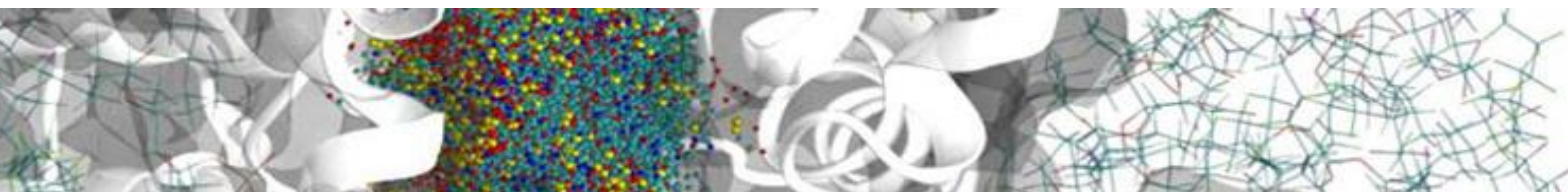# "5 steps to perform molecular dynamics in the Cloud"

Overview

ACECLOUD is the new powerful, flexible way to run ACEMD Molecular Dynamics simulations without the need to buy dedicated GPU computing resources.

Easy-to-use client software makes using AceCloud as simple as running on your own desktop, giving you the power of ACEMD on demand.

AceCloud is available through two price plans for differing usage types.

	Subscription	Pay-As-You-Go
Provides	Reserved capacity	Flexible capacity
Ideal for	Continuous, intensive use.	Occasional or bursty use.
Max Run length*	Unlimited	24 hours
Term*	Monthly reservation	Credit valid for 6 months from purchase
Price (from)*	0.08USD/hr	0.40USD/hr

*Conditions may vary, please consult AWS conditions.

How is it accessed?

AceCloud is available on the AWS Marketplace at
http://aws.amazon.com/marketplace/pp/B01N3SBK3Z

This AMI provides a standalone instance configured to run ACEMD and other Acellera software.

The intuitive AceCloud client abstracts all interactions with AWS, managing the transfer of data to and from S3 and the creation of EC2 virtual machines, making the execution of work through AceCloud as straightforward as running on a local machine.

What do I need?

To access AceCloud, the user need only subscribe to the AceCloud AWS Marketplace product and install the AceCloud client software (supported platforms: Linux, OS X and Windows). The only direct interaction with AWS required is to configure IAM access tokens (full instructions provided). Thereafter, the user runs all their computational work directly

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Visit our website http://www.acellera.com

from the command line of their workstation. Acellera will provide support to the user in all these operations until all is functional on the user infrastructure.

Which Performance may I expect?

Hardware (# GPU cores)	Performance
ACEMD 1 K20 GPU 2496 cores[1]	**100 ns/day**
ACEMD 1 K80 GPU 4992 cores[1]	**120 ns/day**

Model: Dihydrofolate reductase (DHFR) solvated in water, 23558 atoms, periodic boundary conditions, 9 Å cutoff with PME 64x64x64, rigid bonds, long time step scheme 4fs. [1] CUDA3.1 [2] System: X5570 CPUs 2.93 GHz and IB dual rail DDR.

How much does it cost?

AceCloud benefits from "Pay-as-you-go" pricing, with hourly pricing as low as 40¢/hr including EC2 fees. No additional software licenses are required than the license for ACEMD platform (End User License Agreement terms apply).

AceCloud minimizes costs by automatically uses spot Instance pricing, intelligently placing jobs in the lowest cost AWS Regions. With AceCloud, costs are only incurred for the duration of running computations.

Billing for AceCloud computation is directly via the AWS Marketplace.

Where can I get help?

Contact us for any technical or commercial information you may need at info@acellera.com.

Marketplace customers may get support for AceCloud issues by opening an issue on Acellera's HTMD Issue Tracker at https://www.acellera.com/issues

Technical support is included in the license fee covering installation and update