρ, $F_r(\rho) = \rho(F_r) = \rho(F_r') = F_r'(\rho)$. Since F_r, F_r' are polynomials in $\mathbb{R}[\mathcal{P}\mathrm{a}(H)]$, we deduce that $F_r = F_r'$. This completes the proof that Σ_H^D is a Gröbner basis.

Now, any sequence of rewrites leading from F to $S_H F$ corresponds exactly to a division of F by Σ_H^D with remainder F_r, which establishes that $S_H F = F_r = F \bmod \Sigma_H^D$.

The proofs of the next two lemmas parallels exactly those of Lemma A.4 and Lemma A.5 for $S(\cdot)$, but relying on Lemma A.11 instead of Lemma A.3. Their proofs is therefore omitted.

Lemma A.12. *Let H be coherent. For any $E, F \in \mathcal{P}$, $S_H(E+F) = S_H E + S_H F$ and $S_H(E \cdot F) = (S_H E) \cdot (S_H F)$.*

Lemma A.13. *Let H be coherent. For each $x \in X$ and $F \in \mathcal{P}$, $S_H D_x S_H F = S_H D_x F$.*

Proof of Corollary 1. We use the characterizations of ϕ as the unique solution of the IVP $\mathbf{iP}_1 = ((\Sigma_1, X), \rho_1)$ (Theorem A.1) and as a coalgebra morphism (Theorem 1). First, we observe that by Lemma A.9, $\phi(E)(\tau) = \phi(D_\tau E)(\varepsilon)/\boldsymbol{\alpha}! = \phi(\delta_{\Sigma_1}(E,\tau))(\varepsilon)/\boldsymbol{\alpha}!$, where the last equality stems from the definition of δ_{Σ_1} and Lemma A.5. For any F, write $F = F_0 + S_H F$ with $F_0 \in \langle \Sigma_D^H \rangle$ for a suitable D (Lemma A.11): as ϕ is a homomorphism and a solution, we have $\phi(F_0)(\varepsilon) = 0$, hence $\phi(F)(\varepsilon) = \phi(S_H F)(\varepsilon)$. Applying this remark to $F = \delta_{\Sigma_1}(E,\tau)$, we have that $\phi(\delta_{\Sigma_1}(E,\tau))(\varepsilon) = \phi(S_H(\delta_{\Sigma_1}(E,\tau)))(\varepsilon)$. For brevity, let $F_r = S_H(\delta_{\Sigma_1}(E,\tau))$. As $F_r \in \mathcal{P}_0(H) \subseteq \mathcal{P}_0(\Sigma_1)$, we have $\phi(F_r)(\varepsilon) = \rho_1(F_r)$ by definition of coalgebra morphism (14). But, by Theorem A.1, ρ_1 coincides with ρ on elements of $\mathcal{P}_0(H)$, hence $\phi(F_r)(\varepsilon) = \rho_1(F_r) = \rho(F_r)$, which completes the proof of (3).

A.4 Proof of conservative extension

We show that CFPS solutions are a conservative extension of analytic solutions in the classical sense. We first prove this for pure systems, then extend the result to stratified ones.

Pure systems Let $\mathcal{A}$ denote the set of real functions f that are analytic — admit a Taylor expansion — in a neighborhood of $0 \in \mathbb{R}^n$; for definiteness, we take each such function defined over the largest possible open set containing the origin. If $n = 0$, stipulate that $\mathcal{A} \stackrel{\triangle}{=} \{f : \{0\} \to \mathbb{R}\}$. $\mathcal{A}$ induces a commutative coalgebra $C_{\mathcal{A}} = (\mathcal{A}, \delta_{\mathcal{A}}, o_{\mathcal{A}})$, where $\delta_{\mathcal{A}}(f,x) = \frac{\partial f}{\partial x}$ (conventional partial derivative along x) and $o_{\mathcal{A}}(f) = f(0)$. The unique morphism $\mu_{\mathcal{A}} : C_{\mathcal{A}} \to C_{\mathrm{F}}$ (Corollary A.1) is given by (14), that is, for $\tau = \mathbf{x}^{\boldsymbol{\alpha}}$, $\mu_{\mathcal{A}}(f)(\tau) = \frac{1}{\boldsymbol{\alpha}!}\frac{\partial f}{\partial \tau}(0)$. In other words, $\mu_{\mathcal{A}}$ maps the analytic function f into the CFPS obtained from the Taylor expansion of f from 0. Now fix a coherent Σ. Let $\psi : U \to \mathcal{A}$ be a solution of $\mathbf{iP} = (\Sigma, \rho)$, in the classical sense, and assume it analytic. This means, letting the homomorphic extension $\mathcal{P} \to \mathcal{A}$ of ψ be still be denoted by ψ, that

(a) $\psi(u_\tau)(0) = \rho(u_\tau)$ for each $u_\tau \in \mathcal{P}\mathrm{a}(\Sigma)$; and,
(b) $\psi(u_\tau) = \psi(F)$ for each $u_\tau = F$ in Σ^∞.

We want to show that for each $E \in \mathcal{P}$ the Taylor expansion of $\psi(E)$, seen as a CFPS, coincides with $\phi_{\mathbf{iP}}(E)$, the unique solution obtained from Theorem 1: formally, that $\mu_{\mathcal{A}}(\psi(E)) = \phi_{\mathbf{iP}}(E)$. This is a consequence of the following lemma.

Lemma A.14. *Let Σ be finite and coherent. Then any analytic solution ψ is a coalgebra morphism $C_{\mathbf{iP}} \to C_{\mathcal{A}}$.*

Proof. First, by repeating verbatim the proof of Lemma A.6, we check that

$$\text{whenever } E =_\Sigma F \text{ then } \psi(E) = \psi(F). \tag{22}$$

Second, we will exploit the following fact:

$$\text{whenever } F \in \mathcal{P}_0(\Sigma) \text{ then } \psi(F)(0) = \rho(F). \tag{23}$$

This is shown by an induction on F, where the base case $F = u_\tau$ relies on the above definition of solution, part (a). We can now repeat basically the same arguments of the uniqueness part of Theorem 1, as follows. Let $E \in \mathcal{P}$. There are two steps in the proof.

- $\psi(E)(0) = \psi(SE)(0) = \rho(SE) = o_\rho(E)$, where the first equality follows from (22) and the second one from (23).
- For each x, $\frac{\partial \psi(E)}{\partial x} = \psi(\delta_\Sigma(E,x))$. First, we note that $\frac{\partial \psi(E)}{\partial x} = \psi(D_x E)$. This is proven by induction on the size of E: in the base case when $E = u_\tau$, just use the fact that, by the above definition of solution (in the analytic sense), part (b), $\frac{\partial \psi(u_\tau)}{\partial x} = \frac{\partial}{\partial x}\frac{\partial \psi(u)}{\partial \tau} = \frac{\partial \psi(u)}{\partial \tau x} = \psi(u_{\tau x}) = \psi(D_x u_\tau)$; in the induction step, use the fact that ψ is a homomorphism over $\mathcal{P}$, and the differentiation rules of D_x and $\frac{\partial}{\partial x}$ for sum and product. Now applying (22), we get $\psi(D_x E) = \psi(SD_x E) = \psi(\delta_\Sigma(E,x))$, which is the wanted equality.

Proposition 1 (conservative extension for pure systems). *Let Σ be a finite and coherent system and ρ an initial data specification for Σ. Let ψ be an analytic solution of (Σ, ρ). Then $\mu_{\mathcal{A}} \circ \psi = \phi_{(\Sigma,\rho)}$.*

Proof. From the lemma just proven, and since the composition of two coalgebra morphisms is a coalgebra morphism, we have that $\mu_{\mathcal{A}} \circ \psi : C_{\mathbf{iP}} \to C_{\mathrm{F}}$ is a coalgebra morphism. By the uniqueness of such morphism (Corollary A.1), we have $\mu_{\mathcal{A}} \circ \psi = \phi_{(\Sigma,\rho)}$, which is the wanted claim.

Stratified systems In what follows, we let $\mathcal{A}_k$ ($k \geq 0$) denote the set of k-arguments analytic functions defined in a neighborhood of $0 \in \mathbb{R}^k$. For $f \in \mathcal{A}_n$, let $X = \{x_1, ..., x_n\}$ represent the arguments of f, and let $Y \subseteq X$: we let $f_Y \in \mathcal{A}_{|Y|}$ denote the function obtained from f by fixing to 0 the arguments not in Y.

Let us fix a coherent stratified system H and and an initial data specification ρ for H. Let $\psi : U \to \mathcal{A}$ be an analytic solution of (H, ρ), in the classical sense. This means, letting the homomorphic extension $\mathcal{P} \to \mathcal{A}$ of ψ be still be denoted by ψ, that for each $\Gamma_i = (\Sigma_i, X_i) \in \overline{H}$ and for each $u_\tau = F$ in Γ_i^∞:

$$\psi(u_\tau)_{X_i} = \psi(F)_{X_i}\,. \tag{24}$$

Theorem A.2 (conservative extension for stratified systems). *Let H be a coherent stratified system and ρ an initial data specification for H. Let ψ be an analytic solution of (H, ρ). Then $\mu_{\mathcal{A}} \circ \psi = \phi_{(H,\rho)}$.*

Proof. Let $\overline{H} = \{\Gamma_1, ..., \Gamma_k\} \cup \{\Gamma_0\}$, with $\Gamma_i = (\Sigma_i, X_i)$. For each $i = 0, ..., k$, we let $\mu_i : \mathcal{A}_{|X_i|} \to \mathbb{R}[\![X_i]\!]$ denote the final morphism into $\mathbb{R}[\![X_i]\!]$ obtained by turning $\mathcal{A}_{|X_i|}$ into a coalgebra with inputs in X_i and outputs in $\mathbb{R}$ (see previous paragraph). In particular, $\mu_{\mathcal{A}} = \mu_1$. Now, let $\mathbf{iP}_i = (\Gamma_i, \rho_i)$, $i = 0, 1, ...$, be the same sequence of IVPs defined in the proof of Theorem A.1, and $\phi_{\mathbf{iP}_i}$ be the corresponding unique solutions. Let $\psi_i : \mathcal{P}_{\Gamma_i} \to \mathcal{A}_{|X_i|}$ be defined as $\psi_i(E) \stackrel{\triangle}{=} \psi(E)_{X_i}$. We now show that for each $i = 0, ..., k$, ψ_i is an analytic solution — in the classical sense, defined by (a), (b) in the previous paragraph — of $\mathbf{iP}_i$. From this, by invoking Proposition 1 we will have, for each i

$$\phi_{\mathbf{iP}_i} = \mu_i \circ \psi_i\,. \tag{25}$$

From this the thesis will follow by considering $i = 1$, as by Theorem A.1, $\phi_{(H,\rho)} = \phi_{\mathbf{iP}_1}$. We proceed now to actually show that ψ_i is an analytic solution of $\mathbf{iP}_i$. In fact, condition (b) coincides with (24), so we have to check only condition (a). We proceed by induction on a fixed linear order compatible with $\prec$. In the base case, we have $\mathcal{P}\mathrm{a}(\Gamma_i) = \emptyset$, hence condition (a) holds vacuously. In the induction step, consider any $u_\tau \in \mathcal{P}\mathrm{a}(\Gamma_i)$. By definition of ρ_i (cf. proof of Theorem A.1), $\rho_i(u_\tau) = \phi_{\mathbf{iP}_j}(u_\tau)(\varepsilon)$, for the unique j such that $u_\tau \in \mathcal{P}\mathrm{r}(\Gamma_j)$; clearly $j \prec i$. By induction hypothesis, and (25), $\phi_{\mathbf{iP}_j}(u_\tau)(\varepsilon) = \psi_j(u_\tau)(0)$. Now, denoting by $0_i, 0_n$ and 0_j the zero's in $\mathbb{R}^{|X_j|}, \mathbb{R}^n$ and $\mathbb{R}^{|X_i|}$, respectively, we have by definition of ψ_k: $\psi_j(u_\tau)(0_j) = \psi(u_\tau)(0_n) = \psi_i(u_\tau)(0_i)$. To sum up, $\rho_i(u_\tau) = \psi_i(u_\tau)(0)$, hence (a) is proven.

Remark 1 (equational reasoning on analytic solutions). Consider a coherent H, with the additional property that for each initial data specification ρ there exists a unique analytic solution, say $\psi_{(H,\rho)}$, around 0. Then Theorem A.2 ensures that, in terms of valid polynomial equalities, considering analytic solutions or CFPSs makes no difference at all. More precisely, letting $\mathrm{sp}_H^{\mathcal{A}}(P) \stackrel{\triangle}{=} \{E \in \mathcal{P} : \psi_{(H,\rho)}(E) = 0 \text{ for each } \rho \in \mathbf{V}(P)\}$, for such a H we have that $\mathrm{sp}_H^{\mathcal{A}}(P) = \mathrm{sp}_H(P)$.

Unfortunately, not all systems of PDEs posses an analytic solution, even when confining to the polynomial format as we do — in stark contrast with the case of ODEs.

The following example of a linear PDE system is drawn from [15]

$$u_{xx} = u_{xy} + u_{yy} + v$$
$$v_{yy} = v_{xy} + v_{yy} + u$$

with the initial conditions $u(0,y) = u_x(0,y) = \exp(y)$ and $v(x,0) = v_y(x,0) = \exp(x)$. The initial conditions can be easily recast into polynomial form as follows: $u_y(0,y) = u(0,y)$ and $u_{xy}(0,y) = u_x(0,y)$ (similarly for v), with the initial data specified by $P = \{u-1, u_x-1, v-1, v_x-1\}$. This results in a stratified system $H = \{(\Sigma_1,\{x,y\}), (\Sigma_2,\{y\}), (\Sigma_3,\{x\})\}$ that is coherent w.r.t. to the ranking considered in [15]: $u \prec v \prec u_y \prec u_x \prec v_x \prec v_y \prec \cdots$. As a consequence, H has a unique CFPS solution for each initial data specification over $\mathcal{P}a(H) = \{u, u_x, v, v_y\}$. Lemaire [15] shows however that H has no analytic solution. Informally, the reason is that its Taylor coefficients grow too fast as the order of the derivatives grows.

Syntactic formats that guarantee existence and uniqueness of analytic solutions of PDEs IVPs are known: for instance, one has the Cauchy-Kovalevskaya format [18, Ch.2.6], generalized by the Riquier format [22], further generalized by Rust et al. [26].

A.5 Proofs of Section 4

We need need two substitution properties for templates, also to effectively compute (6). These prove the equalities in (5). In what follows, we shall abbreviate S_{Σ_1} as S_1.

Lemma A.15. *Let H be a coherent stratified system. Let π a polynomial template, $v \in \mathbb{R}^s$.*

1. $\delta_{\Sigma_1}(\pi[v],x) = \delta_{\Sigma_1}(\pi,x)[v]$ *for any $x \in X$;*
2. $S_H(\pi[v]) = (S_H\pi)[v]$.

Proof. Let $\pi = \sum_i \ell_i\tau_i$, for distinct monomials $\tau_i \in (X \cup \mathcal{D})^{\otimes}$. Facts (1) and (2) easily follow from the distributivity properties of S_1 (Lemma A.4) and S_H (Lemma A.12). As an example, for (1) we have

$$\begin{aligned}
\delta_{\Sigma_1}(\pi[v],x) &= \delta_{\Sigma_1}\big(\sum_i \ell_i[v]\gamma_i, x\big) \\
&= S_1 \sum_i \ell_i[v] D_x \tau_i \\
&= \sum_i \ell_i[v] S_1 D_x \tau_i \\
&= \sum_i \ell_i[v] \delta_{\Sigma_1}(\tau_i, x) \\
&= \big(\sum_i \ell_i \delta_{\Sigma_1}(\tau_i,x)\big)[v] \\
&= \delta_{\Sigma_1}(\pi,x)[v]\,.
\end{aligned}$$

The proof for (2) is similar.

We finally arrive at the proof of the stabilization property stated in (8).

Lemma A.16 (property (8)). *Let $\mathrm{POST}_H(P_0,\pi) = (V_m, J_m)$, under the hypotheses of Theorem 3. Then for each $j \geq 1$, one has $V_m = V_{m+j}$ and $J_m = J_{m+j}$.*

Proof. We proceed by induction on j. The base case $j = 1$ follows from the definition of m. Assuming by induction hypothesis that $V_m = \cdots = V_{m+j}$ and that $J_m = \cdots = J_{m+j}$, we prove now that $V_m = V_{m+j+1}$ and that $J_m = J_{m+j+1}$. The key to the proof is the following fact

$$(S_H \pi_{\tau x})[v] \in J_m, \ \forall \, |\tau| = m+j, x \in X \text{ and } v \in V_m \,. \tag{26}$$

From this fact the thesis will follow, as we show below.

1. $V_m = V_{m+j+1}$. To see this, observe that for each $v \in V_{m+j} = V_m$ (the equality here follows from the induction hypothesis), it follows from (26) and the definition of J_m that $(S_H\pi_{\tau x})[v]$ can be written as a finite sum of the form $\sum_l h_l \cdot (S_H\pi_{\tau_l})[w_l]$, with $0 \le |\tau_l| \le m$ and $w_l \in V_m$. For each $0 \le |\tau_l| \le m$, $(S_H\pi_{\tau_l})[w_l] \in I_0$ by assumption, from which it easily follows that also $(S_H\pi_{\tau x})[v] = \sum_l h_l \cdot (S_H\pi_{\tau_l})[w_l] \in I_0$. Since fact holds for each τ of size m and $x \in X$, hence for each τ of size $m+1$, it shows that $v \in V_{m+j+1}$, proving that $V_{m+j+1} \supseteq V_{m+j} = V_m$. The reverse inclusion is obvious.

2. $J_m = J_{m+j+1}$. As a consequence of $V_{m+j+1} = V_{m+j} (= V_m)$ (the previous point), we can write
$$\begin{aligned} J_{m+j+1} &= \Big\langle \bigcup_{|\tau| \le m+j} (S_H\pi_\tau)[V_{m+j}] \ \cup \bigcup_{|\xi| = m+j+1} (S_H\pi_\xi)[V_{m+j}] \Big\rangle \\ &= \Big\langle J_{m+j} \cup \bigcup_{|\xi| = m+j+1} (S_H\pi_\xi)[V_{m+j}] \Big\rangle \\ &= \Big\langle J_m \cup \bigcup_{|\xi| = m+j+1} (S_H\pi_\xi)[V_m] \Big\rangle \end{aligned}$$
where the last step follows by induction hypothesis. From (26), we have that for $|\xi| = m+j+1$, $(S_H\pi_\xi)[V_m] \subseteq J_m$, which implies the thesis for this case, as $\langle J_m \rangle = J_m$.

We prove now (26). In this proof, we shall make use of the following equality for S_H and S_1. For each $E \in \mathcal{P}$

$$S_H S_1 E = S_H E \,. \tag{27}$$

In order to check (27), note that as $E = E_0 + S_1 E$, for $E_0 \in \langle \Sigma_1^D \rangle$ and a suitable D (Lemma A.3), by distributivity of S_H (Lemma A.12), one has $S_H E = S_H E_0 + S_H S_1 E$. But $S_H E_0 = 0$, again by distributivity of S_H and since $S_H E_i = 0$ for any equation in $E_i \in \Sigma_1^D$. Let us now proceed to the proof of (26). Fix any $v \in V_m$. First, note that for $|\tau| = m+j$ and $x \in X$, by definition $\pi_{\tau x}[v] = \delta_{\Sigma_1}(\pi_\tau[v], x) = S_1 D_x(\pi_\tau[v])$ (where in the first step we have used Lemma A.15; here $S_1 = S_{\Sigma_1}$). Now consider $S_H\pi_\tau$: by induction hypothesis, $(S_H\pi_\tau)[V_m] = (S_H\pi_\tau)[V_{m+j}] \subseteq J_{m+j} = J_m$, hence $(S_H\pi_\tau)[v]$ can be written as a finite sum $\sum_l h_l \cdot (S_H\pi_{\tau_l}[w_l])$, with $0 \le |\tau_l| \le m$ and $w_l \in V_m$ and $h_l \in \mathcal{P}_0(H)$. Summing up, we have:

$$
\begin{aligned}
(S_H\pi_{\tau x})[v] &= S_H S_1 D_x(\pi_\tau[v]) && (28)\\
&= S_H D_x(\pi_\tau[v]) && (29)\\
&= S_H D_x S_H(\pi_\tau[v]) && (30)\\
&= S_H D_x \sum_l h_l \cdot S_H\pi_{\tau_l}[w_l] && (31)\\
&= S_H \sum_l (D_x h_l)\cdot S_H\pi_{\tau_l}[w_l] + h_l \cdot D_x S_H(\pi_{\tau_l}[w_l]) && (32)\\
&= \sum_l S_H(D_x h_l)\cdot S_H\pi_{\tau_l}[w_l] + h_l \cdot S_H D_x S_H(\pi_{\tau_l}[w_l]) && (33)\\
&= \sum_l S_H(D_x h_l)\cdot S_H\pi_{\tau_l}[w_l] + h_l \cdot S_H D_x(\pi_{\tau_l}[w_l]) && (34)\\
&= \sum_l S_H(D_x h_l)\cdot S_H\pi_{\tau_l}[w_l] + h_l \cdot S_H S_1 D_x(\pi_{\tau_l}[w_l]) && (35)\\
&= \sum_l S_H(D_x h_l)\cdot S_H\pi_{\tau_l}[w_l] + h_l \cdot S_H \delta_1(\pi_{\tau_l}[w_l], x) && (36)\\
&= \sum_l S_H(D_x h_l)\cdot S_H\pi_{\tau_l}[w_l] + h_l \cdot S_H \pi_{\tau_l x}[w_l] && (37)
\end{aligned}
$$

where:

- (28) follows by definition of $\delta_1 = \delta_{\Sigma_1}$;
- (29) follows from (27);
- (30) follows from Lemma A.13;
- (31) follows from the equality for $S_H(\pi_\tau[v]) = (S_H\pi)[v]$ (here we use Lemma A.15) proven above;
- (32) follows from distributing D_x over sum and products, and applying the rules for total derivatives;
- (33) follows from distributing S_H (Lemma A.12) over sums and products, and further noting that $S_H h_l = h_l$, as $h_l \in \mathcal{P}_0(H)$;
- (34) follows again from Lemma A.13;
- (35) follows again from (27);
- (36) follows from the definition of δ_1;
- (37) follows from Lemma A.15.

Now, for each $w_l \in V_m = V_{m+1}$, the term $S_H\pi_{\tau_l x}[w_l]$, with $0 \le |\tau_l x| \le m+1$, is by definition in $J_{m+1} = J_m$. Thus (37) proves that $S_H\pi_{\tau x}[v] \in J_m$, as required.

A.6 Computational details for the POST algorithm in Section 4

We refer the reader to [11, Ch.3,Sect.1,Th.2] for the definition of the technical notion of elimination order; the lexicographic order is one such order. See [3, Lemma 3] for a proof of the following lemma.

Lemma A.17. *Let $\mathbf{z} = \{z_1, ..., z_k\}$ and $\mathbf{a} = \{a_1, ..., a_s\}$ be disjoint sets of indeterminates. Let $B \subseteq \mathbb{R}[\mathbf{z}]$ be a Gröbner basis in $\mathbb{R}[\mathbf{a} \cup \mathbf{z}]$ w.r.t. a monomial elimination order for the a_i s in $\mathbf{a}$. Consider $p \in \mathrm{Lin}(\mathbf{a})[\mathbf{z}]$, seen as a polynomial in $\mathbb{R}[\mathbf{a} \cup \mathbf{z}]$, and $r = p \bmod B$. Then r is linear in $\mathbf{a}$. Moreover, for each $v \in \mathbb{R}^s$, $p[v] \bmod B = r[v]$.*

For $\pi \in \mathrm{Lin}[\mathbf{a}][\mathbb{R}]$, let $\mathrm{coeff}(\pi)$ be the set of coefficients (linear expressions) of π. Recall that for a Gröbner basis B and a polynomial E, E mod B denotes the remainder of the division of E by B. Here we use the fact that $B \subseteq \mathcal{P}_0(H)$ is also a Gröbner over the larger polynomial ring $\mathbb{R}[\{a_1,...,a_s\} \cup \mathcal{P}a(H)]$, which contains also all templates, once an elimination monomial order (e.g. lexicographic) for the a_i s is fixed.

Lemma A.18. *Under the hypotheses of Theorem 3, let $B \subseteq \mathcal{P}_0(H)$ be a Gröbner basis of I_0. Then $V_i = \mathrm{span}\left(\cup_{|\tau|\le i}\mathrm{coeff}((S_H\pi_\tau) \bmod B)\right)$. As a consequence $J_i = \left\langle\ \cup_{|\tau|\le i} (S_H\pi_\tau)[B_i]\ \right\rangle$, where B_i is a basis of V_i.*

Proof. Let $\mathbf{z} = \mathcal{P}a(H)$. Let $B \subseteq \mathcal{P}_0(H)$ be the given Gröbner basis of I_0: B can also be considered as a Gröbner basis in the larger ring $\mathbb{R}[\mathbf{a} \cup \mathbf{z}]$, w.r.t. some elimination order for the parameters a_i s in $\mathbf{a}$. Fix any $\tau \in X^{\otimes}$. Applying Lemma A.17 with $p = S_H\pi_\tau$, we have that for each $v \in \mathbb{R}^s$: $(S_H\pi_\tau)[v] \in I_0$ iff $r^{(\tau)}[v] = 0$, where $r^{(\tau)} \stackrel{\triangle}{=} S_H\pi_\tau \bmod B$; this is true iff $v \in \mathrm{span}(\mathrm{coeff}(r^{(\tau)}))$. Hence, by definition (6), $v \in V_i$ iff $v \in \mathrm{span}(\mathrm{coeff}(r^{(\tau)}))$ for each $|\tau| \le i$. This is in turn equivalent to $v \in \mathrm{span}(\cup_{|\tau|\le i}\mathrm{coeff}(r^{(\tau)}))$, which is the first part of the statement. The last part follows because, for any template π, vector space $V \subseteq \mathbb{R}^s$ and basis B_0 of V, one has $\langle\ \pi[V]\ \rangle = \langle\ \pi[B_0]\ \rangle$.

Remark 2 (on relative completeness). Relative completeness (equality) in part (a) of Theorem 3 is only guaranteed if P_0 is chosen such that $I_0 = \mathbf{I}(\mathbf{V}(P))$, otherwise $\pi[V_m]$ is just a postcondition. When $I_0 = \mathbf{I}(\mathbf{V}(P))$, I_0 is said to be a *real radical* of P. Computing real radicals is a computationally hard problem, in the general case. For a number of special cases relevant to our goals, fortunately, the real radical is trivial. For instance, if P only contains elements of the form $d-e$, for d an indeterminate and e an indeterminate or a constant, then $\langle\ P\ \rangle = \mathbf{I}(\mathbf{V}(P))$, so that $\langle\ P\ \rangle$ is a real radical. Also note that the relative completeness in part (b) of Theorem 3 does *not* depend on having a real radical at hand. See [3] for further discussion on the real radical problem.

A.7 Additional examples

Boundary problems A *boundary problem* prescribes the form of the solution at some specified curve, rather than an initial condition. Any scalar, first order boundary problem can be transformed into an IVP via a suitable change of coordinates, hence becoming amenable to analysis with our algorithm. One can exploit the *method of characteristics* [12, Ch.3] as a systematic recipe for carrying out this transformation. The resulting technique is illustrated via the following example.

Consider the PDE $u_x^2 + u_y^2 = 1$ (the *Eikonal* equation), with the boundary condition $u_{|C} = 0$, where C is the unit circle centered at the origin. According to the method of characteristics, one can transform a boundary problem into a *family* of hopefully simpler ODE IVPs. For our purposes, we need not worry about the details of this transformation (see [16, Ch.2] for a detailed derivation). It suffices to know it results in the following ODE IVPs, depending on a parameter $r \in \mathbb{R}$. Here s is the only independent variable, while x, y, z, p, q are the dependent variables.

$$\begin{array}{lll}
\frac{dx}{ds}(s;r) = 2p & \frac{dy}{ds}(s;r) = 2q & \frac{dz}{ds}(s;r) = 2p^2 + 2q^2 \\
\frac{dp}{ds}(s;r) = 0 & \frac{dq}{ds}(s;r) = 0 & \\
x(0;r) = \cos(r) & y(0;r) = \sin(r) & z(0;r) = 0 \\
p(0;r) = \cos(r) & q(0;r) = \sin(r)\,. &
\end{array}$$

According to the theory of ODEs, for each r the above IVP has a unique solution in a neighborhood of $s = 0$. The union of the solutions' trajectories $(x(s;r), y(s;r), z(s;r))$ represents the solution u of the original problem, in the sense that for each r, and for each s in a neighborhood of 0

$$z(s;r) = u(x(s;r), y(s;r))\,.$$

As $(x(0;r), y(0;r))$ represents a parametrization of the circle C depending on $r \in \mathbb{R}$, the above formula says that we can represent the solution u via z at least locally, that is near the boundary C. Also note that $z(0;r) = 0$, as required by the boundary condition. At this stage, to obtain an explicit formula for u, the method of characteristics prescribes to try the following: (1) solve the given IVPs, obtaining formulae for x, y, z as functions of (s, r); (2) invert the functions x and y, that is express (s, r) in terms of (x, y). This way one can rewrite $z(s;r) = u(x(s;r), y(s;r))$ as a function of x and y alone.

One can avoid to carry out steps (1) and (2) explicitly by exploiting the POST algorithm. In fact, seeing r as an independent *variable*, rather than as a parameter, one can turn the above family of ODE IVPs into a FP, coherent stratified system H of PDEs for the functions $x(s, r), y(s, r), \ldots$: say $H = \{(\Sigma_1, \{s, r\}), (\Sigma_2, \{r\})\}$, for the obvious choices of Σ_1 and Σ_2. Now, one can use POST to systematically search for all valid polynomial relations linking x, y, z. If the resulting polynomial system can be solved for z, obtaining say $z = f(x, y)$, one can deduce $u(x, y) = f(x, y)$, at least for (x, y) sufficiently near to the boundary[11] C. In the present case, we run $\text{POST}_H(P, \pi)$ with $P = \{x - 1, y, z, p - 1, q\}$ (encoding initial values for x, y, z, p, q) and π the complete template of total degree 2 over the variables $\{x, y, z\}$, which has 10 parameters. We get stabilization at $m = 5$ (after about 5s), obtaining a 1-parameter result template π', where $\pi'[1] = x^2 + y^2 - z^2 - 2z - 1 = x^2 + y^2 - (z + 1)^2$. Therefore $x^2 + y^2 = (z + 1)^2$ is the only valid polynomial relation of degree ≤ 2 for this system. Solving for z, we obtain $z = \pm\sqrt{x^2 + y^2} - 1$. The function involving the negative square root does not satisfy the boundary condition, so we deduce that $u = z = \sqrt{x^2 + y^2} - 1$ is the solution of the original problem.

Details for the conservation laws example In Section 5 we have outlined the computation of the conservation laws of an IVP for the wave equation, that is a vector space $(\pi_1[V], \pi_2[V])$ of density-flux pairs. What is actually computed is in fact a *basis* B for this space, that is a finite set of linearly independent pairs that generates $(\pi_1[V], \pi_2[V])$.

[11] Technically, under mild conditions [16, Ch.2] that are satisfied in the present example, the function $G(s, r) \stackrel{\triangle}{=} (x(s, r), y(s, r))$ is locally invertible around $s = 0$. Therefore, for each (x_0, y_0) sufficiently near to the boundary C and for $(s_0, r_0) = G^{-1}(x_0, y_0)$, we have: $u(x_0, y_0) = u(G(s_0, r_0)) = z(s_0, r_0) = f(G(s_0, r_0)) = f(G(G^{-1}(x_0, y_0))) = f(x_0, y_0)$.

We give below the complete list of nontrivial[12] density-flux pairs (Ψ,Φ) in B.

$$\begin{array}{ll}
tu_x + xu_t & -tu_t - xu_x \\
tu_t + xu_x & -tu_x - xu_t \\
-tu_t + u & tu_x \\
\frac{1}{2}u_x^2 + \frac{1}{2}u_t^2 & -u_x u_t \\
u_x u_t & -(\frac{1}{2}u_t^2 + \frac{1}{2}u_x^2) \\
u_t & -u_x \\
u_x v & -u_t v/2 \\
u_x u_t & -u_x^2 + \frac{1}{2}v^2 \,.
\end{array}$$

Of the above eight laws, the last two are specific of the IVP at hand, that is they are not pure for the wave equation. The remaining six are also pure laws for the wave equation. The physical meaning of the densities $\frac{1}{2}u_x^2 + \frac{1}{2}u_t^2$ and $u_x u_t$ has been already discussed in Section 5, the sixth law is just a reformulation of the wave equation itself. The physical meaning of the first three densities is unclear to us.

Remark 3 (pure vs. IVP conservation laws). Methods to search for *pure* conservation laws have traditionally been linked to the existence of symmetries of the system, on account of a celebrated theorem by Emmy Noether [18, Ch.4,Sect.4]. Alternative, direct methods exist that are more widely applicable, like those centered on characteristics [18, Ch.4]. In our context, let us see the given PDE equations as a set of polynomials, $\Sigma = \{u_{\tau_1} - E_1, ..., u_{\tau_k} - E_k\} \subseteq \mathbb{R}[X \cup D]$, for $D \subseteq \mathcal{D}$, with $N \stackrel{\triangle}{=} |X \cup D| < +\infty$. Under suitable technical conditions on Σ (*nondegeneracy*, [18, Ch.4]), the variety $\mathbf{V}(\Sigma) \subseteq \mathbb{R}^N$ coincides with the union of the graphs of the analytic solutions of Σ (and their derivatives in D). Then $\nabla\mathbf{C}$, or more generally any polynomial $G \in \mathbb{R}[X \cup D]$, vanishes on the solutions of Σ if and only if $G \in \mathbf{I}(\mathbf{V}(\Sigma))$. Under the mentioned technical condition, one can assume $G \in \langle\, \Sigma \,\rangle$. The polynomial coefficients Q_j s.t. $G = \sum_j Q_j(u_{\tau_j} - E_j)$ are known as *characteristics*. Characteristics that yield conservation laws can be searched quite effectively by analytical or algebraic means. Unfortunately, it is not obvious how to extend this approach to IVPs. In fact, the subset of the solutions satisfying the given initial conditions, represented in terms of their graphs, may have a complicated geometry, with no algebraic description. Even in cases where such descriptions exist, it is unclear how to build them systematically. This explains why, when searching for IVPs conservation laws, one may have to resort to methods that are more "brute force" in spirit, like the one outlined in Section 5.

[12] A (polynomial) conservation law $\mathbf{C} = (C_1, ..., C_n)$ is *trivial* if it is a linear combination of laws satisfying either of these two conditions: (a) for each i, $D_{x_i}C_i \in \mathrm{sp}_H(P)$; or, (b) $\nabla\mathbf{C} = 0$ as a polynomial in $\mathcal{P}$. See [18, Ch.4,Sect.4]. The code for this example available at `https://github.com/micheleatunifi/PDEPY/blob/master/PDE.py`. The concrete form of the returned basis depends on the underlying platform.