NAMD 3.0 Features, Performance, and Capabilities Part 3

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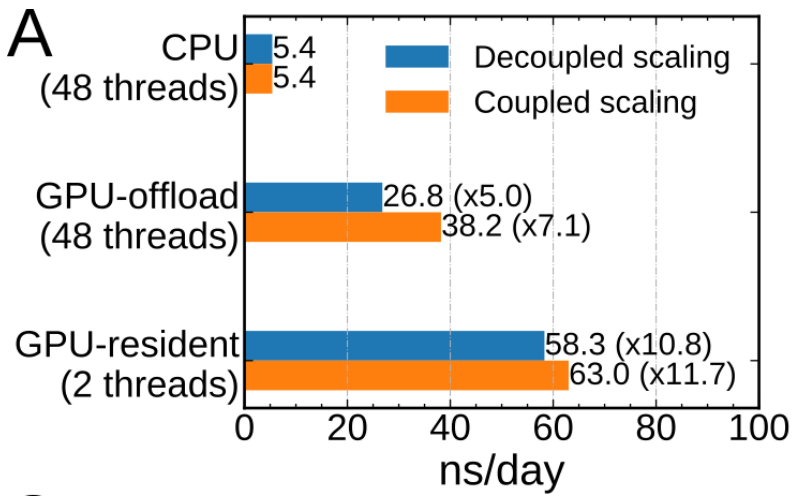
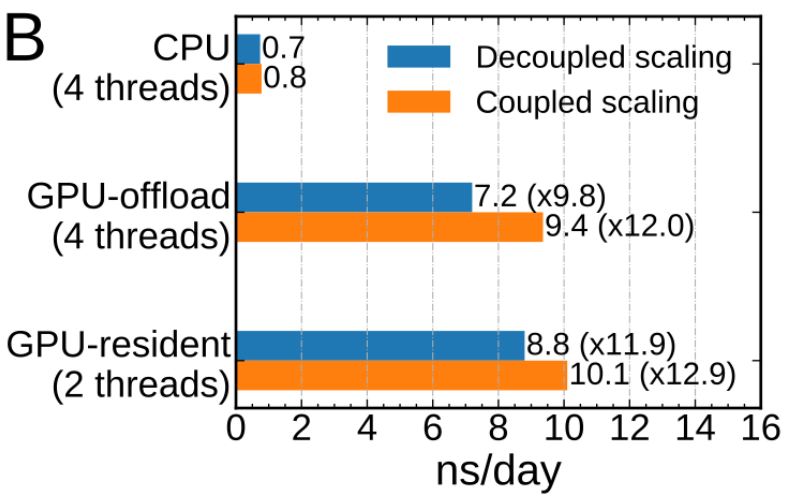
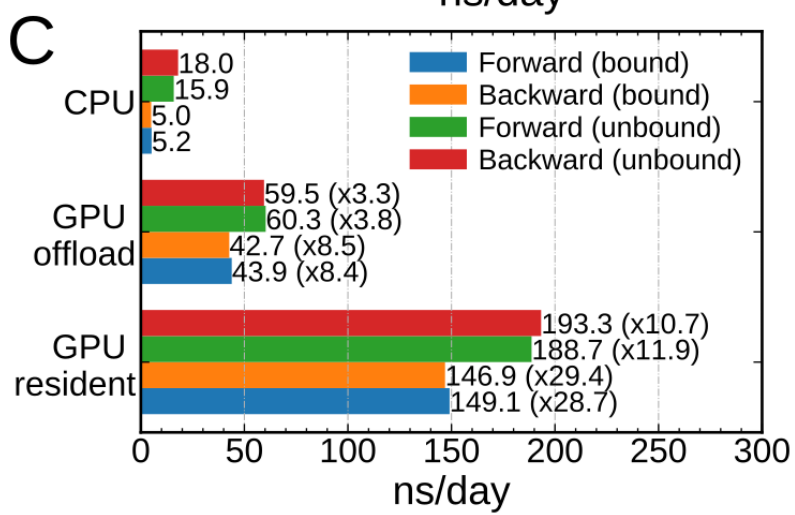
2024 Auburn Workshop

GPU-accelerated FEP/TI Calculation







A. Simulation speeds of the zero-sum transformation on a server;

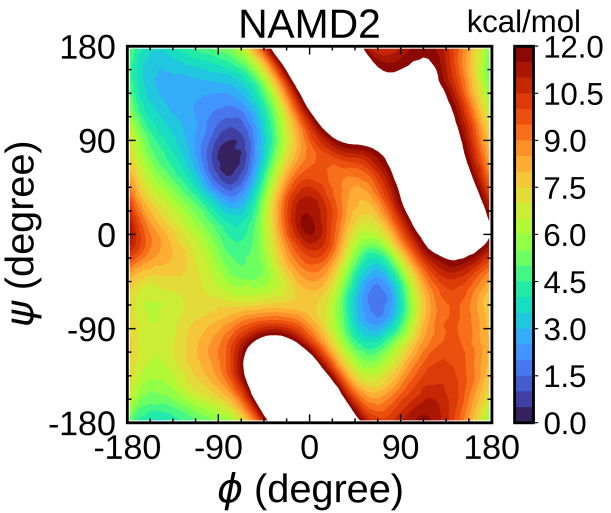
B. Simulation speeds of the zero-sum transformation on a laptop;

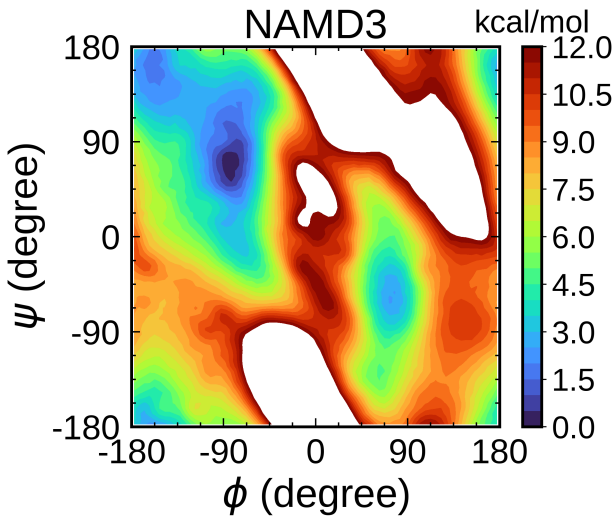
C. Simulation speeds of the Asp-to-Ala mutation of PMI-MDM2 on a server.

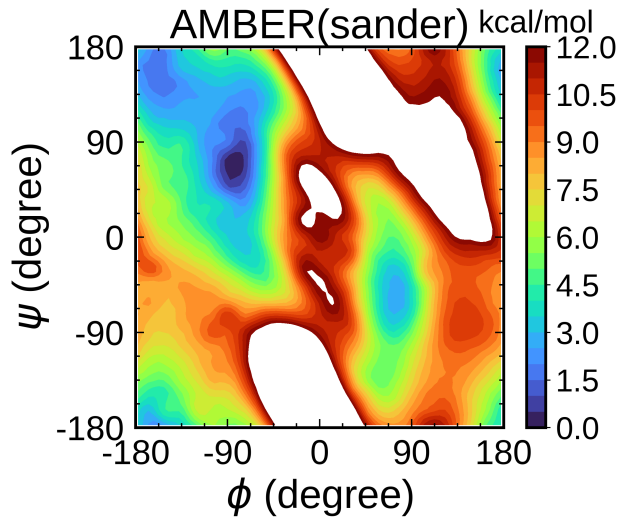
Chen, H.; Maia, J. D. C.; Radak, B. K.; Hardy, D. J.; Cai, W.; Chipot, C.; Tajkhorshid, E. J. Chem. Inf. Model. 2020, 60 (11), 5301–5307.

Better AMBER parm7 format compatibility

- Correctly support CMAP in AMBER ff19SB (parm7 format);
- Follow AMBER's Fortran format specifiers to read the parm7 file;
- **DO NOT USE NAMD2 with AMBER ff19SB in parm7 format (see the example of free-energy landscape of alanine dipeptide below)!**



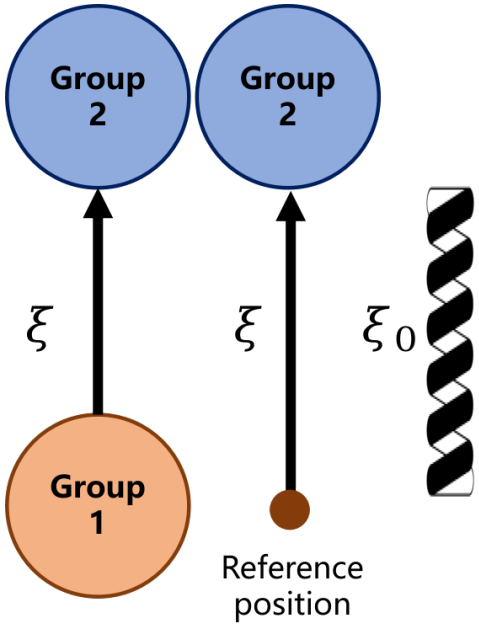




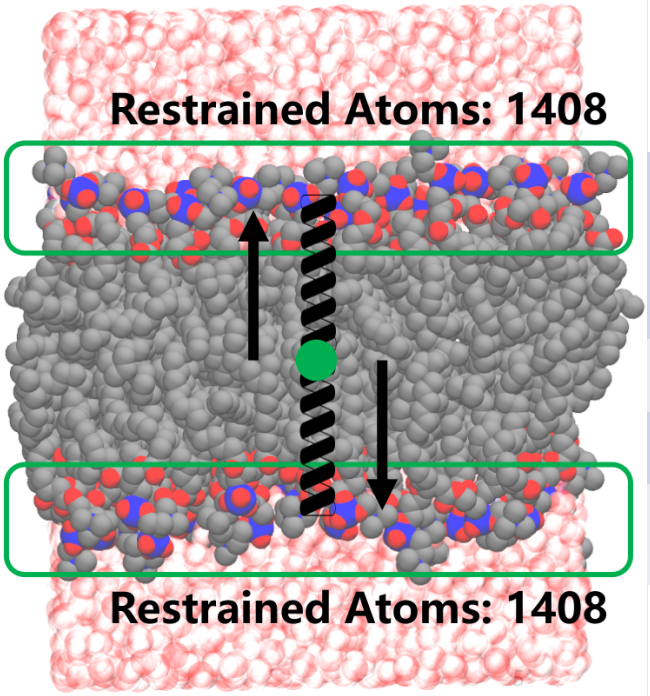
Make feature combinations work

- Replica Exchange with Solute Tempering 2 (REST2) works with NBFIX, AMBER parm7 and Gromacs input formats (by Wei Jiang);
- REST2 now works with LJ potential tail corrections;
- Four-site water models within the GPU-resident mode;
- GPU-resident FEP/TI enhancements:
  - Support van der Waals force switching;
  - GPU atom migration;
  - Fixes on HIP (AMD accelerators);
  - Support for multi-GPU.

GPU-resident group position restraints (by Mohammad Soroush Barhaghi)



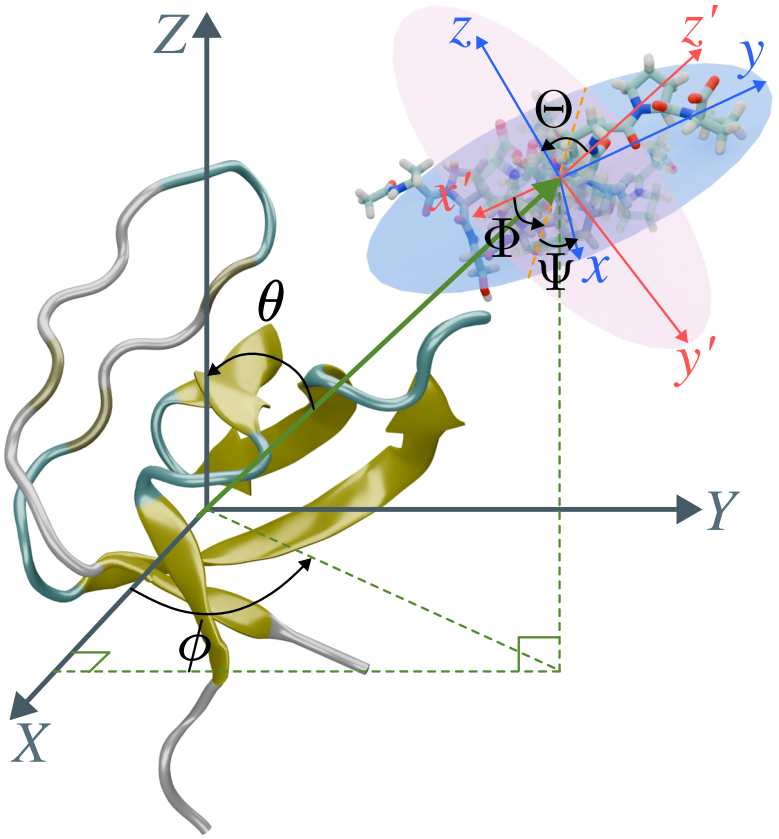
$$E = k(\xi - \xi_0)^n$$



	Simulation (ns/day)		%Performance Lost
NAMD Version	**Without Restraints**	**With Restraints**	**(WO-W)/WO Restraints**
NAMD 2.14	25.2	23.5	6.75%
NAMD 3	69.0	67.6	2.03%
NAMD 3 / NAMD 2.14	2.74	2.88	

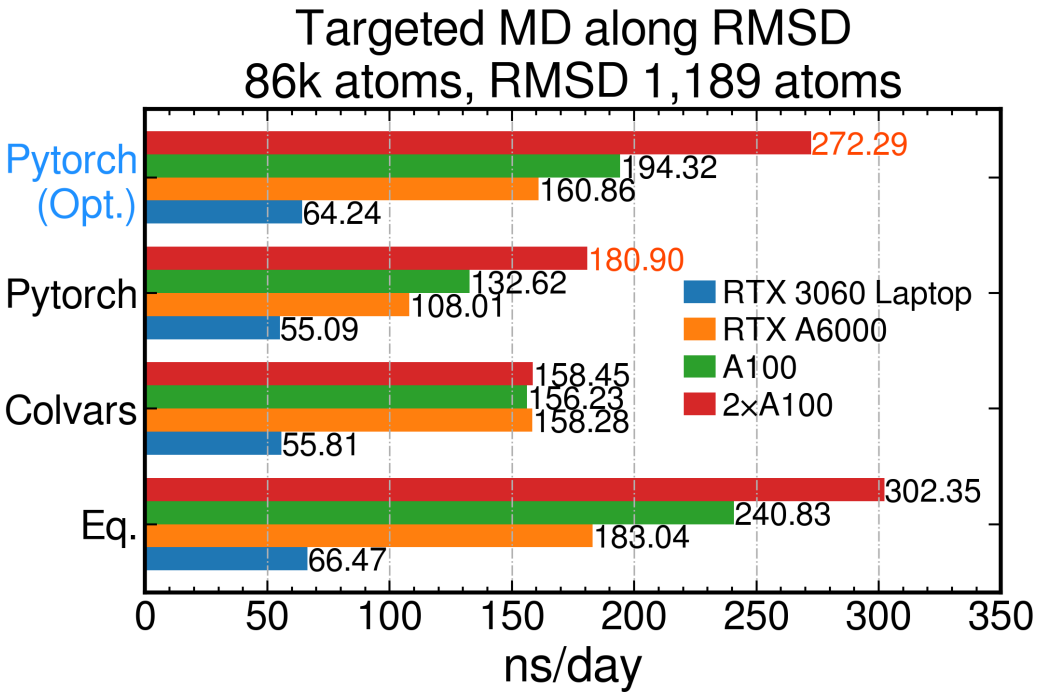
Search "`groupRestraints`" in NAMD 3.0 manual for more details.

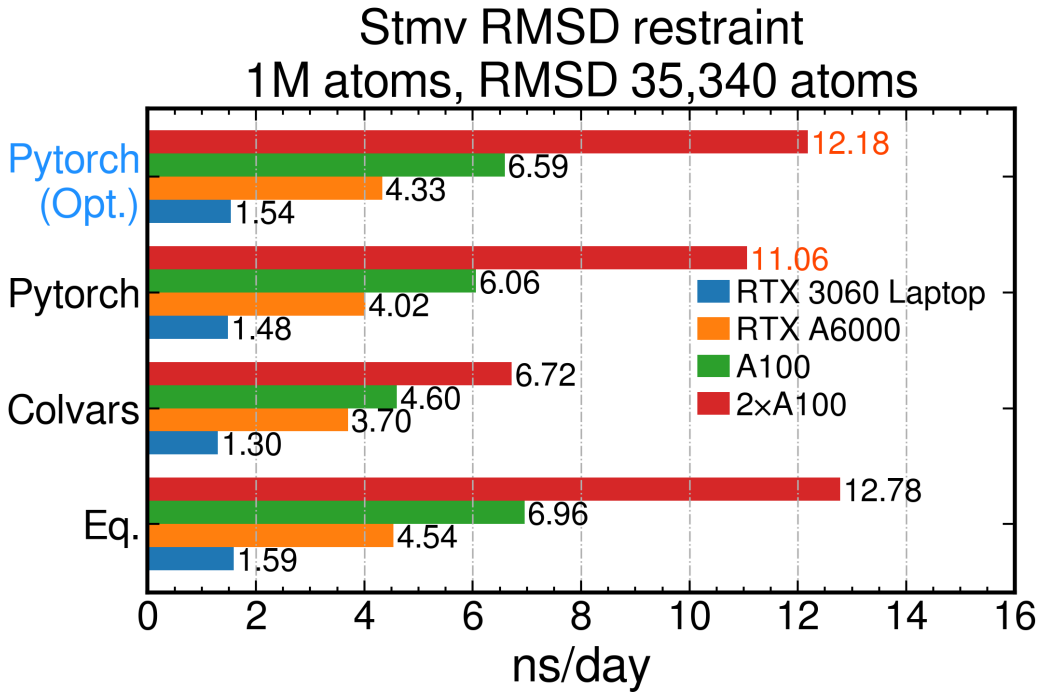
Other significant performance improvements



- Speedup of RMSD, orientation, moving frame of reference calculations in Colvars;
- Tested on laptop with RTX3060 and 8 CPU threads with Abl-SH3:p41 reversible binding (BFEE2):
  - NAMD 2.14 equilibrium simulation without Colvars: 64.83 ns/day;
  - NAMD 2.14: 53.80 ns/day;
  - NAMD 3 (GPU-offload): 60.74 ns/day.

Future developments in NAMD (not in 3.0 yet)



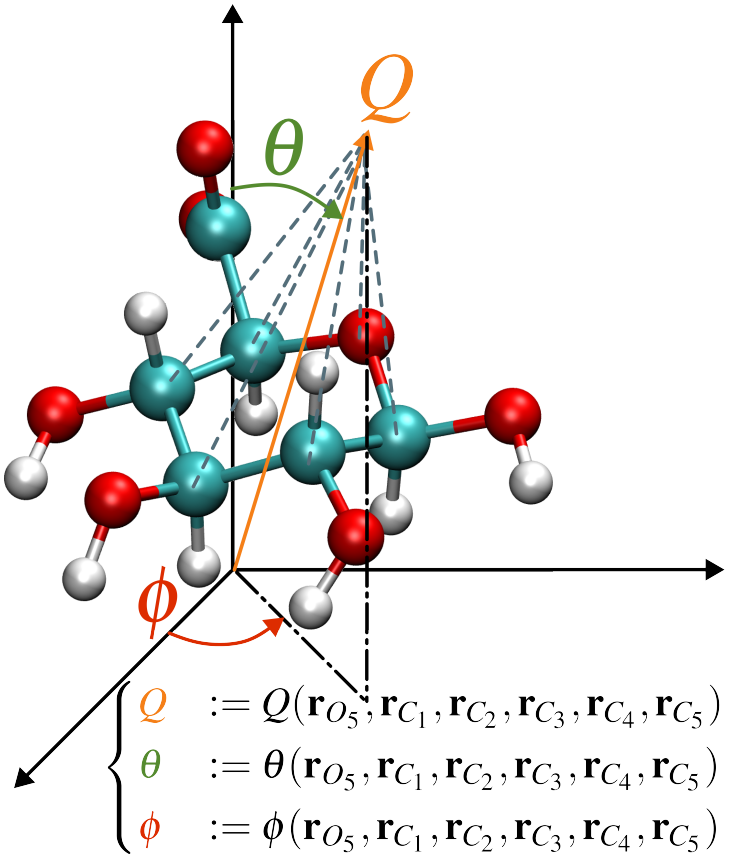


Multi-GPU optimization: PME reciprocal calculation on GPU 0, Pytorch on GPU 1

Pytorch optimizations:

- Converting input positions to float32
- Explicit derivative code instead of using automatic differentiation backward()

Tutorial of customizing collective variables



- A tutorial of
  - Defining customized CVs in NAMD with the help of Colvars,
  - Adding forces to CVs,
  - Performing targeted MD along the CV.
- Example: preparing a glucuronic acid molecule in $^1C_4$ conformation using TMD along the Cremer-Pople CVs.
- https://www.tcbg.illinois.edu/Training/Tutorials/namd/customizing-cvs-in-namd/TCBGTUTORIAL_NAMDCV.pdf

Acknowledgements

Supervisor:

- Emad Tajkhorshid (TCBG)

NAMD developers:

- David Hardy
- Eric Bohm
- Julio Maia (AMD)
- Mohammad Soroush Barhaghi (Schrödinger)

Colvars developers:

- Giacomo Fiorin (NIH)
- Jérôme Hénin (LBT, CNRS)

NVIDIA:

- David Clark
- John Stone

Colaborators:

- Wei Jiang (Argonne National Laboratory)
- Haohao Fu (Nankai University)
- Chris Chipot (Université de Lorraine)
- Benoît Roux (University of Chicago)
- Brian Radak (Tandem AI)
- Wensheng Cai (Nankai University)