Arithmetic constraints :

$$\begin{array}{rcl} \phi & ::= & x{=}\kappa^{(i)}(x_1,\ldots,x_k) \quad | \quad x = x_1 + x_2 \quad | \quad x = x_1 \cdot x_2 \quad | \\ & & x_1 = x_2 \quad | \quad x \in S \quad | \quad \phi \wedge \phi' \quad | \quad \exists x.\phi \end{array}$$

where $i \in$, $\kappa :^k \rightarrow$, x, x_1, x_2 are variables, and $S \subseteq$ a finite set. A solution of an arithmetic constraint ϕ with n variables can be identified with a tuple in ^{n} since we assumed a total order on the variables. Therefore, the solution set (ϕ) of a formula ϕ satisfies $(\phi) \subseteq^n$.

The steady state equations of any reaction network N can be rewritten in linear time to an equivalent arithmetic constraint ϕ_N so that:

$$(\phi_N) =_N$$

It is sufficient to flatten the terms in steady state equations, by introducing new existentially bound variables for all nested subterms. The resulting constraint ϕ_N is clearly equivalent, and thus it satisfies $(\phi_N) =_N$ by Definition **??** of the exchange relation.

A difference constraint : where x is a variable, $d \in$, $S \subseteq$, and $\kappa :^k \rightarrow$:

$$\begin{array}{lrcl} differencerelation & t & ::= & x \mid d \\ setofdifferencerelations & s & ::= & t \mid S \mid s + s' \mid s \cdot s' \mid \kappa(s_1,\ldots,s_k) \\ differenceconstraints & \psi & ::= & t \in s \mid t{=}t' \mid \psi \wedge \psi' \mid \exists x.\psi \end{array}$$

The set of all Δ-*solutions* of a difference constraints ψ with free variables $x_1,\ldots,x_n$ – listed in their order – is the following subset of Δ^n:

$$^{\Delta}(\psi) = \{(\alpha(x_1),\ldots,\alpha(x_n)) \mid \psi = 1\}$$

Difference relations:

$$\begin{array}{l} x = \alpha(x) \\ d = \text{ unique element of } \{d\} \end{array}$$

Sets of difference relations:

$$\begin{array}{ll} t = \{t\} & S = S \\ s \cdot s' = s{\cdot}s' & s + s' = s{+}s' \\ \kappa(s_1,\ldots,s_k) = \kappa(s_1,\ldots,s_k) & \end{array}$$

Difference constraints:

$$\begin{array}{ll} t \in s = (t \in s) & t = t' = (t = t') \\ \psi \wedge \psi' = \psi{\wedge}^{\psi'} & \exists x.\psi = (\exists \delta \in \Delta.\psi\alpha[x/\delta] = 1) \end{array}$$

Figure 1: Semantics of difference constraints over Δ.

Abstract interpretation : We can now abstract from arithmetic constraints by interpreting them as difference constraints:

$$\begin{array}{ll} x{=}\kappa^{(i)}(x_1,\ldots,x_k) =_x \in \kappa(x_1,\ldots,x_k) & x \in S =_x \in S \\ x = x_1 + x_2 =_x \in x_1 + x_2 & \phi \wedge \phi' =_\phi \wedge \phi' \\ x = x_1 \cdot x_2 =_x \in x_1 \cdot x_2 & \exists x.\phi =_\exists x.\phi \\ x_1{=}x_2 =_(x_1{=}x_2) & \end{array}$$

[Soundness] For any arithmetic constraint ϕ and any partition Δ of difference relations, the Δ-solution set of the abstract interpretation of ψ over-approximates the Δ-difference abstraction of the solution set of ϕ, that is:

$$(\phi) \subseteq^\Delta (\phi).$$

We first note that for any two relations $R_1, R_2 \subseteq^n$:

$$(intersect) \qquad (R_1 \cap R_2) \subseteq R_1 \cap R_2$$

This can be verified straightforwardly from the definition of the difference abstraction. It will turn out to be the reason why proper approximations may appear when abstracting conjunctions.

Then we proceed by induction on the structure of arithmetic constraints ϕ. For the variables in the proof, we always assume for simplicity that they are ordered $x_1 x_2 \ldots x_k x$.

Case ϕ is $x = \kappa^{(i)}(x_1,\ldots,x_k)$. By definition of solutions we have that $(\phi) = \{(d_1, \ldots, d_k, d) \in^{k+1} \mid d = \kappa'(d_1,\ldots,d_k),\ \kappa' \sim_\Delta \kappa\}$, i.e., $(\phi) = \{\kappa' \mid \kappa' \sim_\Delta \kappa\}$. Thus, $(\phi) = \kappa$. Furthermore, ϕ is equal to $x{\in}\kappa(x_1,\ldots,x_k)$ so that ${}^\Delta(\phi) = \kappa^\Delta = (\phi)$.

Case ϕ is $x = x_1 + x_2$. This follows, since $\phi = +$. Furthermore ϕ is equal to $x \in x_1 + x_2$ so that ${}^\Delta(\phi) = +$ and thus $\phi =^\Delta (\phi)$.

Case ϕ is $x = x_1 \cdot x_2$. This follows in analogy to the case of addition.

Case ϕ is $x_1 = x_2$. We first note that $\{(d,d) \mid d \in\} = \{(\delta,\delta) \mid \delta \in \Delta\}$ since Δ is a partition of $\times$. We now can conclude as follows: $\phi = \{(d,d) \mid d \in\} = \{(\delta,\delta) \mid \delta \in \Delta\} =^\Delta \phi$.

Case ϕ is $x \in S$. In this case we have $(\phi) = S$, so that $(\phi) = S =^\Delta (x \in S) =^\Delta (\phi)$.

Case ϕ is $\phi_1 \wedge \phi_2$. Hence $(\phi) = (\phi_1) \cap (\phi_2)$ and thus as claimed by (intersect) at the beginning $(\phi) \subseteq (\phi_1) \cap (\phi_2)$. From the induction hypothesis applied to ϕ_1 and ϕ_2, it follows that $(\phi_i) \subseteq (\phi_i)$ for $i = 1, 2$, and thus $(\phi) \subseteq (\phi_1) \cap (\phi_2) \subseteq^\Delta (\phi_1) \cap^\Delta (\phi_2) =^\Delta (\phi)$.

Case ϕ is $\exists x.\phi'$. There case where x does not occur freely in ϕ' is easy, since we can drop the quantifier $\exists x$. Otherwise, we can assume that ϕ' has the free variables $x_1, ..., x_k$ and that $x = x_i$ where $1 \leq i \leq k$. For any set D and tuple set $S \subseteq D^k$ we define the projection $\Pi_x(S) = \{(d_1,\ldots,d_{i-1},d_{i+1},\ldots,d_k) \mid (d_1,\ldots,d_k) \in S\}$. We first note that:

$$(project) \qquad \Pi_x((\phi')) = (\Pi_x((\phi')))$$

All elements of $\times$ belong to some difference in Δ. Based on the equation on projection, we can conclude as follows:

$$\begin{aligned}(\exists x.\phi') &= (\Pi_x((\phi'))) =_{project} \Pi_x((\phi')) \\ &\subseteq_{ind.hyp.} \Pi_x(\phi') = (\exists x.\phi') =^{\Delta} (\exists x.\phi').\end{aligned}$$

If $_N = (\phi_N)$ then $(_N) \subseteq^{\Delta} (\phi_N)$. This follows immediately from Theorem **??**.

The set of Δ-*difference formulas* Ψ is the least set that contains all difference constraints ϕ, all formulas $x \in \Delta'$ where x is a variable and $\Delta' \subseteq \Delta$, and that is closed under the first-order connectives, ie.:

$$\Psi ::= \phi \mid x \in \Delta' \mid \Psi \wedge \Psi' \mid \neg\Psi \mid \exists x.\Psi$$

We define the Δ-difference formula $x = \delta$ as syntactic sugar for $x \in \{\delta\}$ for any $\delta \in \Delta$ and variable x.