

# Big Steps in Higher-Order Mathematical Operational Semantics

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# HO Mathematical Operational Semantics Project

-  Goncharov, Milius, Schröder, Tsampas, and Urbat, "Towards a Higher-Order Mathematical Operational Semantics", POPL 2023
-  Urbat, Tsampas, Goncharov, Milius, and Schröder, "Weak Similarity in Higher-Order Mathematical Operational Semantics", LICS 2023
-  Goncharov, Santamaria, Schröder, Tsampas, and Urbat, "Logical Predicates in Higher-Order Mathematical Operational Semantics", FoSSaCS 2024
-  Goncharov, Milius, Tsampas, and Urbat, "Bialgebraic Reasoning on Higher-Order Program Equivalence", LICS 2024
-  Goncharov, Tsampas, and Urbat, "Abstract Operational Methods for Call-by-Push-Value", POPL 2025
-  Goncharov, Milius, Schröder, Tsampas, and Urbat, "Bialgebraic Reasoning on Stateful Languages", ICFP 2025 (!)

.. and rolling

# Project in Nutshell

- ▶ **Motto:** Make operational semantics more mathematical
- ▶ **Main Idea:** Given operational specification (set of O/S rules), devise methods/properties of the language
- ▶ **Main Tool:** Category theory



- ▶ **Methods:** Abstract logical relations, Abstract Howe's method
- ▶ **Properties:** Compositionality, safety, adequacy
- ▶ **Side-effect:** categorical methods  $\rightsquigarrow$  functional implementation (Haskell, Agda, Rocq)

# Our Hobbyhorse: (Extended) Combinatory Logic

- ▶  $I (= \lambda p. p)$      $K (= \lambda p. \lambda q. p)$      $S (= \lambda p. \lambda q. \lambda r. (p \cdot r) \cdot (q \cdot r))$
- ▶ plus  $S'$ ,  $S''$  and  $K'$  for partially reduced terms

Small-step semantics (cf. [lazy  \$\lambda\$ -calculus](#)<sup>†</sup>):

$$K \xrightarrow{p} K'(p) \quad K'(p) \xrightarrow{q} p \quad S''(p, q) \xrightarrow{r} (p \cdot r) \cdot (q \cdot r) \quad \dots$$
$$\frac{p \rightarrow p'}{p \cdot q \rightarrow p' \cdot q} \quad \frac{p \xrightarrow{q} p'}{p \cdot q \rightarrow p'}$$

(Example:  $K \cdot I \cdot K \cdot S \rightarrow K'(I) \cdot K \cdot S \rightarrow I \cdot S \rightarrow S$ )

- ✓ Language is purely algebraic, yet higher order
- ✓ Well suited for presentation because of simplicity
- ✗ Technically different from  $\lambda$ -calculus (but bear with me)

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<sup>†</sup> Abramsky, "The lazy  $\lambda$ -calculus".

# Big-Step Semantics

- ▶ Notion of **value**:  $v, w ::= I \mid K \mid S \mid K'(t) \mid S'(t) \mid S''(s, t)$
- ▶ Evaluation relation:  $\Downarrow \subseteq Terms \times Values$
- ▶ Big-step rules:

$$\frac{}{v \Downarrow v} \quad \frac{s \Downarrow I \quad t \Downarrow v}{s \cdot t \Downarrow v} \quad \frac{s \Downarrow K'(r) \quad r \Downarrow v}{s \cdot t \Downarrow v}$$

$$\frac{s \Downarrow S''(r, q) \quad (r \cdot t)(q \cdot t) \Downarrow v}{s \cdot t \Downarrow v} \quad \dots$$

**Equivalence** of Big-Step and Small-Step:  $t \Downarrow v \iff t \rightarrow^* v \wedge v \text{ is a value}$

② How to prove it abstractly?

↳ ② How to interpret it abstractly?

# How to prove

$t \Downarrow v \iff t \rightarrow^* v \wedge v \text{ is a value}$

abstractly?

# Abstract Higher-Order GSOS

# A Bit of Category Theory

From the programming perspective:

- ▶ **(Endo-)functor** is a type constructor, e.g.  $FX = X \times X$
- ▶ **Natural transformation**  $\alpha: F \rightarrow G$  is a polymorphic function  $\alpha_X: FX \rightarrow GX$ , e.g.  $swap: X \times X \rightarrow X \times X$
- ▶ **Algebra** is a map  $a: FX \rightarrow X$ , e.g. the free algebra of  $\Sigma$ -terms  $\iota: \Sigma(\Sigma^*X) \rightarrow \Sigma^*X$  over variables  $X$ , and  $\mu\Sigma := \Sigma^*\emptyset$
- ▶ **Monad** is such a functor  $T$  that morphisms  $(f: X \rightarrow TY)_{X, Y \in \mathcal{C}}$  form a category, e.g. for  $T = \mathcal{P}$  we obtain the **category of relations**

# Dinaturality

Given two functors  $F, G: \mathcal{C}^{\text{op}} \times \mathcal{C} \rightarrow \mathcal{D}$ ,  $\alpha = (\alpha_{X,Y}: F(X, Y) \rightarrow G(X, Y))_{X,Y \in \mathcal{C}}$  is a dinatural transformation if

$$\begin{array}{ccccc} & & F(X, X) & \xrightarrow{\alpha_{X,X}} & G(X, X) \\ F(f, \text{id}) \swarrow & & & & \searrow G(\text{id}, f) \\ F(Y, X) & & & & G(X, Y) \\ \searrow F(\text{id}, f) & & F(Y, Y) & \xrightarrow{\alpha_{Y,Y}} & G(Y, Y) \\ & & & \nearrow G(f, \text{id}) & \end{array}$$

commutes for any  $f: X \rightarrow Y$

**Example:** evaluation transformation  $\text{ev}: C^X \times X \rightarrow C$

# Higher-Order (Abstract) GSOS

A **higher-order GSOS law** in category  $\mathcal{C}$  consists of

- ▶ **Signature functor**  $\Sigma: \mathcal{C} \rightarrow \mathcal{C}$
- ▶ **Behaviour functor**  $B: \mathcal{C}^{\text{op}} \times \mathcal{C} \rightarrow \mathcal{C}$
- ▶ Family  $(\rho_{X,Y}: \Sigma(X \times B(\boxed{X}, Y)) \rightarrow B(X, \Sigma^*(X + Y)))_{X,Y}$  **natural** in  $Y$ , **dinatural** in  $X$

generalizing **first-order GSOS** <sup>†</sup>

For **combinatory logic**:

- ▶  $\mathcal{C}$  – category of sets
- ▶  $\Sigma X = \coprod_{f \in Ops} X^{\text{arity}(f)}$ ,  $Ops = \{S, S', S'', K, K', I, \cdot\}$
- ▶  $B(X, Y) = Y^X + Y$
- ▶  $\rho$  is induced by rules of operational semantics

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<sup>†</sup> Turi and Plotkin, "Towards a Mathematical Operational Semantics".

# Combinatory Logic as HO-GSOS

For example,

$$\frac{p \rightarrow p'}{p \cdot q \rightarrow p' \cdot q}$$

$$\frac{p \xrightarrow{q} p'}{p \cdot q \rightarrow p'}$$

correspond to

$$\rho((p, p') \cdot (q, \_)) = p' \cdot q$$

$$\rho((p, f) \cdot (q, \_)) = f(q)$$

$$\left( \rho_{X,Y}: \Sigma(X \times (Y + Y^X)) \rightarrow \Sigma^\star(X + Y) + (\Sigma^\star(X + Y))^X \right)$$

# Operational Model

- ▶ We generally obtain **operational model**  $\gamma: \mu\Sigma \rightarrow B(\mu\Sigma, \mu\Sigma)$  by structural recursion  
(=initially of  $\mu\Sigma$ )
- ▶ Explicitly:

$$\gamma = B(\text{id}, \nabla^\sharp) \cdot \rho \cdot \Sigma \langle \text{id}, \gamma \rangle \cdot \iota^{-1}$$

- ▶ For combinatory logic:  $\gamma: \mu\Sigma \rightarrow \mu\Sigma \cup (\mu\Sigma \rightarrow \mu\Sigma)$ ,

$$\gamma(p) = \begin{cases} p' \in \mu\Sigma & \text{if } p \rightarrow p' \\ f \in \mu\Sigma \rightarrow \mu\Sigma & \text{if } \forall x. p \xrightarrow{x} f(x) \end{cases}$$

# Separation

# Strict and Lazy Arguments

In big-step, we cannot frivolously inspect operands:

$$\frac{s \Downarrow K'(r) \quad r \Downarrow v}{s \cdot t \Downarrow v}$$

behaves differently from

$$\frac{s \Downarrow K'(r) \quad t \Downarrow w \quad r \Downarrow v}{s \cdot t \Downarrow v}$$

Separating example:  $K'(I) \cdot \Omega$  (where  $\Omega$  is divergent term, e.g.  $(S \cdot I \cdot I) \cdot (S \cdot I \cdot I)$ )

**Solution:** make do with binary  $\Sigma: \mathcal{C} \times \mathcal{C} \rightarrow \mathcal{C}$ , for strict and lazy arguments

# Separation

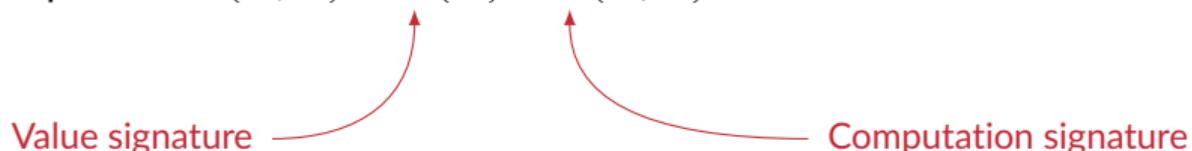
In  $t \Downarrow v \iff t \rightarrow^* v \wedge v \text{ is a value}$  we need to define multistep semantics  $\rightarrow^*$  and values

**Solution:**

- ▶ Involve  $\omega$ -continuous monad  $T$ , i.e such monad that morphisms  $X \rightarrow T(Y + X)$  can be iterated, so that we can define  $\rightarrow^*$  as least fixpoint

**Examples:**  $TX = X + 1$ ,  $TX = \mathcal{P}X$ , monad of probabilistic sub-distributions

- ▶ Assume separation  $\Sigma(X, Y) = \Sigma^v(Y) + \Sigma^c(X, Y)$



## Separated Abstract HO-GSOS

Given  $D: \mathcal{C}^{\text{op}} \times \mathcal{C} \rightarrow \mathcal{C}$ ,  $\Sigma_v: \mathcal{C} \rightarrow \mathcal{C}$ ,  $\Sigma_c: \mathcal{C} \times \mathcal{C} \rightarrow \mathcal{C}$  and a monad  $T$ , **separated abstract HO-GSOS** consists of

$$\rho_X^v: \Sigma_v X \rightarrow D(X, \Sigma^* X)$$

$$\rho_{X,Y}^c: \Sigma_c(X \times (TD(X, Y) + TY), X) \rightarrow T\Sigma^*(X + Y)$$

dinatural in  $X$  and natural in  $Y$ , and a **distributive law**  $\chi_{X,Y}: \Sigma_c(TX, Y) \rightarrow T\Sigma_c(X, Y)$

This is exact **refinement** of abstract HO-GSOS

## Separated Abstract HO-GSOS: Properties

- ▶ Combinatory logic is separated (and so many others)
- ▶ Operational model gets separated to

$$\gamma^v: \Sigma_v \mu\Sigma \rightarrow TD(\mu\Sigma, \mu\Sigma)$$

$$\gamma^c: \Sigma_c(\mu\Sigma, \mu\Sigma) \rightarrow T\mu\Sigma$$

(**Slogan:** Values behave as values, computations as computations)

- ▶ We can define abstract multi-step semantics  $\beta: \mu\Sigma \rightarrow T(\Sigma^v \mu\Sigma)$
- ▶ Monad can be used for modelling other effects, e.g. add **erratic choice** with

$$p + q \rightarrow p \quad p + q \rightarrow q \quad (T = \mathcal{P})$$

# Abstract Big-Step SOS

## Abstract Big-Step SOS

- Abstract big-step SOS is a natural transformation

$$\xi: \Sigma_c(\Sigma_v X, X) \rightarrow T(\Sigma^* X)$$

- Corresponding operational model  $\zeta: \mu\Sigma \rightarrow T(\Sigma_v \mu\Sigma)$  can be defined by recursion (neither structural, nor tail) thanks to assumptions on  $T$
- Assuming that  $T = \text{Id}$ ,  $\xi$  captures two kinds of rules:

$$\frac{}{g(p_1, \dots, p_n) \Downarrow g(p_1, \dots, p_n)} \quad (g \in \Sigma_v)$$

$$\frac{p_1 \Downarrow g_1(p_1^1, \dots, p_{n_1}^1) \dots p_k \Downarrow g_k(p_1^k, \dots, p_{n_k}^k) \quad t \Downarrow v}{f(p_1, \dots, p_k, \dots, p_n) \Downarrow v} \quad (f \in \Sigma_c, g_i \in \Sigma_v)$$

where precisely  $k$  first arguments are strict

# Separation isn't Enough

- Under separability, one still can do wild things, like

$$\frac{p \rightarrow p'}{f(p) \rightarrow g(p')} \quad \frac{p \xrightarrow{p} p'}{f(p) \rightarrow p'}$$

violating the principle:  $p \Downarrow v \wedge f(v) \Downarrow w \implies f(p) \Downarrow w$

↳  $t \Downarrow v \iff t \rightarrow^* v \wedge v$  is a value easily fails

- **Solution:** **strong separation condition**, abstracting the following: if a rule has at least one premise of the form  $x_k \rightarrow x'_k$  then the conclusion of the rule must be

$$f(x_1, \dots, x_n, y_1, \dots, y_m) \rightarrow f(x'_1, \dots, x'_n, y_1, \dots, y_m)$$

where either  $x_i \rightarrow x'_i$  occurs in the premise, or else, the premise contains a labeled transition for  $x_i$ , in which case  $x'_i = x_i$

## Main Result

**Theorem:** Every separated abstract HO-GSOS  $(\rho^v, \rho^c, \chi)$

- ▶ induces abstract big-step SOS law  $(\xi, \chi)$ , and
- ▶ if  $(\rho^v, \rho^c, \chi)$  is strongly separated, then multi-step semantics and big-step operational model agree:

$$\beta = \zeta$$

## Example: Call-by-Value

Call-by-value combinatory logic: combinators as before, plus

$$\frac{t \rightarrow t'}{t \cdot s \rightarrow t' \cdot s} \quad (a)$$

$$\frac{t \xrightarrow{r} t' \quad s \rightarrow s'}{t \cdot s \rightarrow t \cdot s'} \quad (b)$$

$$\frac{t \xrightarrow{s} t' \quad s \xrightarrow{r} s'}{t \cdot s \rightarrow t'} \quad (c)$$

But no rule

$$\frac{t \rightarrow t' \quad s \rightarrow s'}{t \cdot s \rightarrow t' \cdot s'}$$

Hence, no strong separation. Solution: replace (b)-(c) with

$$\frac{s \xrightarrow{r} s'}{s \cdot t \rightarrow s \bullet t}$$

$$\frac{s \rightarrow s'}{t \bullet s \rightarrow t \bullet s'}$$

$$\frac{t \xrightarrow{r} t'}{s \bullet t \rightarrow s \bullet t}$$

$$\frac{t \rightarrow t'}{t \bullet s \rightarrow t' \bullet s}$$

$$\frac{t \xrightarrow{s} t'}{t \bullet s \rightarrow t'}$$

This produces “pretty-big-step semantics”<sup>†</sup>

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<sup>†</sup> Charguéraud, “Pretty-Big-Step Semantics”.

# Languages with Binders

Consider  $\lambda$ -calculus:

Small-step rules:

$$\frac{}{(\lambda x. p)q \rightarrow p[q/x]} \quad (\beta)$$

$$\frac{p \rightarrow p'}{pq \rightarrow p'q} \quad (\text{app})$$

Big-step rules:

$$\frac{}{\lambda x. p \Downarrow \lambda x. p}$$

$$\frac{p \Downarrow \lambda x. p' \quad p'[q/x] \Downarrow v}{pq \Downarrow v}$$

We need to decompose  $(\beta)$  to

$$\frac{p[q/x] = p'}{\lambda x. p \xrightarrow{q} p'}$$

$$\frac{p \xrightarrow{q} p'}{pq \rightarrow p'}$$

Space of substitution actions

So,  $p[q/x] = p'$  becomes new kind of transitions (!)

**Solution:** Upgrade  $\rho^v$  to  $\rho_{X,Y}^v: \Sigma_v(X \times (X \multimap Y)) \rightarrow D(X, \Sigma^*(X + Y))$  use a presheaf category as  $\mathcal{C}$ , for modeling languages with binders<sup>†</sup>

<sup>†</sup> Fiore, Plotkin, and Turi, "Abstract Syntax and Variable Binding".

# Conclusions

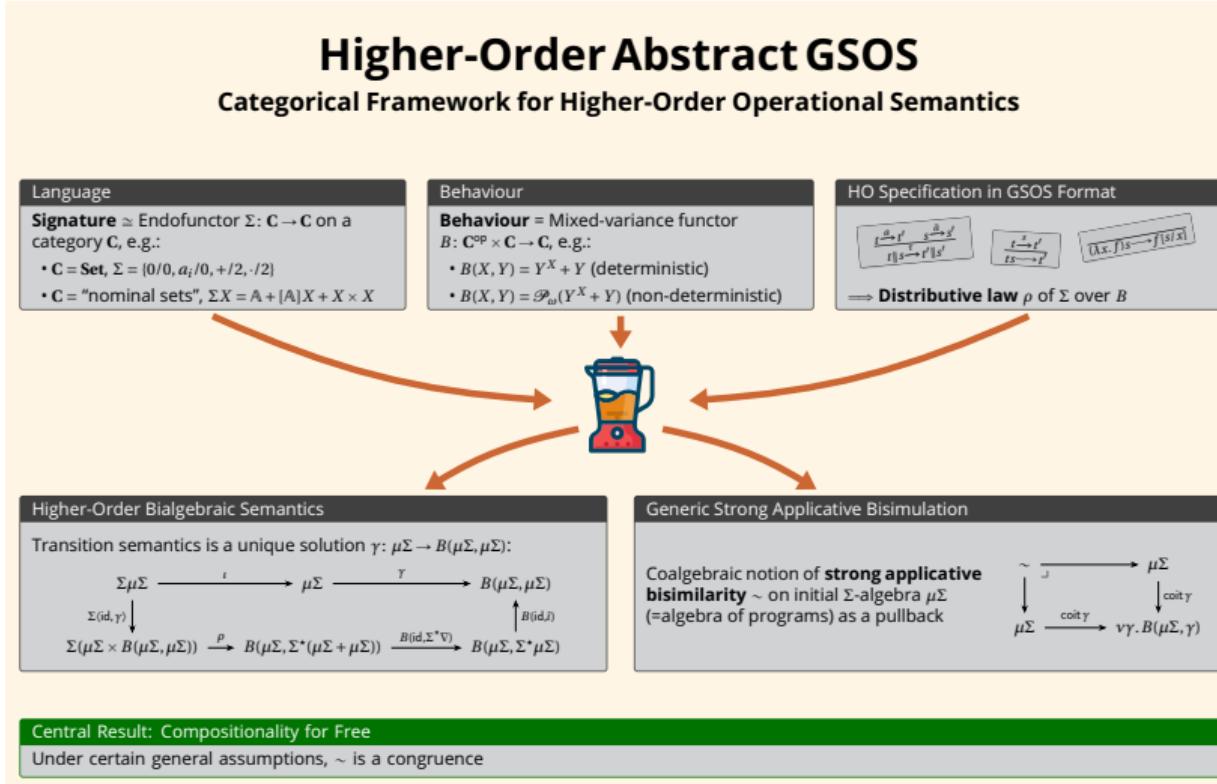
- ▶ Abstract notions of small-step/big-step semantics
- ▶ A general and abstract  $t \Downarrow v \iff t \rightarrow^* v \wedge v \text{ is a value}$
- ▶ Functional implementation in Haskell (artifact – see QR code)

## Further Work:

- ▶ Cost semantics, probabilistic semantics (by varying  $T$ )
- ▶ Equivalence for stateful semantics ( $T = \text{state monad?}$ )
- ▶ Other uses of (strong) separation (compositionality of observational equivalences?)
- ▶ Proof formalization, bridging gap between mathematical theory and implementation beyond purely algebraic signatures



# Thank You for Your Attention!



# Representing Rules

For  $\mathcal{C} = Set$ ,  $\Sigma X = \coprod_{f \in Ops} X^{\text{arity}(f)}$ ,  $B(X, Y) = Y^X + Y$ , HO-GSOS precisely correspond to sets of rules of the form<sup>†</sup>:

$$\frac{(x_j \rightarrow y_j)_{j \in W} \quad (x_i \xrightarrow{z} y_i^z)_{i \in \overline{W}, z \in \{x_1, \dots, x_n\}}}{f(x_1, \dots, x_n) \rightarrow t}$$

or

$$\frac{(x_j \rightarrow y_j)_{j \in W} \quad (x_i \xrightarrow{z} y_i^z)_{i \in \overline{W}, z \in \{x, x_1, \dots, x_n\}}}{f(x_1, \dots, x_n) \xrightarrow{x} t}$$

$$(W \subseteq \{1, \dots, n\}, \overline{W} = \{1, \dots, n\} \setminus W)$$

**Proof Idea:** Yoneda-style argument

 Generally, HO-GSOS vastly abstract this situation

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<sup>†</sup> Goncharov, Milius, Schröder, Tsampas, and Urbat, "Towards a Higher-Order Mathematical Operational Semantics".

# Operational Model

- ▶ Operational model  $\gamma: \mu\Sigma \rightarrow B(\mu\Sigma, \mu\Sigma)$  abstracts derivability of one-step transitions  
 $p \rightarrow p'$ ,  $p \xrightarrow{t} p'$
- ▶ It is a unique solution to

$$\begin{array}{ccc} \Sigma(\mu\Sigma) & \xrightarrow{\iota} & \mu\Sigma \\ \downarrow \Sigma(\text{id}, \gamma) & & \downarrow \gamma \\ \Sigma(\mu\Sigma \times B(\mu\Sigma, \mu\Sigma)) & \xrightarrow{\rho} & B(\mu\Sigma, \Sigma^*(\mu\Sigma + \mu\Sigma)) \xrightarrow{B(\text{id}, \nabla^\sharp)} B(\mu\Sigma, \mu\Sigma) \end{array}$$

- ▶ Alternatively:  $\gamma = B(\text{id}, \nabla^\sharp) \cdot \rho \cdot \Sigma(\text{id}, \gamma) \cdot \iota^{-1}$  (structural recursion)
- ▶ For combinatory logic:  $\gamma(p) = p'$  iff  $p \rightarrow p'$   
and  $\gamma(p) = f$  iff  $\forall x. p \xrightarrow{x} f(x)$

Separated Abstract HO-GSOS  
and Abstract BSSOS  
in Haskell

# Free Functors, and Signatures

```
1  data Free s x = Res x | Cont (s (Free s x))
2  type Initial s = Free s Void
3
4  newtype Mrg s x = Mrg (s x x)
5  sigOp = Cont . Mrg
6
7  data SepSig' sv sc x y = SigV (sv y) | SigC (sc x y)
8  type SepSig sv sc      = Mrg (SepSig' sv sc)
```

# Values, Computations, Behaviours

```
1 type InitialV sv sc = sv (Initial (SepSig sv sc))  
2 type InitialC sv sc = sc (Initial (SepSig sv sc))  
3  
4  
5 data SepBeh d x y = BehV (d x y) | BehC y
```

## SepHOGSOS Type Class

```
1 class (MixFunctor d, Functor sv, Bifunctor sc) => SepHOGSOS sv sc d where
2   rhoV :: sv x -> d x (Free (SepSig sv sc) x)
3   rhoC :: sc (x, SepBeh d x y) x
4                           -> Free (SepSig sv sc) (Either x y)
```

# Operational Model

```
1 gammaV :: InitialV sv sc ->
2     d (Initial (SepSig sv sc)) (Initial (SepSig sv sc))
3 gammaV t = mvmap id join $ rhoV t
4
5 gammaC :: Proxy d ->
6     InitialC sv sc -> Initial (SepSig sv sc)
7 gammaC (p :: Proxy d) t =
8     (rhoC @_ @_ @d $ first (id &&& gamma) t) >>= nabla
9     where
10    nabla = either id id
11    gamma (Cont (Mrg (SigV v))) = BehV $ gammaV v
12    gamma (Cont (Mrg (SigC c))) = BehC $ gammaC p c
```

# Multi-Step Semantics

```
1  beta :: (Functor sv, Bifunctor sc, MixFunctor d, SepHOGSOS sv sc d) =>
2    Proxy d -> Initial (SepSig sv sc) -> InitialV sv sc
3
4  beta (p :: Proxy d) (Cont (Mrg (SigV v))) = v
5  beta (p :: Proxy d) (Cont (Mrg (SigC c))) =
6    beta p (gammaC p c)
```

# XCL Signature

```
1  data XCLV x
2      = S
3      | K
4      | I
5      | S' x
6      | K' x
7      | S'' x x
8
9  data XCLC x y
10     = Comp x y
```

# XCL as SepHOGSOS

```
1 instance SepHOGSOS XCLV XCLC (->) where
2   rhoV S = sigOp . SigV . S' . Res
3   rhoV K = sigOp . SigV . K' . Res
4   rhoV I = Res
5   rhoV (S' t) = sigOp . SigV . S'' (Res t) . Res
6   rhoV (K' t) = const (Res t)
7   rhoV (S'' t s) = \r -> sigOp $ SigC $ Comp
8     (sigOp $ SigC $ Comp (Res t) (Res r))
9     (sigOp $ SigC $ Comp (Res s) (Res r))
10
11  rhoC (Comp (_, BehC s) r) =
12    sigOp (SigC $ Comp (Res $ Right s) (Res $ Left r))
13  rhoC (Comp (_, BehV f) r) = Res (Right $ f r)
```

# BSSOS Type Class

```
1  class (Functor sv, Bifunctor sc) => BSSOS d sv sc where
2    xi :: sc (sv x) x -> Free (SepSig sv sc) x
3
4    zeta' :: Initial (SepSig sv sc) -> InitialV sv sc
5    zeta' (Cont (Mrg (SigV v))) = v
6    zeta' (Cont (Mrg (SigC c))) = zeta' @d $ join $ xi @d $ first (zeta' @d
7      ) c
8
9    zeta :: InitialC sv sc -> InitialV sv sc
10   zeta = zeta' @d . sigOp . SigC
```

# From SepHOGSOS to BSSOS

```
1 instance (SepHOGSOS sv sc d) => BSSOS d sv sc where
2   xi :: sc (sv x) x -> Free (SepSig sv sc) x
3   xi t = rhoCV (bimap ((sigOp . SigV &&
4                         mx_second @d join . rhoV)
5                         . fmap return)
6                         return t)
7   >>= nabla
8 where nabla = either id id
```

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