Electronic Supplementary Material (ESI) for Digital Discovery. This journal is © The Royal Society of Chemistry 2022

## **Supporting Information**

Alejandro Becerra,<sup>1,2,3</sup> Oscar Homero Diaz-Ibarra,<sup>4</sup> Kyungjoo Kim,<sup>4</sup> Bert Debusschere<sup>4</sup>, Eric A. Walker<sup>5,6,\*</sup>

<sup>1</sup>Institute for Artificial Intelligence and Data Science, The State University of New York at Buffalo, 14260, USA

<sup>2</sup>Data Intensive Studies Center, Tufts University, Medford, MA 02155, USA

<sup>3</sup>Department of Mathematics, Tufts University, Medford, MA 02155, USA

<sup>4</sup>Sandia National Laboratories, Livermore, CA 94551, USA

<sup>5</sup>Department of Chemical and Biological Engineering, The State University of New York at Buffalo, 14260, USA

<sup>6</sup>Linde plc, 175 E Park Dr, Tonawanda, NY 14150

	Т	$\theta_{H_2}$	$\theta_{0_2}$	$\theta_0$	$\theta_{OH}$	$\theta_{H_2O}$	$\theta_{H}$	$\theta_{HO_2}$	$\theta_{H_2 \theta_2}$	$\theta_{Ar}$
Т	-1.624	-2.344	-7.429	-9.496	2.736	2.226	-5.849	-3.234	-4.525	6.921
	E+00	E+01	E+01	E+08	E+10	E+02	E+09	E+06	E+07	E+01
$\theta_{H_2}$	-2.190	-1.163	-1.814	-3.737	-1.329	1.214	2.170	-1.210	6.429	5.475
	E-05	E-02	E-03	E+05	E+06	E-03	E-02	E+02	E-04	E-04
$\theta_{0_2}$	-3.476	-1.845	-2.879	2.170	-1.234	1.912	-2.117	5.840	-5.573	8.690
	E-04	E-01	E-02	E-02	E-02	E-02	E+07	E+01	E+00	E-03
$\theta_{O}$	3.580	3.807	1.723	-2.966	1.638	5.642	8.565	-2.170	-2.106	-1.793
	E-13	E-11	E-11	E+06	E-02	E-11	E+06	E-12	E-12	E-12
$\theta_{OH}$	0.000	0.000	0.000	3.153	-1.121	7.787	9.105	0.000	1.088	0.000
	E+00	E+00	E+00	E+06	E+07	E-05	E+06	E+00	E+04	E+00
$\theta_{H_2 0}$	0.000	0.000	0.000	0.000	1.188	-8.248	0.000	0.000	0.000	0.000
	E+00	E+00	E+00	E+00	E+07	E-05	E+00	E+00	E+00	E+00
A.,	1.095	5.813	9.068	1.868	6.646	-6.070	-6.670	6.236	-3.215	-2.737
°Н	E-05	E-03	E-04	E+05	E+05	E-04	E+05	E+01	E-04	E-04
$\theta_{HO_2}$	3.586	1.903	2.969	-2.238	1.273	-1.972	4.171	-2.042	1.151	-8.963
	E-04	E-01	E-02	E-02	E-02	E-02	E+06	E+03	E+01	E-03
$\theta_{H_2 0_2}$	0.000	0.000	0.000	0.000	0.000	0.000	0.000	2.042	-1.089	0.000
	E+00	E+00	E+00	E+00	E+00	E+00	E+00	E+03	E+04	E+00
$\theta_{Ar}$	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	E+00	E+00	E+00	E+00	E+00	E+00	E+00	E+00	E+00	E+00

Table S1. Table of Jacobian values. Temperature is available from TChem but was not modeled with an equation in the example reduced models.

Table S2. Table of RHS values.

Table S3. Table of initial state vector values.

Т	-8.369E+01
$\theta_{H_2}$	-1.124E-03
$\theta_{0_2}$	-1.784E-02
$\theta_{O}$	8.762E-12
$\theta_{OH}$	0.000E+00
$\theta_{H_2 0}$	0.000E+00
$ heta_{H}$	5.618E-04
$\theta_{HO_2}$	1.840E-02
$\theta_{H_2 \theta_2}$	0.000E+00
$\theta_{Ar}$	0.000E+00

Т	1200
$\theta_{H_2}$	0.05
$\theta_{0_2}$	0.45
θο	0
θ <sub>OH</sub>	0
$\theta_{H_2O}$	0
$\theta_{H}$	0
$\theta_{HO_2}$	0
$\theta_{H_2 0_2}$	0
$\theta_{Ar}$	0.5



Figure S1. Fidelity of quantum solution based upon angle between vectors in 2x2 matrix A. For the blue points in (b), the first row of each matrix A was the vector  $\begin{bmatrix} 1 & 0 \end{bmatrix}$  and the second row of  $\frac{\pi}{2}$ 

each matrix A was a rotation of this vector by some angle  $\theta$  (increments of  $\overline{16}$  radians). For the red points in (b), these rows are permuted. In other words, the first row and the second row are



swapped.

Figure S2. Fidelity of quantum solution with random orthogonal matrices *A*.



Figure S3. Fidelity of quantum solution to linear systems of equations (Ax = b) with random orthonormal matrices *A*.



Figure S4. Fidelity of quantum solution to linear systems of equations (Ax = b) with random



diagonal matrices A.

Figure S5. Fidelity of quantum solution to linear systems of equations (Ax = b) with random matrices *A* and select vectors  $b = \lambda v$  (for some eigenvalue  $\lambda$  and eigenvector *v* pair of *A*).



Figure S6. Fidelity of quantum solution to linear systems of equations (Ax = b) with random matrices *A* of the forms shown above. (a) Two-dimensional. (b) Four-dimensional.