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Diff Studio: Ecosystem for Interactive Modeling by Ordinary Differential Equations

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Software

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Summary

Ordinary differential equations (ODEs), typically formulated as initial value problems (IVPs), are widely used to model the dynamics of complex systems. They are utilized in many domains, including physical processes (Chicone, 2006), biochemical kinetics (Ingalls, 2013), drug delivery systems (Mircioiu et al., 2019), cloud computing (Ghomi et al., 2019), and population dynamics (Hastings, 2013).

While a broad ecosystem of mature numerical solvers exists, effective **interactive exploration**, **reproducible computation**, and **collaborative model development** remain difficult to achieve - particularly in browser-based environments. Most existing tools are designed around desktop or scripting workflows and provide limited support for real-time interaction, model sharing, or collaborative analysis.

Diff Studio is a **browser-native environment for solving and exploring IVPs**, designed to support interactive, collaborative, and reproducible ODE modeling without custom software development or local environment setup. It enables users to define models declaratively, explore their behavior interactively, and share fully reproducible simulations through the browser.

Diff Studio consists of two components: 1. **Diff Grok**: general-purpose high-performance TypeScript library for solving ODE systems defined in a declarative form 2. **Diff Studio**: web application that integrates Diff Grok into the **Datagrok** scientific computing platform. It provides autogenerated user interface, rich interactive visualizations, and the ability to manage ODE models and simulations.

Statement of need

ODEs can be solved either analytically or numerically. Analytic methods provide exact solutions but apply only to limited classes of problems and are often impractical due to their complexity (Hairer et al., 2008). Numerical methods, which compute approximate solutions, are therefore the dominant approach. A wide range of such methods has been developed (Hairer et al., 2008; Hairer & Wanner, 2002) and is available in established scientific computing tools, including SUNDIALS (Gardner et al., 2022; Hindmarsh et al., 2005), Julia DifferentialEquations (Rackauckas & Nie, 2017), SciPy (Virtanen et al., 2020), Maple (Maplesoft, 2025), Mathematica (Wolfram Research Inc., 2024), Matlab (The MathWorks Inc., 2022), and deSolve (Soetaert et al., 2010).

These tools provide robust and efficient solvers but are primarily designed for **desktop or scripting-centric workflows**. In practice, scientific modeling is often exploratory: researchers iteratively adjust parameters, inspect transient behavior, compare scenarios, and refine model structure. Collaboration across teams and institutions is also common. Existing solutions typically require local installation, environment configuration, and custom scripting, which complicates sharing models and reproducing results. Building interactive analysis tools on top of these systems often requires substantial additional programming effort, shifting focus away from scientific inquiry toward software engineering.

Diff Studio addresses these limitations by providing a **browser-native**, **interactive modeling environment** that combines numerical performance with ease of use. It supports low-code model definition, immediate visual feedback, and seamless sharing of fully reproducible simulations via the web.

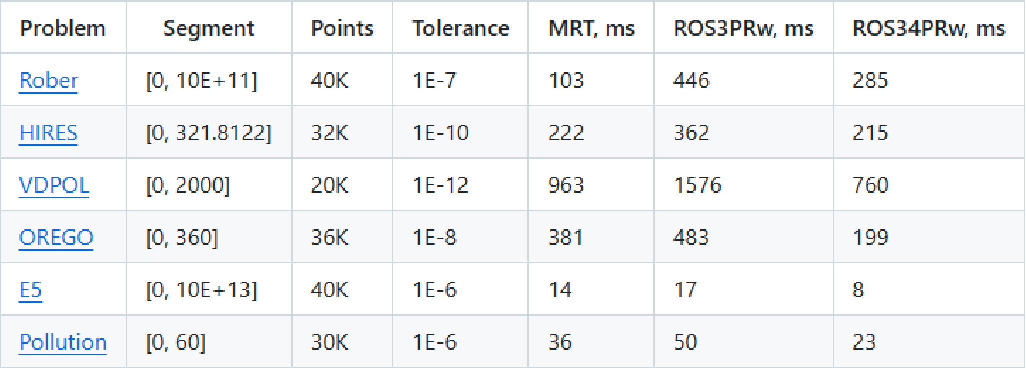
The solution: Diff Studio

Delivering high-performance ODE modeling in the browser introduces additional technical challenges. Approaches based on WebAssembly (*WebAssembly Specification*, 2025) or Pyodide (*Pyodide*, 2025) enable reuse of existing numerical libraries but impose important trade-offs. WebAssembly offers near-native performance for code written in C/C++ or Rust, but typically requires recompilation when equations or model structure change, limiting flexibility during iterative model design. Pyodide provides a WebAssembly-based Python environment that supports NumPy and SciPy but incurs large download sizes, potential performance overhead, and less seamless integration with browser APIs and reactive user interfaces.

In contrast, pure JavaScript and TypeScript solutions integrate naturally with the browser execution model and user interface frameworks. However, existing libraries such as Math.js (*MathJS*, 2025) and odex-js (*Odex-Js* , 2025) expose low-level APIs and generally require programming expertise from end users.

Diff Studio adopts a TypeScript-native approach combined with declarative modeling to eliminate the need for programming expertise while preserving performance and flexibility. Its core numerical engine, Diff Grok, provides:

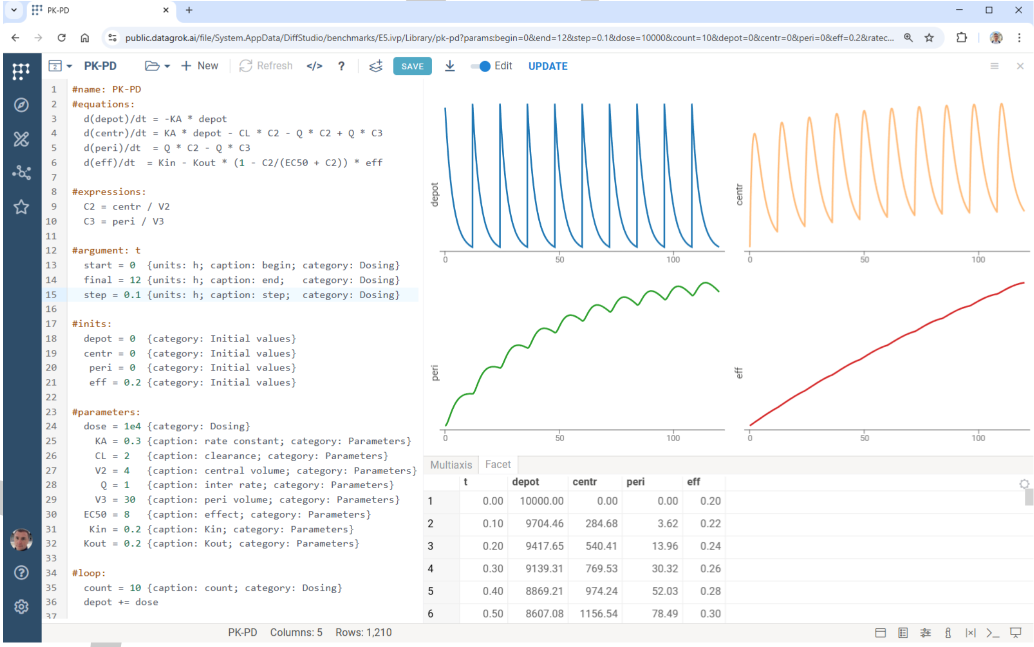
- **Solving tools**: A collection of numerical methods. Diff Grok implements the modified Rosenbrock triple (MRT) (Shampine & Reichelt, 1997), ROS3PRw (Jax et al., 2021), and ROS34PRw (Rang, 2015) methods, supporting both stiff and non-stiff systems. Performance was benchmarked on standard test problems including Robertson (Robertson, 1966), HIRES (Schäfer, 1975), VDPOL (Pol (van der), 1926), OREGO (Hairer & Wanner, 2002), E5 (Hairer & Wanner, 2002), and Pollution (Verwer, 1994). The results demonstrate near-real-time performance suitable for interactive exploration (see Figure 1).
- **Computational pipelines**: Support for multi-stage modeling and solving workflows executed in web workers, enabling parallel computation. These pipelines are used for parameter optimization and sensitivity analysis directly in the browser.
- **Declarative modeling language**: A domain-specific language for specifying IVPs as text, including equations and annotated model inputs. This representation supports automatic interface generation.



Problem	Segment	Points	Tolerance	MRT, ms	ROS3PRw, ms	ROS34PRw, ms
Rober	[0, 10E+11]	40K	1E-7	103	446	285
HIRES	[0, 321.8122]	32K	1E-10	222	362	215
VDPOL	[0, 2000]	20K	1E-12	963	1576	760
OREGO	[0, 360]	36K	1E-8	381	483	199
E5	[0, 10E+13]	40K	1E-6	14	17	8
Pollution	[0, 60]	30K	1E-6	36	50	23

Figure 1: Diff Grok performance: computational time comparison.

Diff Studio integrates Diff Grok into the Datagrok platform, providing a complete web application for ODE modeling. It includes an equations editor (Figure 2), an autogenerated interactive user interface (Figure 3), and rich visualization capabilities.


PK-PD
public.datagrok.ai/file/System.AppData/DiffStudio/benchmarks/E5.ivp/Library/pk-pd?params:begin=0&end=12&step=0.1&dose=10000&count=10&depot=0&centr=0&peri=0&eff=0.2&ratec...
PK-PD
New
Refresh
</>
?
SAVE
Edit
UPDATE
depot
centr
peri
eff
0
50
100
Multiaxis
Facet

```
#name: PK-PD
#equations:
  d(depot)/dt = -KA * depot
  d(centr)/dt = KA * depot - CL * C2 - Q * C2 + Q * C3
  d(peri)/dt  = Q * C2 - Q * C3
  d(eff)/dt  = Kin - Kout * (1 - C2/(EC50 + C2)) * eff

#expressions:
  C2 = centr / V2
  C3 = peri / V3

#argument: t
  start = 0  {units: h; caption: begin; category: Dosing}
  final = 12 {units: h; caption: end;   category: Dosing}
  step = 0.1 {units: h; caption: step;  category: Dosing}

#inits:
  depot = 0  {category: Initial values}
  centr = 0  {category: Initial values}
   peri = 0  {category: Initial values}
   eff = 0.2 {category: Initial values}

#parameters:
  dose = 1e4 {category: Dosing}
    KA = 0.3 {caption: rate constant; category: Parameters}
    CL = 2   {caption: clearance; category: Parameters}
    V2 = 4   {caption: central volume; category: Parameters}
     Q = 1   {caption: inter rate; category: Parameters}
    V3 = 30  {caption: peri volume; category: Parameters}
  EC50 = 8   {caption: effect; category: Parameters}
   Kin = 0.2 {caption: Kin; category: Parameters}
  Kout = 0.2 {caption: Kout; category: Parameters}

#loop:
  count = 10 {caption: count; category: Dosing}
  depot += dose
```

	t	depot	centr	peri	eff
1	0.00	10000.00	0.00	0.00	0.20
2	0.10	9704.46	284.68	3.62	0.22
3	0.20	9417.65	540.41	13.96	0.24
4	0.30	9139.31	769.53	30.32	0.26
5	0.40	8869.21	974.24	52.03	0.28
6	0.50	8607.08	1156.54	78.49	0.30

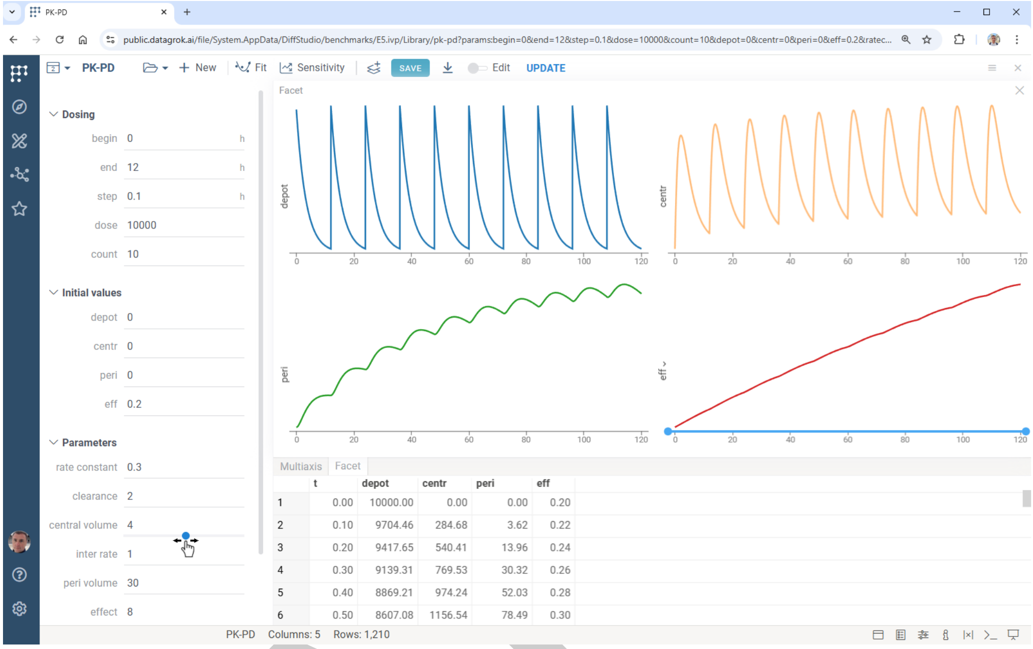
PK-PD Columns: 5 Rows: 1,210

Figure 2: Pharmacokinetic–pharmacodynamic simulation in Diff Studio, showing the declarative model specification, numerical solution, and interactive visualization.

A defining feature of Diff Studio is its real-time interactivity. Whenever a user adjusts a parameter or moves a slider, the system automatically recomputes the solution and updates all visualizations. Diff Grok enables these updates to occur almost instantaneously, supporting rapid hypothesis testing and intuitive exploration of model behavior.

Diff Studio also emphasizes reproducibility and collaboration. Models, parameter settings, and results can be shared via URLs, allowing collaborators to reproduce simulations without installing software or configuring environments. Shared models remain fully interactive, enabling continued exploration and comparison.

Beyond basic simulation, Datagrok provides built-in sensitivity analysis and parameter optimization, allowing users to study parameter influence and fit models to data. Together, these capabilities position Diff Studio as a centralized, browser-based hub for ODE-driven modeling, exploration, and collaboration.


PK-PD
public.datagrok.ai/file/System.AppData/DiffStudio/benchmarks/E5.ivp/Library/pk-pd?params:begin=0&end=12&step=0.1&dose=10000&count=10&depot=0&centr=0&peri=0&eff=0.2&ratec...
PK-PD
New
Fit
Sensitivity
SAVE
Edit
UPDATE
Facet
depot
centr
peri
eff
0
20
40
60
80
100
120
Multiaxis
Facet

Dosing

begin 0 h

end 12 h

step 0.1 h

dose 10000

count 10

Initial values

depot 0

centr 0

peri 0

eff 0.2

Parameters

rate constant 0.3

clearance 2

central volume 4

inter rate 1

peri volume 30

effect 8

	t	depot	centr	peri	eff
1	0.00	10000.00	0.00	0.00	0.20
2	0.10	9704.46	284.68	3.62	0.22
3	0.20	9417.65	540.41	13.96	0.24
4	0.30	9139.31	769.53	30.32	0.26
5	0.40	8869.21	974.24	52.03	0.28
6	0.50	8607.08	1156.54	78.49	0.30

PK-PD Columns: 5 Rows: 1,210

Figure 3: Diff Studio in model exploration mode, showing the autogenerated user interface with live parameter controls.

Availability

- Diff Grok: https://github.com/datagrok-ai/diff-grok
- Diff Studio: https://github.com/datagrok-ai/public/tree/master/packages/DiffStudio
- Run Diff Studio online: https://public.datagrok.ai/apps/DiffStudio
- Interactive tutorial: https://public.datagrok.ai/apps/tutorials/Tutorials/Scientificcomputing/Differentialequations

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Conflicts of interest

The authors declare no conflict of interest.

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