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Studying the Computational Performance of CSP Analysis on Heterogeneous Computing Platforms

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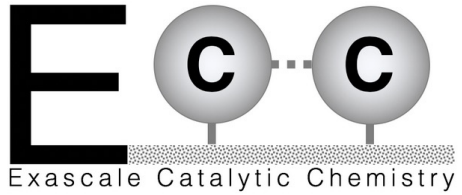

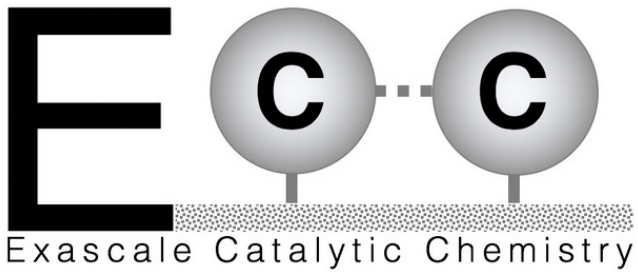

https://ecc-project.sandia.gov/

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Motivation

- The computational singular perturbation (CSP) method was first introduced by Lam and Goussis (1988).
- This method is useful for dynamical systems with wide range of time scales.
- It has been applied in gas phase kinetic modeling, as well as biochemical modeling for diagnostics and model simplification.
- CSP analysis for gas-phase and surface chemistry models has been implemented in open-source code, CSPlib: https://github.com/sandialabs/CSPlib.

Computational Singular Perturbation (CSP) Analysis

- CSP basis vectors decouple the fast and slow subspaces.
- Eigenvectors of the Jacobian, i.e. $J_{ij} = \frac{\partial g_i(\boldsymbol{y})}{\partial y_j}$, provide first order decoupling of the fast and slow subspaces.
- For chemical systems, CSP indices measure contribution of reactions in the slow/fast subspace (Importance indices) and mode amplitudes (Participation index).

ODE:

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{g}(\boldsymbol{y}) \qquad \boldsymbol{y} \in \mathbb{R}^N \quad \boldsymbol{y}(t=0) = \boldsymbol{y}_0$$

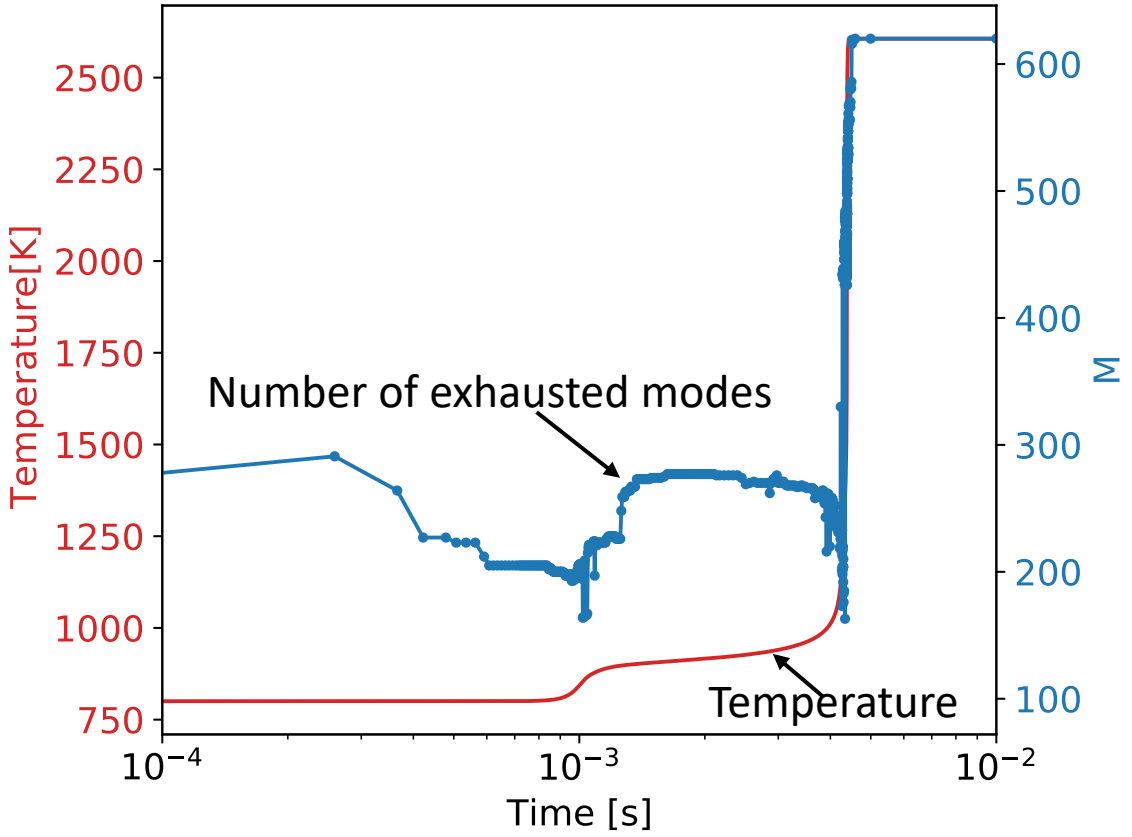
Expand RHS in CSP basis:

$$\boldsymbol{g} = \boldsymbol{a}_1 f^1 + \cdots + \boldsymbol{a}_N f^N$$

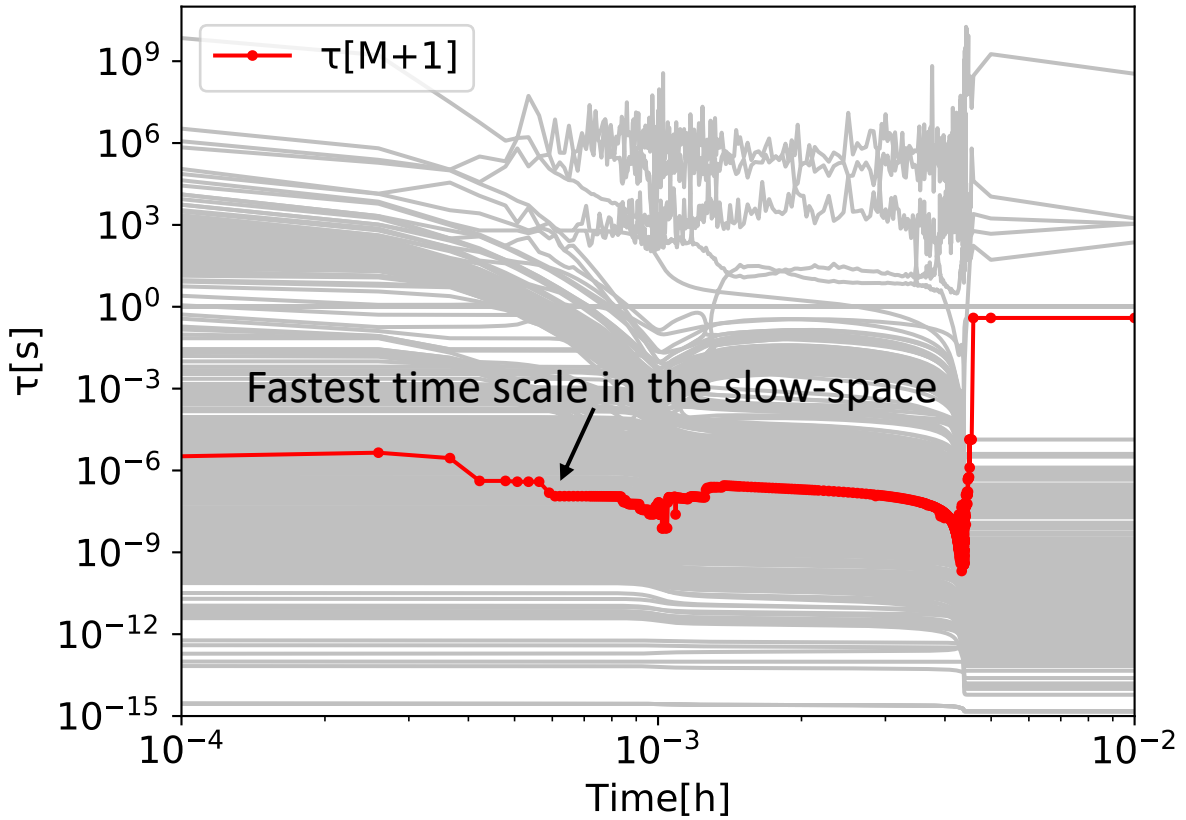
$$\boldsymbol{g} = \underbrace{\sum_{i=1}^{M} \boldsymbol{a}_i f^i}_{g_{\text{fast}} \approx 0} + \underbrace{\sum_{i=M+1}^{N} \boldsymbol{a}_i f^i}_{g_{\text{slow}}}$$

D. Goussis, H. Lam (1988--), M. Valorani ('90s--). Comb. Sci. Tech.; Comb. Flame; Comb. Theo. Mod.

CSP Helps Uncover the Dynamics of Complex Kinetic Models



Number of inactive models during the ignition for n-heptane.



Kinetic models exhibit a wide range of time scales.

https://combustion.llnl.gov/mechanisms/alkanes/n-heptane-detailed-mechanism-version-3
Number of species : 654 Number of reactions: 2827

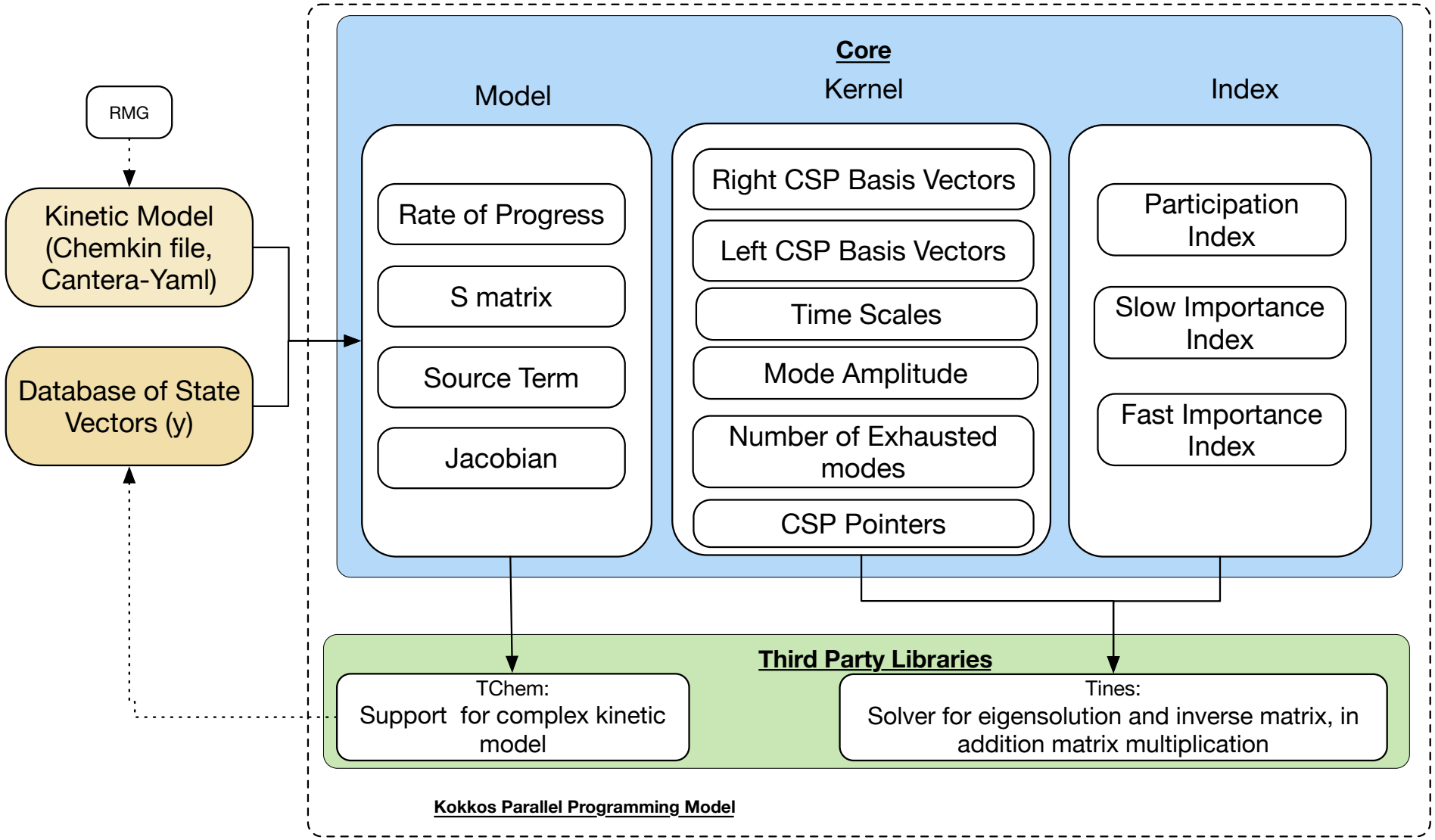
We Extend the CSP Method to Handle DAE Systems.

- CSP analysis for DAE/ODE of catalysis systems has been implemented in the open-source code, CSPlib: https://github.com/sandialabs/CSPlib.
- In CSPlib, computations can be executed on modern computing platforms, i.e, GPUs and many-core CPUs.

Oscar Diaz-Ibarra, Kyungjoo Kim, Cosmin Safta, Judit Zador & Habib N. Najm (2021) Using computational singular perturbation as a diagnostic tool in ODE and DAE systems: a case study in heterogeneous catalysis, Combustion Theory and Modelling, DOI: 10.1080/13647830.2021.2002417

Schematic of CSPlib

github.com/sandialabs/csplib



CSP Tasks in the Kernel/Index Class Are Linear Algebra Operations, E.G., Eigensolver, Matrix Inversion, Matrix-Matrix Multiplication.

CSPlib task	Type of operation	Library
Right CSP Basis Vectors	Right eigenvectors of Jacobian	Tines/LAPACK
Left CSP Basis Vectors	Matrix inverse of right eigenvectors	Tines/LAPACK
Time Scales	Multiplicative inverse of eigenvalues	CSPlib
Mode Amplitude	Dense matrix-vector multiplication	Tines
Number of Exhausted Modes	Iterative search	CSPlib
CSP Pointer	Element-wise matrix multiplication	CSPlib
Participation Index	Dense matrix-matrix multiplication	CSPlib/Tines
Slow Importance Index	Dense matrix-matrix multiplication	CSPlib/Tines
Fast Importance Index	Dense matrix-matrix multiplication	CSPlib/Tines

https://github.com/sandialabs/TChem

Rate of progress, S matrix, Source term, and Jacobian (TChem routines) are non-linear operations.

Tines

Time Integration, Newton and Eigensolver

https://github.com/sandialabs/Tines

CSPlib uses Kokkos as parallel programing model.

"Kokkos Core implements a programming model in C++ for writing performance portable applications targeting all major HPC platforms."

https://github.com/kokkos/kokkos

To effectively use modern computer platforms, CSPlib computes many CSP analyses in parallel, i.e., batched computation.

```
Kokkos::TeamPolicy<exec_space> policy(nBatch, Kokkos::AUTO());
Kokkos::parallel_for("UserCode", policy,
  KOKKOS_LAMBDA(const member_type& member) {
  const ordinal_type i = member.league_rank();
  // do something with ith work item
  // ...
  // compute model/kernel/index task
  compute_CSPlib_task(member, t, p, Y, ... );
});
```

Kokkos offers:

- Parallel computing patterns
- Data management (View)
- Backend: CUDA, HIP, SYCL, HPX, OpenMP and C++ threads

A single version of CSPlib is used for both CPU and GPU, mapping the code to OpenMP and CUDA backends respectively.

Case Study: Testbed Machine Specification

Processor	IBM Power9 2x20@3.6GHz	NVIDIA V100 80 SM@1.5GHz
# Threads	4 SMT/core	max 2048/SM
Cache	120 MB	6 MB L2
Memory	320 GB	16 GB
Compiler	GNU 7.2	NVCC 10.1
Exec. Space	OpenMP	CUDA

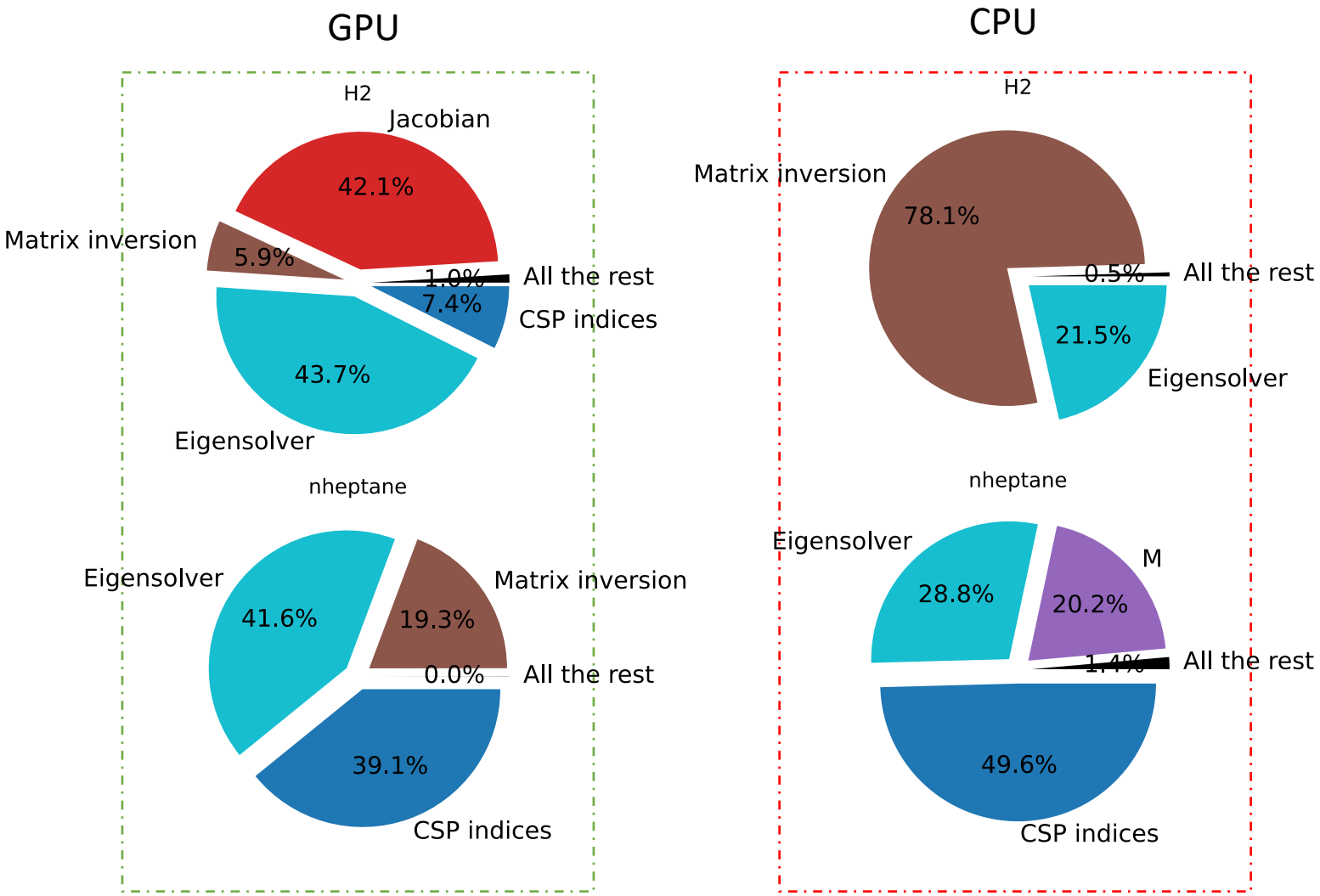
CSPlib copies database from host to device when the CSP analysis starts.

Case Study: Chemical Kinetic Models

Model	# Species	# Reactions	Reference
H_2	8	19	Yetter et al. (1991)
CO	14	33	Ranzi et al. (2012)
GRIMech 3.0	53	325	GRI-Mech v3.0 (2011)
n-dodecane	106	420	Luo et al. (2014)
n-heptane	654	2827	Mehl et al. (2011)

- Constant pressure ignition reactor configuration (from TChem)
- Batch parallel computation (vary the number of input states)

Eigensolver is the most expensive task in the CSP analysis, as expected.



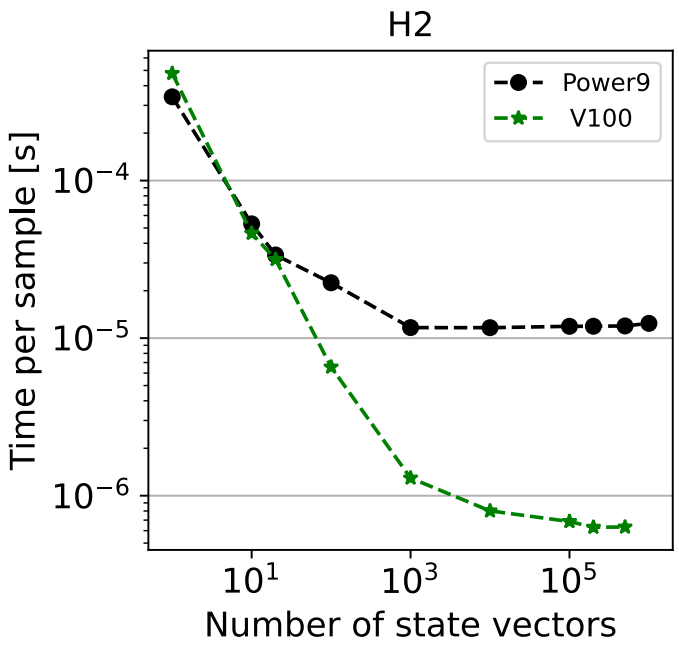
"All the rest": tasks with less than 0.5 % w.r.t. total time.

- Kinetics models size affects the performance of CSPlib in GPUs/CPUs.
- The computation of CSP indices is significant for large kinetic models because of the number of species and reactions.
  - H2 : 500, 000 state vectors
  - n-heptane : 100 state vectors
  - Read/write files is not included.

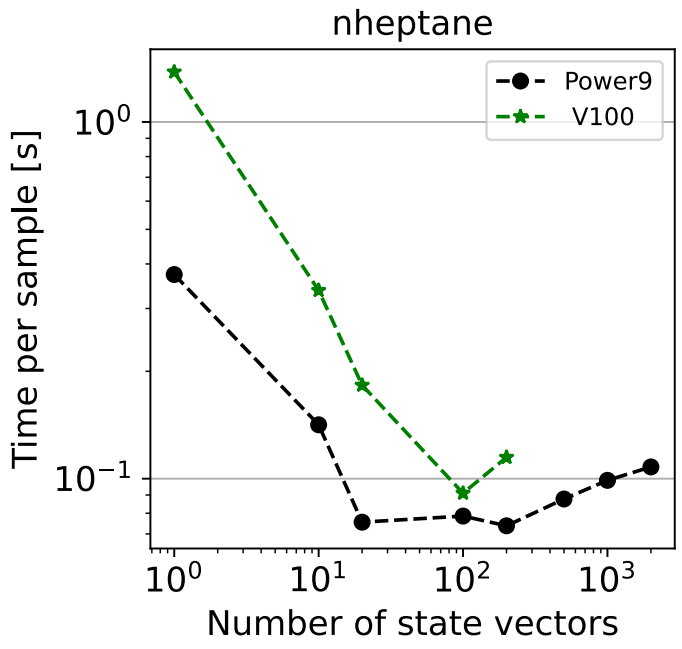
https://github.com/kokkos/kokkos-tools/tree/master/profiling/simple-kernel-timer-json

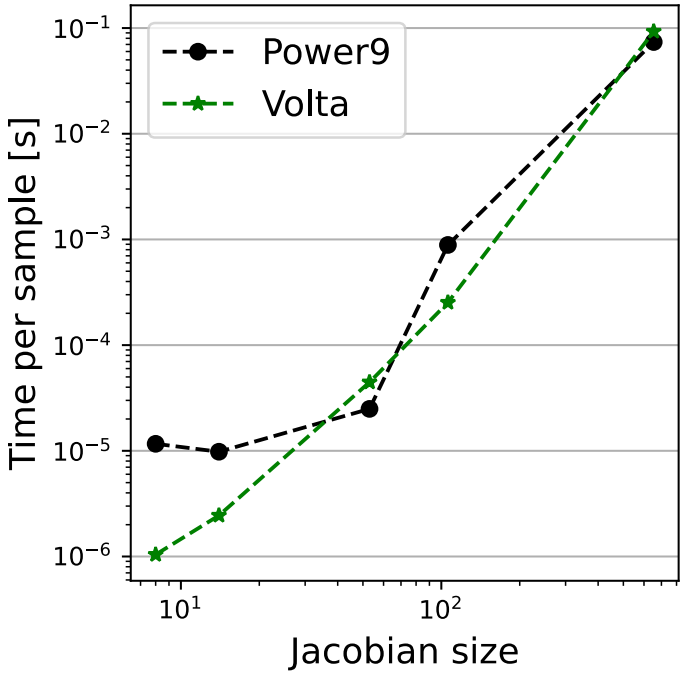
GPU Eigensolver Is Faster Than the LAPACK Routine for Small Kinetic Models.

H2: 9 variables



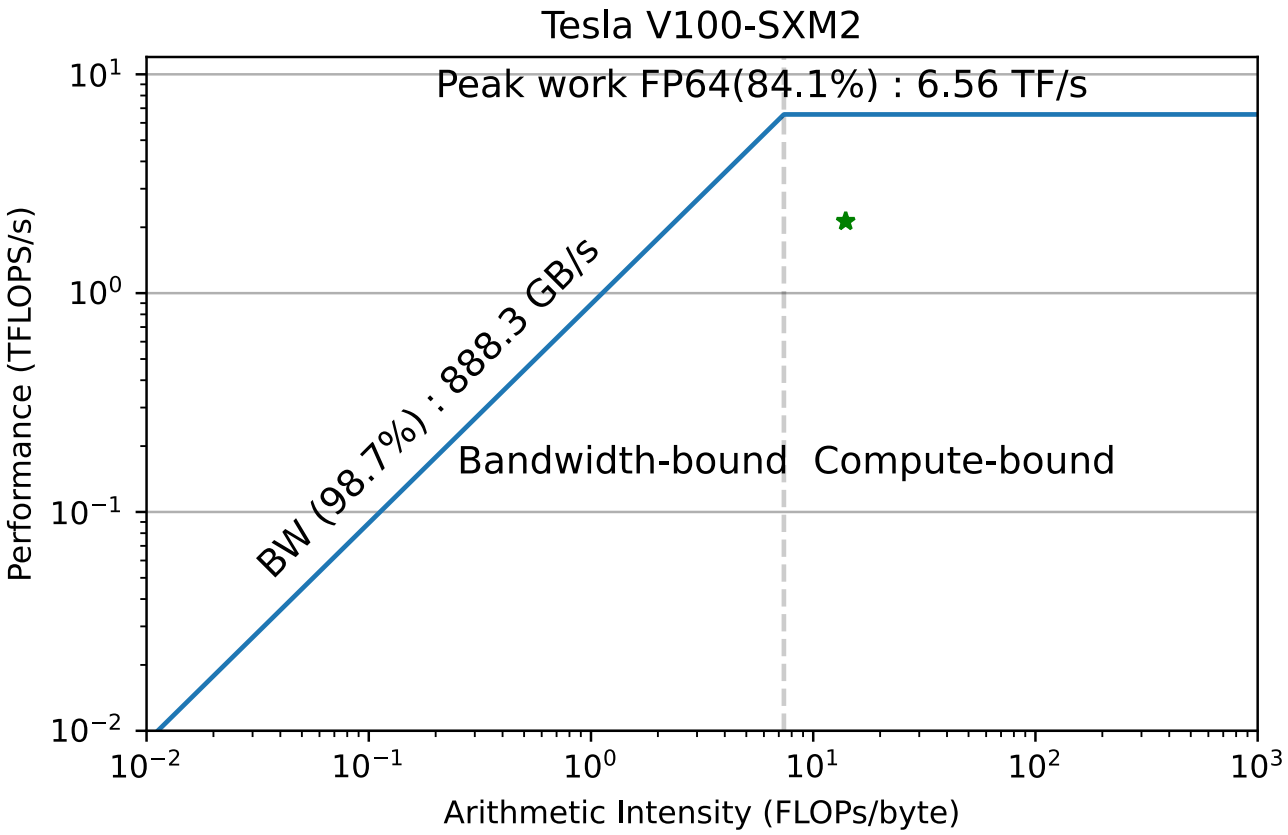
N-heptane: 655 variables





Due to limitations of GPU memory, the number of state vectors for large kinetic model cannot be increased.

How Does CSPlib Compare with Peak Performances in GPUs?



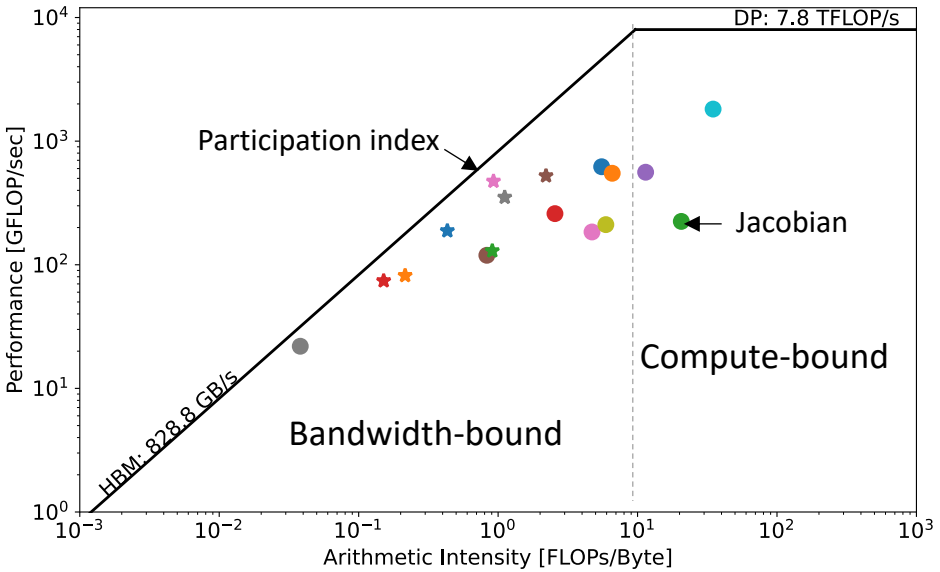
- Arithmetic Intensity (AI): ratio of total floating-point operations (FLOPs) to the total data movement (Bytes).
- Performance FLOPs/s : computational throughput.

- To compare application performance vs machine capabilities.
- To track code progress.
- Information: run time, the total number of FLOPs performed and bytes moved.
- Profiling data is produced by Nsight Compute (NVIDIA) to produce roofline charts.

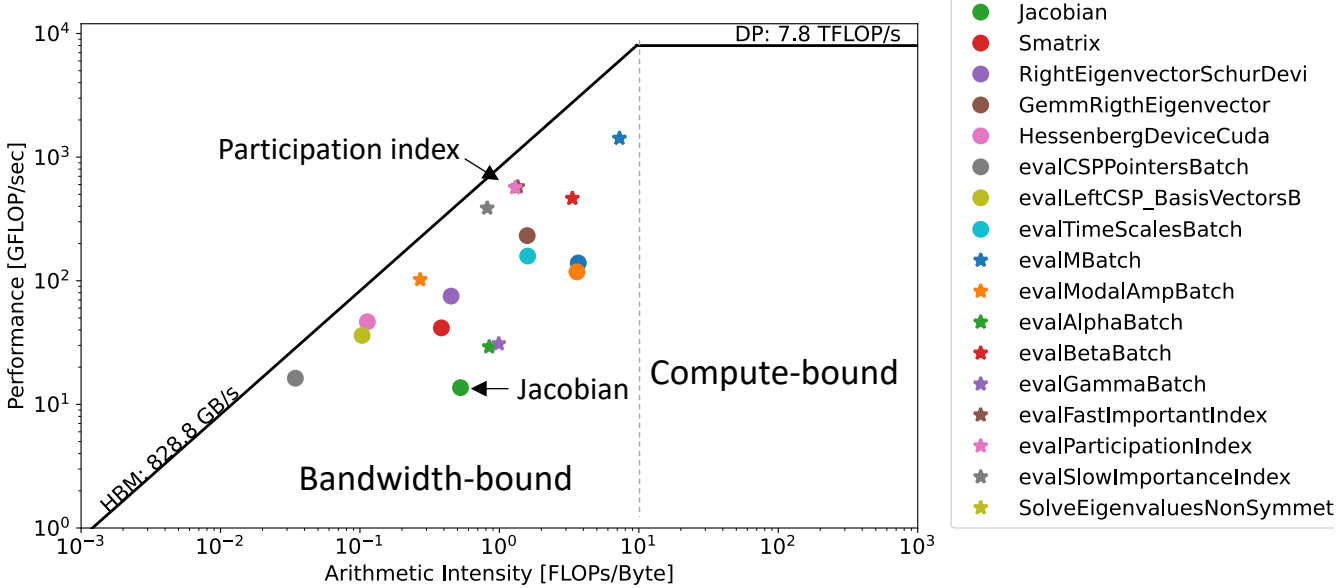
Documentation:
https://docs.nersc.gov/tools/performance/roofline/

https://gitlab.com/NERSC/roofline-on-nvidia-gpus

According to Roofline Model, Most of The CSP Tasks Are Considered to Be Bandwidth-bound.



H2: 9 variables/19 reactions
Batch size : 500,000 samples



N-heptane: 655 variables/ 2827 reactions
Batch size : 100 samples

Many tasks are close to peak performance, e.g, Participation index.

Conclusions

- We developed an open-source code, CSPlib, and analyzed its performance on modern computing platforms using wall-clock time profiles and roofline charts.
- The most expensive tasks in CSPlib are: eigensolver, matrix inversion, and Jacobian evaluation; which are expected in the CSP analysis.
- According to Roofline model, most of the CSP tasks are considered to be bandwidth-bound.
- GPU implementations of CSPlib (TChem/Tines) are faster that the CPU implementation for small kinetic models (H2, CO, GRI3).