CS205: Final Project

William Burke, Drake Deuel, Esmail Fadae, Jamila Pegues

Chemistry on grain surfaces in space

Simulation of stochastic chemical processes on a grain surface in a cloud of gas

The Chemistry

4 processes govern the dynamics of particles on grain surfaces:

- Adsorption - sticks to surface
- Desorption (Thermal) - leaves surface
- Diffusion - moves around surface
- Reaction - forms a new molecule with another particle

All of the processes are experimentally observed to be Poisson Processes whose rates depend on known parameters.

The equations governing the rates are nonlinear, but they do not change with time. This means we can precompute.

$$R_{des} = \nu \exp\left(\frac{-E_{bind,a}}{kT_{gr}}\right) \qquad R_{diff} = \nu \exp\left(\frac{-E_{surf,a}}{kT_{gr}}\right) \qquad R_{ads} = s_a v_a n_a \pi r_{gr}^2$$

$$\nu = \sqrt{\frac{2N_s E_{bind,a}}{\pi^2 m_a}} \qquad \nu = \sqrt{\frac{2N_s E_{surf,a}}{\pi^2 m_a}} \qquad v_a = \sqrt{\frac{8kT_{gas}}{\pi m_a}}$$

Poisson Processes

Assumptions

- The number of events in a fixed interval follows a Poisson distribution
- The number of events in disjoint intervals are independent

$$P(k=0) = \frac{e^{-\lambda t}(\lambda t)^k}{k!} = e^{-\lambda t}$$

$$P(k>0) = 1 - e^{-\lambda t}$$

$$P(k>0) = 1 - e^{-(\lambda_{desorbtion} + \lambda_{diffusion})t}$$

$$P(desorbtion|event) = \frac{\lambda_{desorbtion}}{\lambda_{desorbtion} + \lambda_{diffusion}}$$

$$P(diffusion|event) = \frac{\lambda_{diffusion}}{\lambda_{desorbtion} + \lambda_{diffusion}}$$

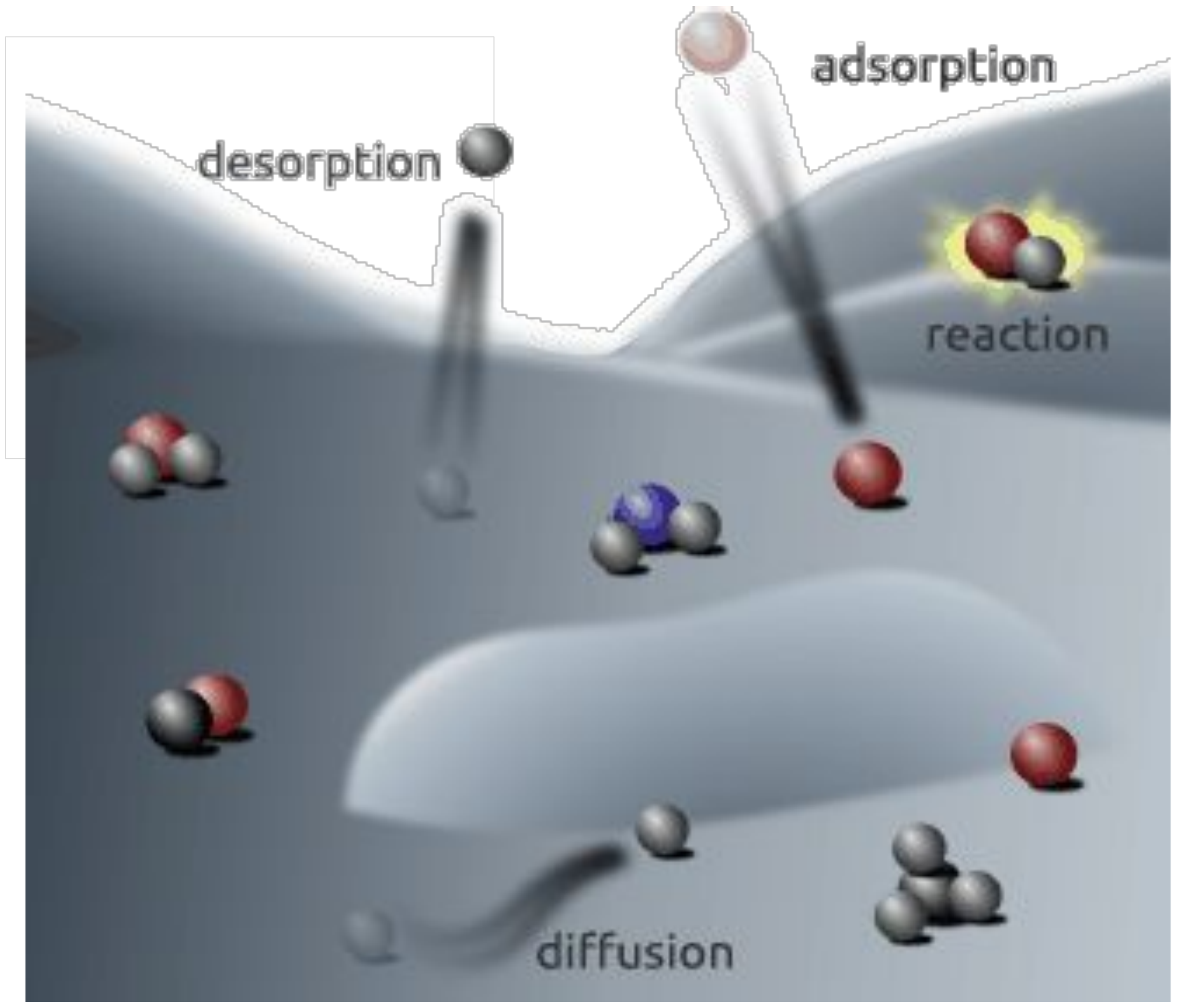
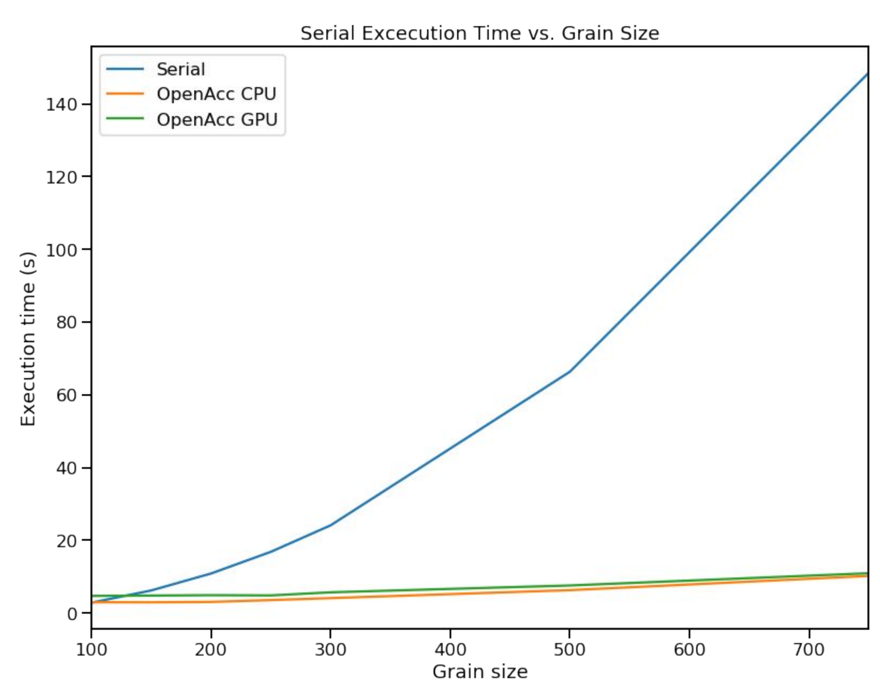
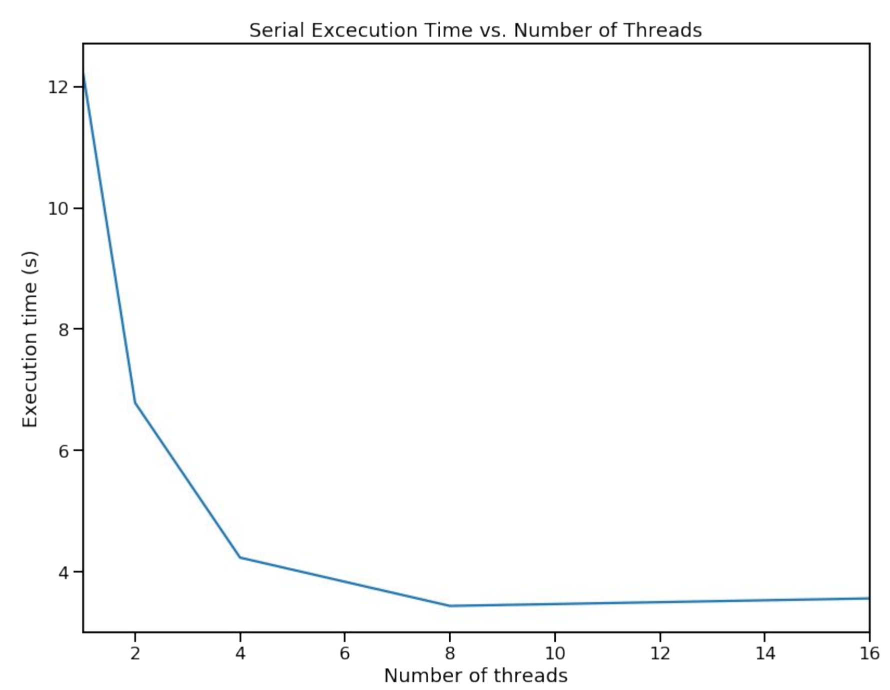


Figure 1 of Cuppen et al. 2017.

Parallelization: OpenACC Approach





Our simplest parallelization approach was an OpenACC implementation of a single node multi-threaded CPU, shared memory parallel design.

Features:

- easy portability to a GPU parallel model random numbers for sampling
- linear scaling as thread count increased
- Using shared memory parallelization allowed us to not worry about separate copies of our matrix becoming out of sync.

Overheads (pgprof analysis):

- Fork - [CUDA memcpy HtoD]
- Waits - [CUDA memcpy DtoH]
- Synchronization

Our GPU compute implementation involved changing our data management strategy to limit the memory copy from host to device overhead. We used OpenACC pragma data clause to copyin our two matrices after initialization, then maintained local copies in GPU memory

Features:

- Large number of threads
- Good speedup
- Still using shared memory in this implementation meant no communication to synchronize separate matrix copies.

Parallelization: MPI Approach

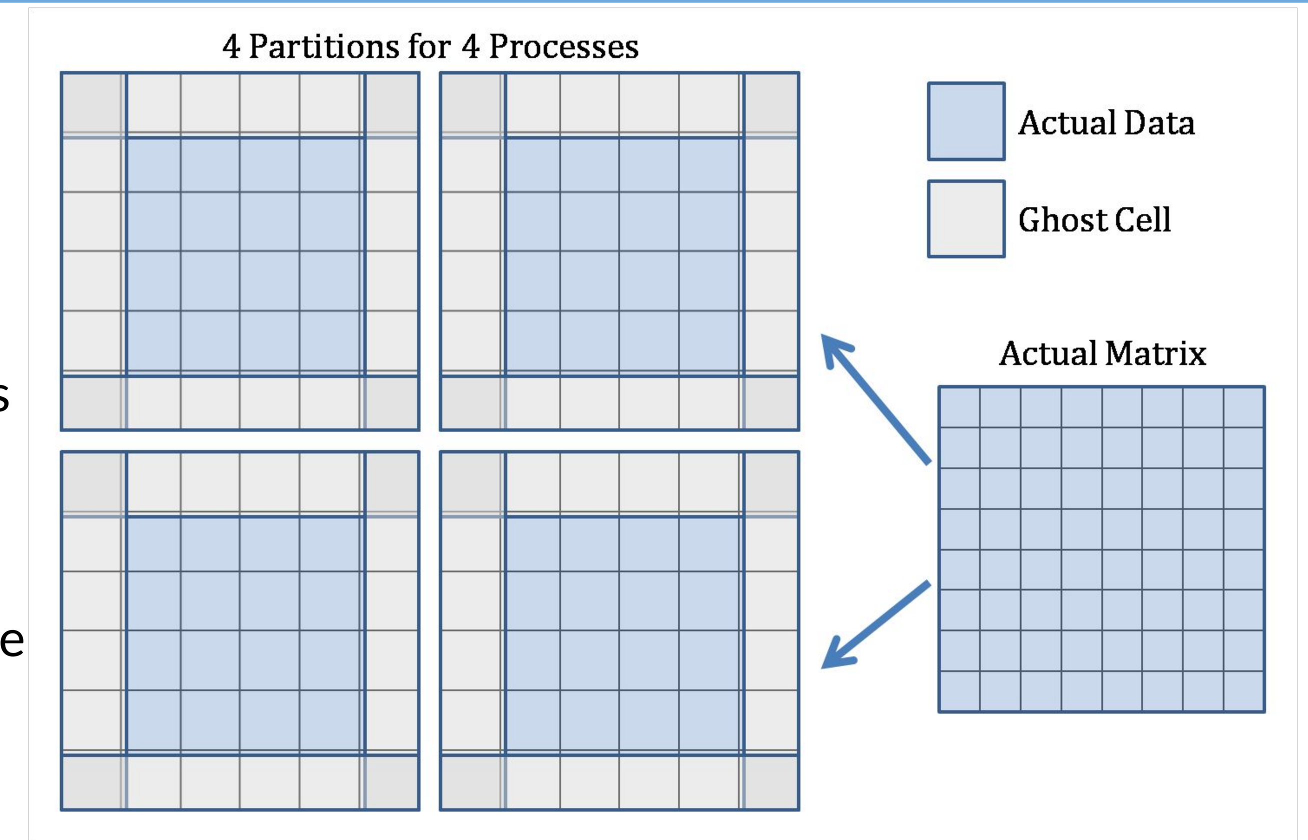
System Setup: AWS t2.2xlarge

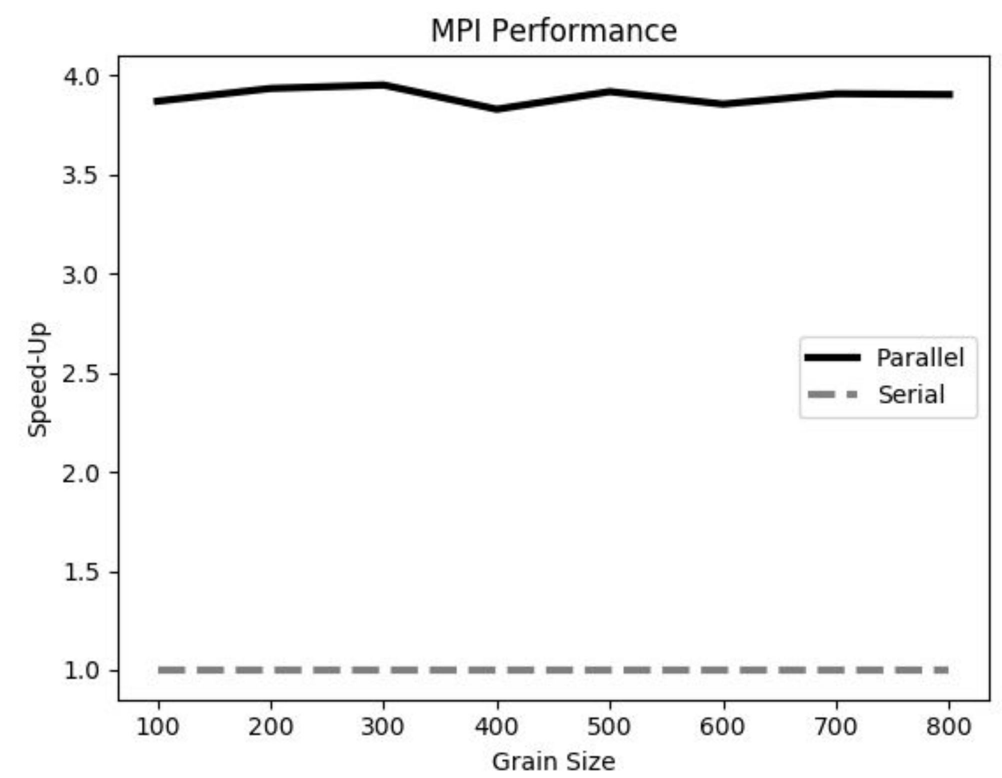
Techniques:

- Divide grain surface across multiple processors
- Communicate at specific points via ghost cells

Major challenges:

- Message-passing across surface partitions
- Handling ghost cells



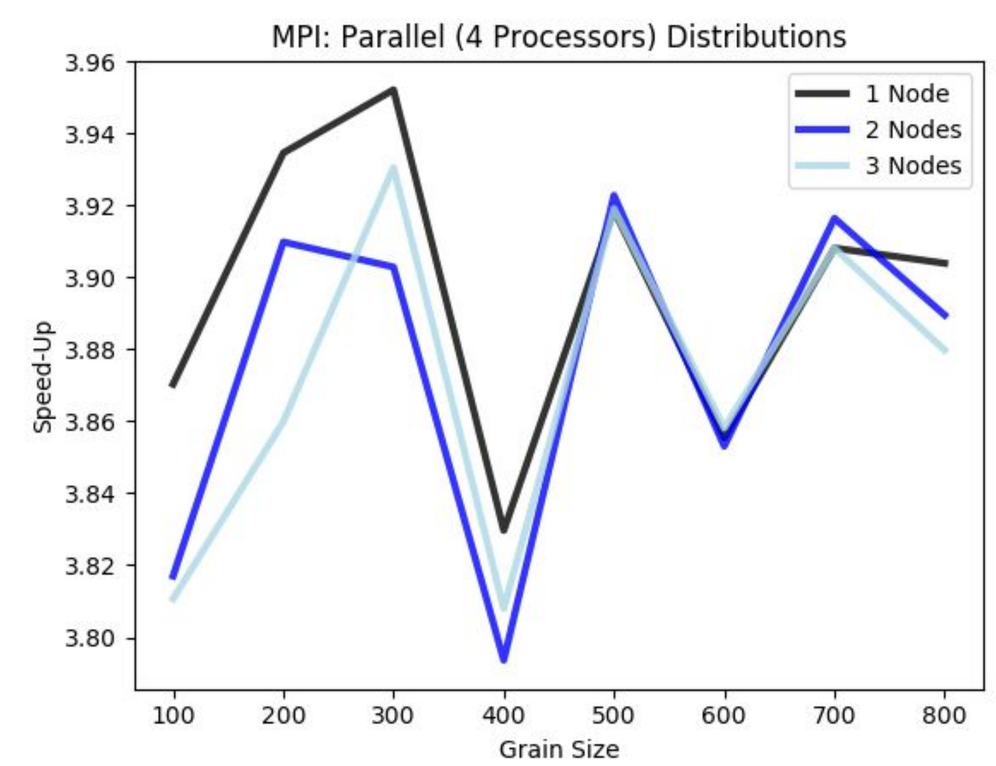


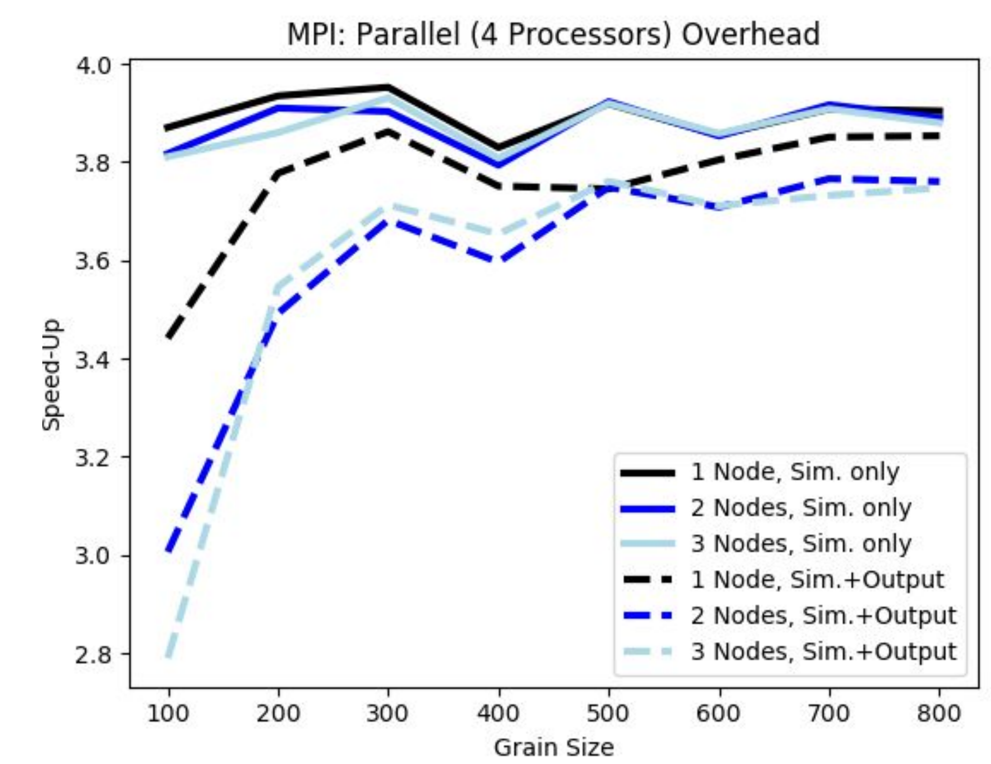
Consistent simulation performance across node cluster.

Consistent speed-up of simulation with increasing problem size.

Gathering data from different processors significantly affects speed-up.

Magnitude of effect decreases for larger problem size.





Citations and Links

Github: https://github.com/ddeuel/CS205

Sarah Ballard. Predicted Number, Multiplicity, and Orbital Dynamics of TESS M-dwarf Exoplanets.

J. K. Blitzstein and J. Hwang. Introduction to Probability. CRC Press, Taylor Francis Group, 2015.

Q. Chang, H. M. Cuppen, and E. Herbst. Continuous-time random-walk simulation of H2 formation on interstellar grains. , 434(2):599–611, May 2005.

Qiang Chang and Eric Herbst. Interstellar Simulations Using a Unified Microscopic-Macroscopic Monte Carlo Model with a Full Gas-Grain Network Including Bulk Diffusion in Ice Mantles. , 787(2):135, Jun 2014.

H. M. Cuppen, C. Walsh, T. Lamberts, D. Semenov, R. T. Garrod, E. M. Penteado, and S. Ioppolo. Grain Surface Models and Data for Astrochemistry. Oct 2017.

Ricker et al. The Transiting Exoplanet Survey Satellite Mission. In American Astronomical Society Meeting Abstracts Jun 2014.

Wakelam et al.H2 formation on interstellar dust grains: The viewpoints of theory, experiments, models and observations. Molecular Astrophysics Dec 2017.