CelOWS: uma arquitetura orientada a serviços para definição, pesquisa e reuso de modelos biológicos

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***Abstract**: The amount of information generated by research in biological science has lead to an intensive use of models. Mathematical and computational modeling need accurate description to share, reuse and simulate models as formulated by original authors. In this paper we introduce the Cell Component Ontology - CelO, an ontology expressed in OWL-DL. This ontology captures both the structure of a cell model and the properties of functional components. We are using this ontology in a Web project where the use of CelO allows describing, reasoning, querying and composing CellML models. It aims to improve reuse and composition of existent components and allow semantic validation of new models.*

***Resumo:** A quantidade e variedade de informações geradas pelas ciências biológicas têm levado a um uso intenso de modelos na área. Neste contexto, tanto a modelagem matemática quanto a modelagem computacional necessitam de uma descrição acurada que permita que esses modelos sejam compartilhados, reutilizados e simulados tal como foram formulados por seus criadores. Neste artigo, apresentamos a Cell Component Ontology CelO, uma ontologia expressa em OWL-DL, que captura tanto a estrutura do modelo de uma célula quanto as propriedades dos seus componentes funcionais. A ontologia CelO é utilizada em uma arquitetura orientada a serviços para descrever, realizar inferências e consultar os modelos CellML. O objetivo principal da arquitetura é facilitar o reuso e a composição dos componentes existentes e permitir a validação semântica de novos modelos.*

1. Introdução

[illegible]

[illegible]

[illegible]

E [illegible] CeML [CeML 2008] [illegible] XML (*eXte* [illegible] *e*) CeML [illegible] M ML (*e* [illegible] *e*) [illegible] CeML [illegible] N [illegible] CeML [illegible]

P [illegible] CeOWS CeOWS [illegible] CeO (*e* [illegible] *e* [illegible]) O [illegible] CeOWS [illegible] O [illegible] CeO [illegible] OWL-DL [Be [illegible] fe 2004] [illegible]

N [illegible] 2 [illegible] CeML A [illegible] 3 [illegible] CeO [illegible] A [illegible] CeOWS [illegible] 4 A [illegible] 5 e [illegible] 6 [illegible]

2. Conceitos Relacionados

Ontologia

U [illegible] [G [illegible] 1994][B [illegible] 1997] Ne [illegible] “f [illegible] (exe [illegible]); “ex [illegible]” [illegible] “ [illegible] ; “ [illegible] ” [illegible] “ [illegible] z çã ” [illegible]

A [illegible] í [illegible] A [illegible]

[illegible]

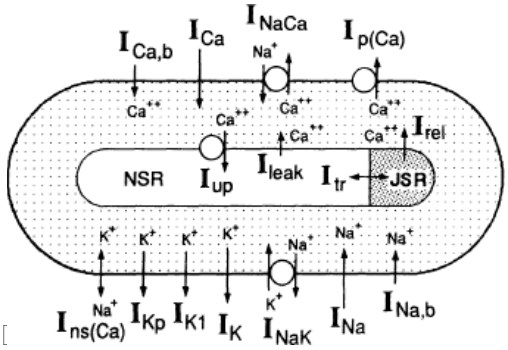
Ex[illegible] OWL ([illegible]) OWL [illegible] W3C [illegible] SWRL ([illegible]) [H[illegible]k 2004] SWRL [illegible] OWL.

Modelos biológicos

N[illegible] ex[illegible] “[illegible]” C[illegible] A[illegible] ex[illegible]

Eletrofisiologia da célula cardíaca

O[illegible] [N[illegible]ke[illegible] H[illegible] 2006] O[illegible] C[illegible] 1[illegible] L[illegible]-R[illegible]y II[illegible] [L[illegible] R[illegible]y 1994] D[illegible] ex[illegible] à[illegible] E[illegible] CeML[illegible]



b. Currents through the L-type Ca^{2+} channel

$I_{Ca,t}=I_{Ca}+I_{Ca,K}+I_{Ca,Na}$;

$I_{Ca}=d\cdot f\cdot f_{Ca}\cdot I_{Ca}$; $I_{Ca,K}=d\cdot f\cdot f_{Ca}\cdot \bar{I}_{Ca,K}$; and $I_{Ca,Na}=d\cdot f\cdot f_{Ca}\cdot \bar{I}_{Ca,Na}$.

For ion S, including Ca^{2+}, Na^+, and K^+,

$$\bar{I}_S=P_S\cdot z_s^2\cdot\frac{VF^2}{RT}\cdot\frac{\gamma_{si}\cdot[S]_i\cdot\exp(z_sVF/RT)-\gamma_{so}\cdot[S]_o}{\exp(z_sVF/RT)-1};$$

$P_{Ca}=5.4\times10^{-4}$ cm/s; $\gamma_{Cai}=1$; $\gamma_{Cao}=0.341$;

$P_{Na}=6.75\times10^{-7}$ cm/s; $\gamma_{Nai}=\gamma_{Nao}=0.75$;

$P_K=1.93\times10^{-7}$ cm/s; $\gamma_{Ki}=\gamma_{Ko}=0.75$;

$f_{Ca}=1/[1+([Ca^{2+}]_i/K_{m,Ca})^2]$; $K_{m,Ca}=0.6$ μmol/L;

$d_\infty=1/\{1+\exp[-(V+10)/6.24]\}$;

$\tau_d=d_\infty\cdot\{1-\exp[-(V+10)/6.24]\}/[0.035\cdot(V+10)]$;

$f_\infty=1/\{1+\exp[(V+35.06)/8.6]\}+0.6/\{1+\exp[(50-V)/20]\}$;

$$\tau_f=1/\left(0.0197\cdot\exp\{-[0.0337\cdot(V+10)]^2\}+0.02\right);$$

$\alpha_d=d_\infty/\tau_d$; $\beta_d=(1-d_\infty)/\tau_d$; $\alpha_f=f_\infty/\tau_f$; and $\beta_f=(1-f_\infty)/\tau_f$.

Figura 1. Diagrama e equações modelo Luo-Rudy II, extraídas do artigo original [LUO, RUDY 1994].

CellML

Ce ML [illegible] XML [illegible] O [illegible] C [illegible] exe [illegible] D [illegible] çã [illegible]

U [illegible] URI (*e* *e* *e Ide* *fie*) E çõe [illegible] ex [illegible] M ML [illegible] U [illegible] çõe U [illegible] ([illegible] f [illegible] úl [illegible] / [illegible]) [illegible] C exõe [illegible] ã [illegible]

3. Cell Component Ontology - CelO

O je [illegible] CelO [illegible] O [illegible] ex [illegible] çã [illegible] z [illegible] çã [illegible] We [illegible] A [illegible] f [illegible] çõe [illegible] çã [illegible] Ce ML [illegible] AGOS [B [illegible] 2006] e PCE [PCE 2008] [illegible] w kf w [illegible]

3.1. Classes

A [illegible] CelO [illegible] (2) E [illegible]:

- **SI** [illegible]: G [illegible] ez [illegible] à [illegible]
- [illegible]: C [illegible] í [illegible] B [illegible]
- [illegible]: C [illegible]

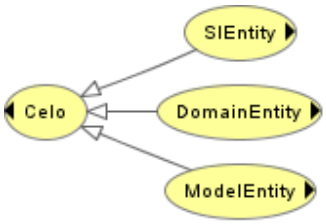


Figura 2. Nível topo da ontologia CelO.

Ne [illegible] ex [illegible] CeWS A [illegible] :// [illegible] fjf [illegible]

A [illegible] (3) [illegible] O [illegible] CeML [illegible]

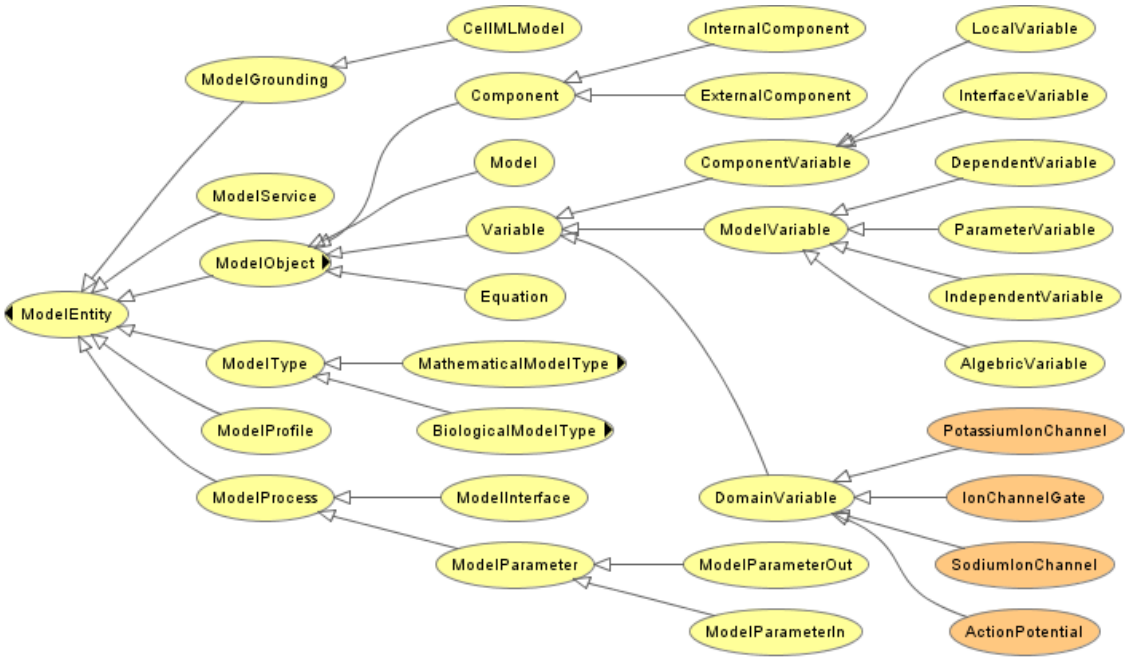


Figura 3. Classe ModelEntity da ontologia CelO.

U [illegible] CeOWS [illegible] we [illegible] “exe [illegible]) A [illegible] S [illegible] OWL-S [M [illegible] 2004] [illegible] we U [illegible] S [illegible]

[illegible] f [illegible] URI [illegible] CeML [illegible] ej [illegible] (I) [illegible] (I) [illegible] E [illegible]

[illegible] j [illegible] je [illegible] q [illegible] M ML V [illegible]

[illegible]

3.2. Regras Semânticas

[illegible]

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De[illegible]e[illegible]e[illegible]e[illegible]e[illegible]
[illegible]e[illegible]) ^ [illegible]h[illegible]De[illegible] [illegible]2) ^ [illegible]De[illegible]e[illegible]U[illegible]3) ^
[illegible]h[illegible]N[illegible]e[illegible]3[illegible] [illegible]4) ^ [illegible]w[illegible]Eq[illegible]I[illegible]eC[illegible]e[illegible]2[illegible] [illegible]4) ^ [illegible]e[illegible]e[illegible]e[illegible]3[illegible] [illegible]
[illegible]5) → [illegible]e[illegible]h[illegible]Me[illegible]e[illegible] [illegible]5)
Se [illegible] v[illegible]áve[illegible] [illegible] [illegible] [illegible] [illegible] [illegible]e[illegible]e [illegible] [illegible]he [illegible]2 q[illegible]e é [illegible] [illegible] [illegible]e [illegible]4 [illegible]e
[illegible] [illegible]e [illegible]3 q[illegible]e [illegible]e [illegible] [illegible] [illegible]ez[illegible] [illegible]5[illegible] e[illegible]ã[illegible] [illegible] v[illegible]áve[illegible] [illegible] [illegible]e [illegible] [illegible]ez[illegible] [illegible]5
[illegible]e[illegible]e[illegible]e[illegible]e[illegible]e[illegible]e[illegible]e[illegible]e[illegible]e[illegible])[illegible]
[illegible]e[illegible]) ^ [illegible]e[illegible]h[illegible]De[illegible] [illegible]2) ^ [illegible]e[illegible]Che[illegible]E[illegible]3) ^
[illegible]e[illegible]h[illegible]N[illegible]e[illegible]3[illegible] [illegible]4) ^ [illegible]w[illegible]Eq[illegible]I[illegible]eC[illegible]e[illegible]2[illegible] [illegible]4) ^
[illegible]e[illegible]h[illegible]eU[illegible] [illegible]5) ^ [illegible]e[illegible]h[illegible]N[illegible]e[illegible]5[illegible] [illegible]6) ^ [illegible]w[illegible]Eq[illegible]6[illegible]
"[illegible]e[illegible]e[illegible]") → [illegible]e[illegible]h[illegible]D[illegible]E[illegible] [illegible]3)
Se [illegible] v[illegible]áve[illegible] [illegible] [illegible] [illegible] [illegible] [illegible]e[illegible]e [illegible] [illegible]he [illegible]2 q[illegible]e é [illegible] [illegible] [illegible]e [illegible]4 [illegible]e [illegible]
e[illegible]e[illegible] q[illegible]í[illegible] [illegible]3 e e[illegible] v[illegible]áve[illegible] [illegible]ã[illegible] é [illegible]e[illegible] e[illegible] é [illegible] [illegible] e[illegible]e[illegible]
q[illegible]í[illegible] [illegible]vé[illegible] [illegible] [illegible]e[illegible]e h[illegible]D[illegible]E[illegible]
[illegible]e[illegible]â[illegible]e[illegible]B[illegible]E[illegible]y[illegible]
[illegible]e[illegible]) ^ [illegible]e[illegible]h[illegible]De[illegible] [illegible]2) ^ [illegible]e[illegible]B[illegible]E[illegible]3) ^
[illegible]e[illegible]h[illegible]N[illegible]e[illegible]3[illegible] [illegible]4) ^ [illegible]w[illegible]Eq[illegible]I[illegible]eC[illegible]e[illegible]2[illegible] [illegible]4) →
[illegible]e[illegible]h[illegible]D[illegible]E[illegible] [illegible]3)
Se [illegible] v[illegible]áve[illegible] [illegible] [illegible] [illegible] [illegible] [illegible]e[illegible]e [illegible] [illegible]he [illegible]2 q[illegible]e é [illegible] [illegible] [illegible]e [illegible]4 [illegible]e
[illegible] e[illegible]e [illegible]ó[illegible] [illegible]3[illegible] e[illegible]ã[illegible] [illegible] v[illegible]áve[illegible] [illegible] é [illegible] à e[illegible]e [illegible]ó[illegible] [illegible]vé[illegible]
[illegible] [illegible]e[illegible]e h[illegible]D[illegible]E[illegible]
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Figura 4 Exemplos de regras usadas com a ontologia CelO.

4. CelOWS: uma arquitetura para aplicações em e-science

[illegible]

O [illegible] je [illegible] CeloWS [illegible] e [illegible] f [illegible] e [illegible] e [illegible] e [illegible] e [illegible] çã [illegible] çã [illegible] e exe [illegible] çã [illegible] ([illegible] çã) [illegible] e [illegible] z [illegible] E [illegible] e f [illegible] e e CeloWS [illegible] e [illegible]:

- Re [illegible] e [illegible] ze [illegible] e [illegible] e [illegible] e [illegible] (e [illegible]) [illegible] e [illegible] e [illegible] e â [illegible] e [illegible] z [illegible] e [illegible] e [illegible] e [illegible] e [illegible] e [illegible] e [illegible] e [illegible] e [illegible] e [illegible]
- Pe [illegible] e [illegible] e [illegible] e â [illegible] ex [illegible] e [illegible] e [illegible]
- C [illegible] çã [illegible] e [illegible] e [illegible] e [illegible] e [illegible] ex [illegible] e [illegible] e [illegible] e [illegible] ze [illegible] e [illegible]
- Exe [illegible] çã [illegible] e [illegible] e [illegible] ej [illegible] ã [illegible] e [illegible] fe [illegible] e [illegible] e [illegible] e [illegible] çã [illegible] e [illegible] e [illegible] e [illegible] e [illegible]

C [illegible] j [illegible] e [illegible] çã [illegible] e â [illegible] e [illegible] e [illegible] e [illegible] f [illegible] e [illegible] e [illegible] çã [illegible] e [illegible] e [illegible] efe [illegible] e [illegible] e [illegible] e [illegible] fe [illegible] e [illegible] j ex [illegible] e [illegible] z [illegible] e f ex [illegible] e [illegible] e [illegible] e [illegible] e [illegible] e [illegible] e [illegible] e [illegible] e-[illegible] e [illegible]

CeloWS [illegible] e [illegible] e [illegible] e ç we [illegible] I [illegible] e [illegible] e [illegible] çã [illegible] e [illegible] e f [illegible] e [illegible] e [illegible] e [illegible] e w kf w [illegible] e íf [illegible] e [illegible] C [illegible] e [illegible] e [illegible] e [illegible] e ç we [illegible] e [illegible] e exe [illegible] e [illegible] e (e f [illegible] e [illegible] e [illegible] e [illegible] e [illegible]) [illegible] f [illegible] e [illegible] z çã [illegible] exe [illegible] çã [illegible] e [illegible]

U [illegible] ã [illegible] e [illegible] e [illegible] CeloWS [illegible] e [illegible] 5 N f [illegible] *I* [illegible] *e* [illegible] e [illegible] URI [illegible] e CeloA [illegible] e [illegible] (*e*) [illegible]:

- [illegible] **WS**: I [illegible] e [illegible] e ç we [illegible] e [illegible] e [illegible] e [illegible] e [illegible] çã [illegible] e [illegible] e [illegible] e [illegible] e [illegible] e f [illegible] e [illegible] e [illegible] e [illegible] e ç [illegible] f [illegible] e [illegible] çã [illegible] fe [illegible] e [illegible] j ex [illegible] e [illegible]
- **B** [illegible] **k** [illegible]: [illegible] e [illegible] e [illegible] e [illegible] e ç [illegible] e [illegible] CeloWS [illegible] e [illegible] e [illegible] (CeloWS-DB) e exe [illegible] çã [illegible] e fe [illegible] e [illegible] çã [illegible] e CellML [illegible]
- [illegible]: [illegible] e [illegible] e f [illegible] e [illegible] çã [illegible] e [illegible] e [illegible] e [illegible] e [illegible] e [illegible] e [illegible] e ç we [illegible]

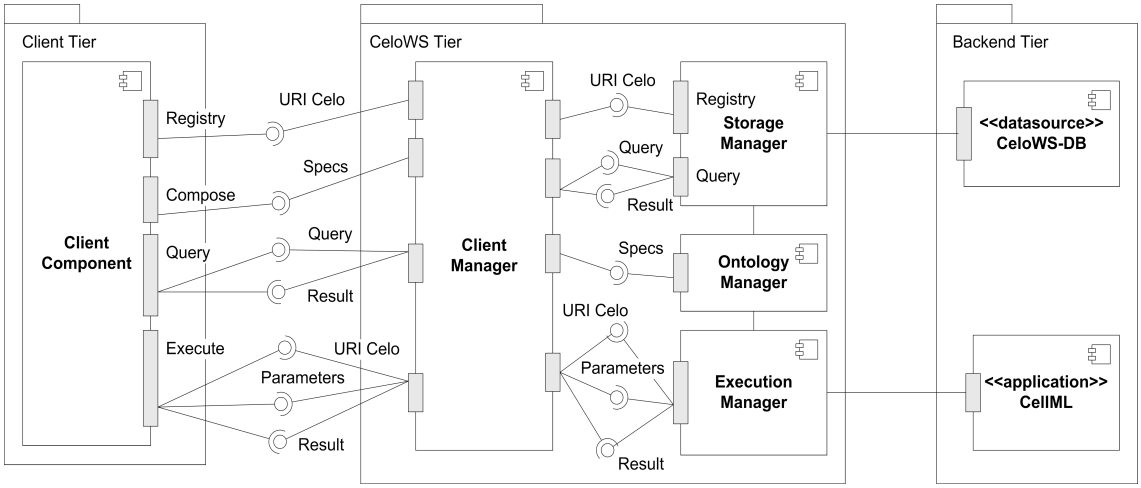

Figura 5 - Visão geral da arquitetura do framework CeloWS.

[illegible]

- **R**[illegible]: [illegible]
- [illegible]
- **Q**[illegible]: [illegible] SPARQL [SPARQL 2008] [illegible]
- [illegible]

[illegible]

- [illegible]
- **S**[illegible]: [illegible]
- [illegible] API ([illegible]) [illegible]
- [illegible]

4.3. Cenários de uso

[illegible]

- [illegible]
- [illegible]
- [illegible]

e [illegible] e [illegible] í [illegible] e [illegible] e [illegible] z [illegible] e [illegible] z [illegible] e [illegible] e [illegible] â [illegible] e [illegible]

- O [illegible] e [illegible] e [illegible] z [illegible] e [illegible] z [illegible] ex [illegible] e [illegible] çã [illegible] e [illegible] e [illegible] j [illegible] ex [illegible] e [illegible] U [illegible] e [illegible] CeML [illegible] e [illegible] e [illegible] e [illegible] çã [illegible] O [illegible] e [illegible] çã [illegible] e [illegible] e [illegible] ex [illegible]

A [illegible] z çã [illegible] efe [illegible] f [illegible] CeOWS [illegible] e [illegible] çã [illegible] e [illegible] çõe [illegible] f [illegible] z [illegible] e f [illegible] f [illegible] e [illegible] e [illegible] ç [illegible] fe e [illegible] CeOWS [illegible]

4.4. Testes do protótipo

P [illegible] e e [illegible] çã [illegible] f [illegible] e CeOWS [illegible] f [illegible] í [illegible] O [illegible] e e [illegible] e ç [illegible] e [illegible] e [illegible] çã [illegible] e [illegible] e [illegible]

[illegible] **çã** [illegible] **:** P [illegible] çã [illegible] e [illegible] z [illegible] f [illegible] 8 ([illegible]) [illegible] e [illegible] CeML C [illegible] exe [illegible] e [illegible] "A M [illegible] f [illegible] f [illegible] e H [illegible] k [illegible]-H x ey E [illegible] A [illegible] e [illegible] P [illegible] k [illegible] je [illegible] e A [illegible] P [illegible] e-M ke [illegible] P [illegible] e [illegible]" [illegible] e e [illegible] 6 [illegible] e [illegible] D [illegible] e C [illegible] e e UML [illegible] O [illegible] e e [illegible] e e e [illegible] exõe [illegible] (e [illegible] z [illegible] exõe [illegible] e [illegible] e [illegible] â e [illegible] e f e [illegible])

C [illegible] e e [illegible] 8 [illegible] e e : [illegible] *e* [illegible] *e* [illegible], [illegible] *e*, [illegible] *e* [illegible], [illegible] _ [illegible] *e*, [illegible] _ [illegible] *e* [illegible] *e*, [illegible] *d* [illegible] _ [illegible] *e*, [illegible] *d* [illegible] _ [illegible] *e* [illegible] *e*, [illegible] *d* [illegible] _ [illegible] *e* [illegible] *e* N [illegible] e [illegible] e [illegible] f [illegible] - e 8 [illegible] CeML ([illegible] e [illegible] ô [illegible]) [illegible] e [illegible] 8 [illegible] e [illegible] CeO O [illegible] efe e e [illegible] e [illegible] ô [illegible] e [illegible] e [illegible] e [illegible] CeO [illegible] e [illegible] e ã [illegible] í e [illegible] je [illegible] ([illegible] :// e [illegible] fjf [illegible])

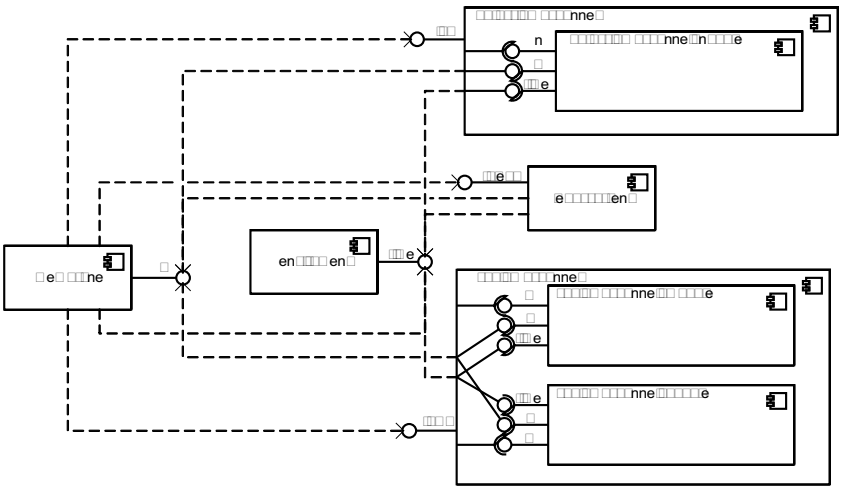

Figura 6 - Modelo usado nos testes com o protótipo.

A [illegible] çã [illegible] e [illegible] ô [illegible] je [illegible] e e í f [illegible] e CeOWS A [illegible] e çã [illegible] e [illegible] z çã [illegible] e [illegible] e e ex [illegible] e [illegible] çã [illegible] e [illegible] e [illegible] z [illegible] e [illegible] ex [illegible] A [illegible]

[illegible] [illegible]çã[illegible]z [illegible] [illegible] [illegible] [illegible]e [illegible]CellML [illegible] [illegible] [illegible]e [illegible] [illegible]e [illegible] [illegible]e [illegible] [illegible]e [illegible]ef[illegible]e [illegible] exã[illegible] [illegible] [illegible]e [illegible] [illegible]e [illegible]

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Figura 7 - Arquivo de configuração para composição do modelo.

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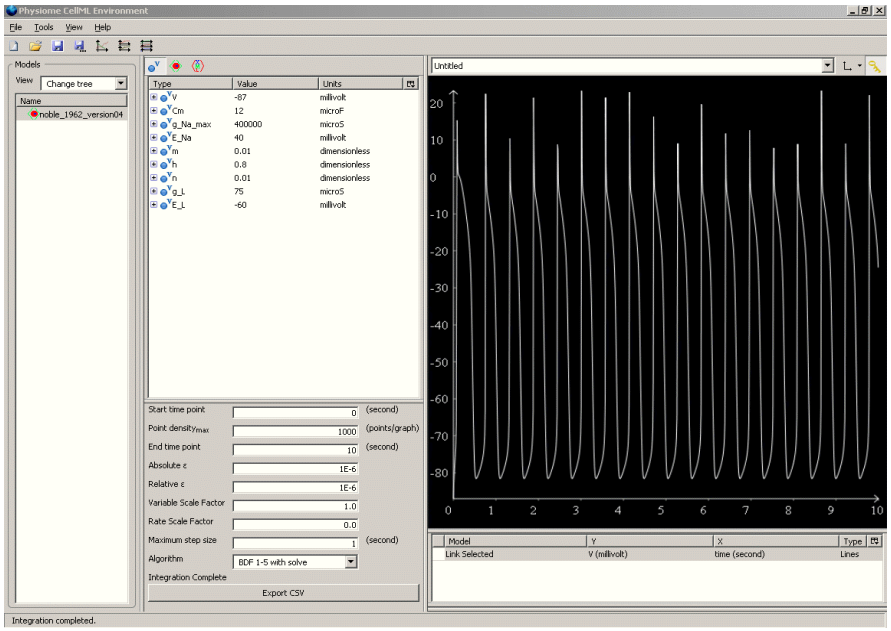

Figura 8. Gráfico V x time gerado usando o modelo CellML original.

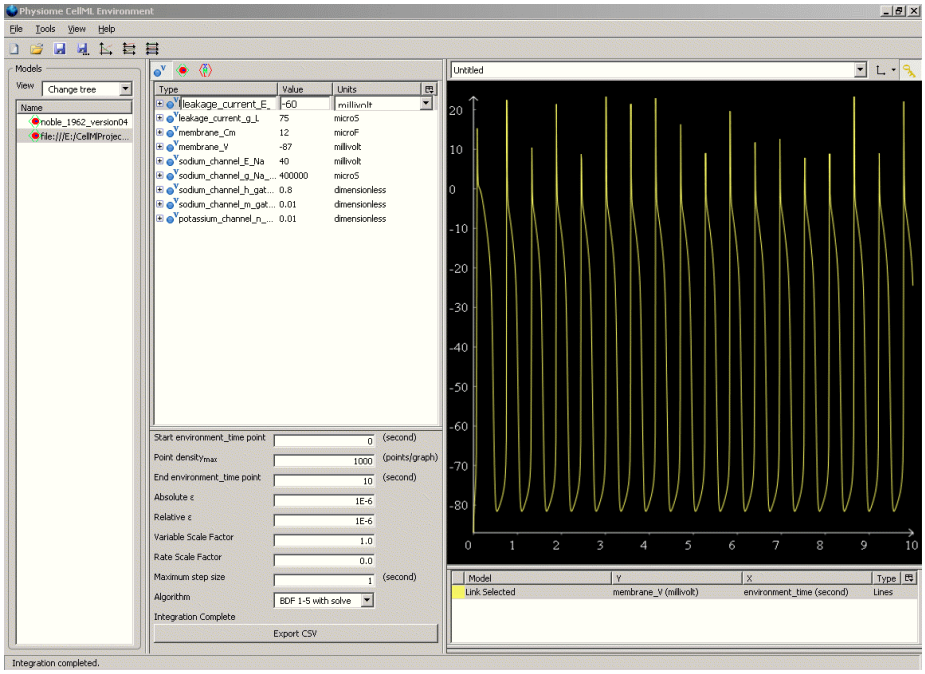

Figura 9- Gráfico V x time gerado usando o modelo CellML gerado a partir do modelo CelO.

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[illegible] WHERE {
[illegible]
}
```

Figura 10 - Consultas SPARQL para buscas no repositório de ontologias.

4.5. Detalhes de Implementação

[illegible]

5. Trabalhos Correlatos

[illegible]

[illegible]

[illegible]

6. Considerações Finais

[illegible]

[illegible]

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