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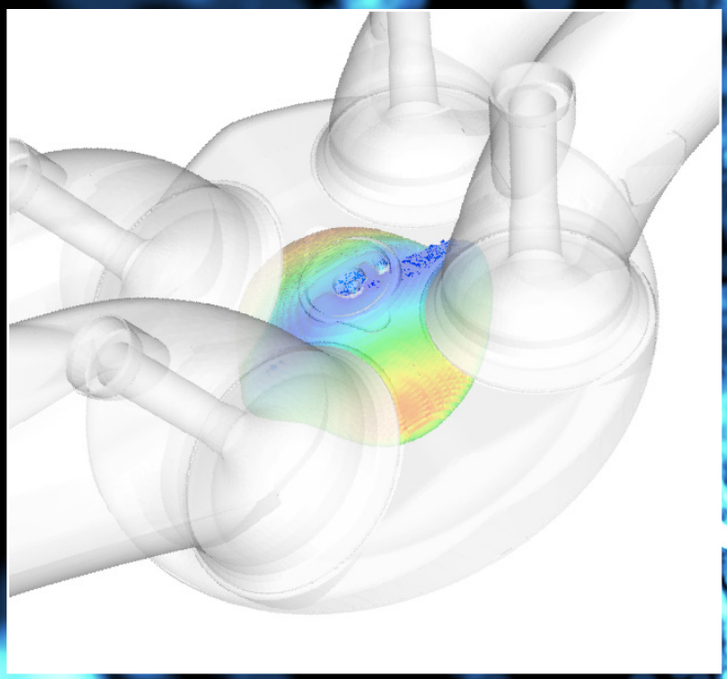
Zero-order Reaction Kinetics (Zero-RK)



Prepared for:

2015 R&D 100 Award Entry

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Zero-order Reaction Kinetics (Zero-RK)

Video link: see attached mp4 file.

1. General Entry Information

A. Product brand name and name of submitting organization(s).

Zero-order Reaction Kinetics (Zero-RK)

Lawrence Livermore National Laboratory

B. Short description of the product (maximum 25 words).

Zero-RK is a software package that dramatically decreases time to solution for scientific and engineering simulations involving chemically reacting systems such as internal combustion engines.

C. Product Photo(s).

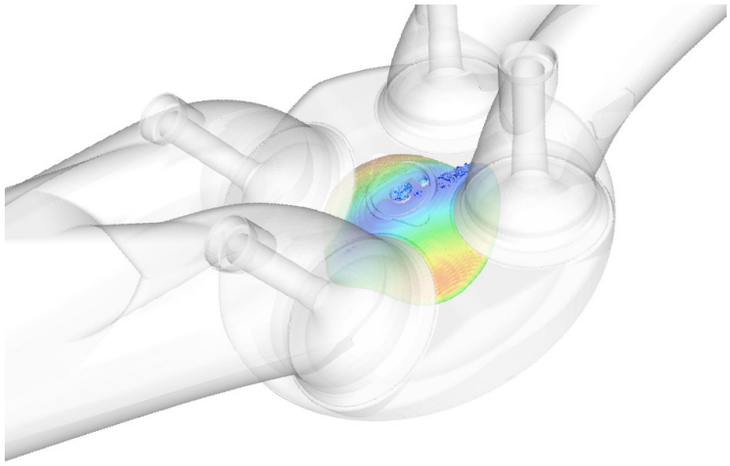

Figure 1: Zero-Order Reaction Kinetics (Zero-RK) logo alongside a simulation of the flame propagation in an internal combustion engine using ConvergeCFD combined with LLNL's Zero-RK solver. The spark ignition engine is port-injected with iso-octane, a gasoline surrogate, and represents a typical U.S. automotive design.

D. Price in U.S. dollars.

Zero-RK has a variable license structure at rates between $1,000 and $100,000 per year depending on the licensing organization, number of users, and use cases.

2. Product Description

A. What does the product or technology do? Describe the principal applications of this product.

Zero-order Reaction Kinetics (Zero-RK) is a software package that simulates chemically reacting systems in a computationally efficient manner. The fundamental advance embodied in Zero-RK is the numerical approach, which results in orders-of-magnitude reduction in simulation time while maintaining the accuracy of the results (detailed in Section 2B). The increased efficiency also allows combustion design engineers and researchers to include more detailed chemistry models in their simulations to better capture the real fuels and reactor systems being analyzed. Simulations range from zero- and quasi-dimensional simulations of constant volume and piston–cylinder devices up to full-scale simulations of industrial devices with complex 3D boundaries via direct coupling to computational fluid dynamics (CFD) codes (see Figure 2). Zero-RK also has the ability to perform sensitivity analysis for the development of chemical kinetic methods. Examples of its applicability include simulations of fundamental research devices such as shock tubes and rapid compression machines, and commercial applications such as internal combustion engines, gas turbines, rocket engines, and industrial burners.

B. How does the product operate? Describe the materials, composition, construction, theories or mechanism of action.

Zero-RK calculates the thermo-physical properties, reaction rate coefficients, and production rates necessary to simulate the evolution of species in a chemically reacting system. Species are the molecules representing the initial reactants, final products, and the stable and unstable intermediates in the reacting system. In a methane burner, for example, the methane fuel (CH_4) reacts with oxygen (O_2) to form the products water (H_2O) and carbon dioxide (CO_2). While this process can be modeled by a single global reaction for the four species, greater accuracy is achieved by resolving the intermediate species that are formed during the fuel conversion. This includes stable intermediate species like carbon monoxide (CO), formaldehyde (CH_2O) and hydrogen peroxide (H_2O_2), and highly reactive radical species like atomic hydrogen (H), atomic oxygen (O) and the hydroxyl radical (OH).

Resolving these intermediate species is critical to accurately predict the ignition properties and pollutant emissions (e.g., NOx and soot) for commercial combustion applications. However, the use of detailed fuel chemistry for transportation fuels has had limited use in commercial combustor design because of the prohibitive computational cost. Zero-RK directly addresses this challenge and allows design calculations to use more than ten times the number of intermediate

chemical species for the same computational cost as the best commercial solver (see Figure 3).

The highest fidelity models for realistic transportation fuels (e.g., gasoline and diesel) require thousands of intermediate species to be resolved. Zero-RK has been designed to calculate the necessary chemistry quantities in a computationally efficient manner by use of carefully designed algorithms that minimize the number of necessary operations while taking advantage of memory cache and vector arithmetic capabilities present in modern computing processors. In addition, when solving for reacting systems involving large numbers of species, Zero-RK employs a sparse, adaptive preconditioning (SAP) strategy to dramatically reduce the cost of implicit integration. The SAP strategy is employed in the context of Krylov subspace methods within a backward-difference formula (BDF) stiff integration scheme with variable order and step sizes. Krylov subspace methods have been employed in other fields and allow for iterative solution of large systems of equations in a matrix-free manner, dramatically reducing the computational cost of solution. BDF schemes have been proven to efficiently and robustly integrate stiff systems of equations by accurate estimation of derivative information. Zero-RK combines the Krylov subspace method and BDF schemes with an adaptively constructed preconditioner for chemical systems. Krylov subspace methods generally require preconditioning to ensure fast convergence of the iterative solution and the SAP strategy developed within Zero-RK provides good preconditioning while being very inexpensive to calculate. The SAP strategy solves the same system of equations as previous techniques for integration of chemical systems without any loss of accuracy. This is in contrast to species reduction techniques commonly used to lower the simulation cost when using competing packages.

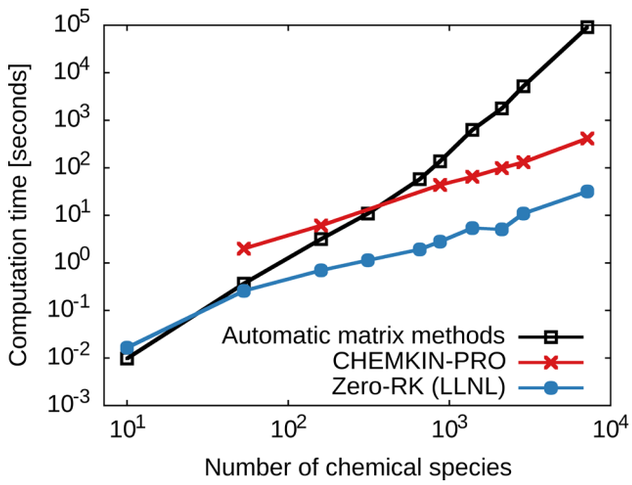

Figure 2: Zero-Order Reaction Kinetics (Zero-RK, shown in blue) is 10–14 times faster than Reaction Design's CHEMKIN-PRO, and several orders of magnitude faster than the automatic matrix techniques typically found with solvers like Cantera, OpenFOAM, and CHEMKIN II.

3. Product Comparison

A. Supply a matrix or table showing how the key features of your product compare to existing products or technologies. Use numerical figures to represent performance metrics. For price, and capital and operating costs, use actual dollar amounts or a relative scale ($$, $$$) to show a comparison.

Package	Cost (US Dollars)	Features	Interface	Benchmark Time [seconds][1] (lower is better)	Error [-][2]
Zero-RK	Variable ($1,000–$100,000 per year)	Thermo-physics; Kinetics; 0D reactors; Quasi-dimensional engine models; Sensitivity analysis; Couples with computational fluid dynamics coupling	Text	28–34	1.0e-8
Cantera	Free	Thermo-physics; Kinetics; 0D reactors; 1D flames	Text	63,0000–120,000	1.0e-8
Chemkin Pro	Contact Vendor	Thermo-physics; Kinetics; 0-D reactors; 1D flames; Sensitivity analysis; Couples with computational fluid dynamics	Graphical	360–500	1.0e-8

[1] The benchmark used is the ignition delay time calculation for 2-methylnonadecane ($C_{20}H_{42}$), a heavy diesel component, in a constant volume reactor with 7,200 species.
[2] The error compared is the local relative error, which is used in time step control and is estimated by the integrator for all compared packages. The error is a user selectable tolerance. The error tolerance used in our comparison is small enough that calculated engineering quantities of interest will be essentially identical between the packages.

B. Describe how your product improves upon competitive products or technologies. Describe limitations of your product.

The key innovation inherent in Zero-RK is the sparse, adaptive precondition (SAP) method (detailed above in Section 2B), which dramatically reduces the cost of integration for chemical systems comprised of many species. In addition, Zero-RK incorporates efficient algorithms for evaluating species' thermo-physical functions and chemical reaction rates. The resulting improvement in simulation turn-around time is dramatic in many applications. For example, Figure 3 shows how solution time scales with the number of included chemical species in zero-dimensional reactor simulations. For the largest system analyzed, the reduction in simulation time for Zero-RK compared to the best competing commercial package is over ten times. Compared to Cantera, the best free alternative, Zero-RK achieves a four-thousand-fold reduction in simulation time. These simulation time reductions translate directly to other reactor configurations. For one case, Zero-RK has been used to develop a rapid compression machine model for Argonne National Laboratory that runs in minutes instead of days. When

coupled with sophisticated computational fluid dynamics (CFD) packages like Convergent Science Inc.'s ConvergeCFD, Zero-RK based models can reduce the chemistry cost by a factor of seven for realistic transportation fuels (see Figure 3). One limitation is a fewer number of features relative to competing packages as detailed in Table 1. This limitation is acceptable because Zero-RK is coupled to detailed CFD, which allows for many different reactor configurations to be studied, and supports the largest user base.

4. Summary (maximum 200 words)

Zero-Order Reaction Kinetics (Zero-RK) is a software package for simulating chemically reacting systems. Zero-RK's algorithms dramatically reduce the time to results for many commercial applications, providing in some cases a three-orders-of-magnitude reduction in simulation time (e.g., 4,000x speedup shown in Figure 3). Zero-RK's feature set, including simulation of zero- and quasi-dimensional reactor systems, reaction sensitivity analyses, and coupling to CFD packages, allows users to simulate a wide variety of systems and devices. These systems include internal combustion engines for automotive and heavy-duty platforms, gas turbines, rocket engines, and industrial burners. Zero-RK is offered for license at a reasonable rate commensurate with its capabilities and offers much higher performance than its competitors.

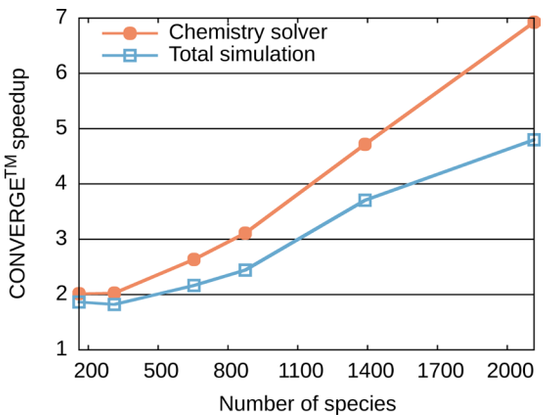

Figure 3: The chemistry solver speedup factor (orange) is shown using LLNL's Zero-RK solver coupled with Convergent Science's ConvergeCFD. Also shown is the overall simulation speedup (blue) for an advanced combustion engine running in the homogeneous charge compression ignition (HCCI) mode.

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6. Affirmation

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