

Interactive Molecular Dynamics (IMDv3) in Practice: MD Packages and Performance

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This talk will cover how **IMDv3 works in practice**: how IMDv3 is implemented in various Simulation (MD) engines, how we can use it while running simulations, and how well it performs with physical systems of scientific interest.

- 1 IMDv3 implementation in MD engines
- 2 IMDv3 usage with GROMACS, LAMMPS and NAMD
- 3 Benchmarking IMDv3 modified simulations
- 4 Comparing streaming with file I/O

IMDv3 Functionality in Various MD Engines

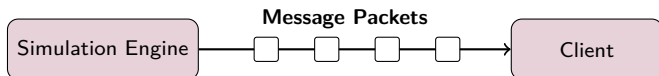
Source Code Modifications

- IMDv3 was implemented by appending new methods to existing code modules pertaining to IMDv2
- The IMDv2 code template and structure was maintained and only changed where needed
- Enabled the user to switch between v2 and v3 implementations
- The modified source codes were tested for consistency and against unchanged versions of the codebases

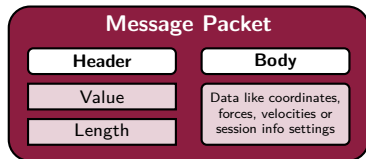
IMDv3 Functionality

- IMDv3 features were added in accordance with the new v3 protocol
- Functions and modules added – provide the ability to stream (send) specific information
- Ability to control streaming settings through MD engine input configuration file

Streaming Data with IMDv3 Protocol



- Data is streamed and sent in the form of packets which contain a *header* and a *body*



- Value** sets the type of Message/information being sent in the body
- Length** sets the length of that information
- Simple messages like IMD_GO, IMD_DISCONNECT, IMD_KILL do not have a body
- Others like IMD_FCOORDS or IMD_VELOCITIES have long array-like data within their bodies

IMD Message type	enum
IMD_DISCONNECT	0
IMD_ENERGIES	1
IMD_FCOORDS	2
IMD_GO	3
IMD_KILL	4
IMD_HANDSHAKE	5
IMD_TRATE	6
IMD_MDCOMM	7
IMD_PAUSE	8
IMD_IOERROR	9
IMD_SESSIONINFO	10
IMD_INFO	11
IMD_TIME	12
IMD_BOX	13
IMD_FORCES	14
IMD_VELOCITIES	15
IMD_WAIT	16

- IMD_HANDSHAKE** – special case i.e. length variable contains the version info
- IMD_SESSIONINFO** – establishes streaming session parameters between MD engine and server

Configuring MD engine input for streaming

- **IMD_SESSIONINFO** – special message packet, contains setting options for streaming process
- Settings configured by the user in simulation input file

Header:

```
20 (int32) Value: Session info
7 (int32) Length: Number of
configuration options in the body
```

Body:

```
<val> (int8) Are line packets sent?
<val> (int8) Are IMD energy block
packets sent?
<val> (int8) Are coords/momenta
packets sent?
<val> (int8) Are velocities packets
sent?
<val> (int8) Are force packets sent?
<val> (int8) Are box packets sent?
<val> (int8) Are time packets sent?
```

- Similar input functionality available in other MD engines

- For eg. NAMD's input file would look like:

```
# IMD parameters
# standard IMD parameters
# IMDon streaming -- on or off
IMDon      yes
# IMDport -- port number to listen on
IMDport    8888
# IMDfreq -- frequency to send data
IMDfreq    1
# IMDwait -- wait for client connection before starting
            simulation
IMDwait     on

# IMD version -- 2 for VMD and 3 for latest protocol
IMDversion 3
# IMD session info settings
# IMDsendPositions -- sending positions of entire system
IMDsendPositions  yes
# IMDsendEnergies -- sending energies and bonded, non-bonded and
                    other contributions
IMDsendEnergies   yes
# IMDsendTime -- sending time information (time, dt, step)
IMDsendTime       yes
# IMDsendBoxDimensions -- sending box dimensions (lattice
                        vectors a, b, c). If box dimensions are not defined,
                        default unit box is sent
IMDsendBoxDimensions  yes
# IMDsendVelocities -- sending velocities of entire system
IMDsendVelocities     yes
# IMDwrapPositions -- wrap positions to box; applicable when
                    IMDsendPositions is yes
IMDwrapPositions      no
```

NAMD
Scalable Molecular Dynamics

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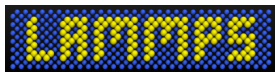
```
# IMD parameters
# standard IMD parameters
# IMDon streaming -- on or off
IMDon          yes
# IMDport -- port number to listen on
IMDport        8888
# IMDfreq -- frequency to send data
IMDfreq        1
# IMDwait -- wait for client connection before starting
               simulation
IMDwait        on

# IMD version -- 2 for VMD and 3 for latest protocol
IMDversion     3

# IMD session info settings
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IMDsendPositions  yes
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IMDwrapPositions  no
```

NAMD
Scalable Molecular Dynamics

Configuring MD engine input for streaming



- The input file in LAMMPS can be set with a line that takes care of various IMDv3 settings

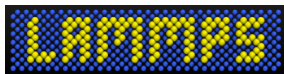
```
## IMD settings
# https://docs.lammps.org/fix_imd.html
fix 2 all imd 8888 trate 1 version 3 unwrap off time on box on coordinates on velocities on forces on
```



- For GROMACS the mdp file is modified with requisite IMDv3 settings, which can then be assembled into a binary tpr using grompp


```
; IMD parameters
IMD-group    = System      ; group to send to IMD
IMD-nst      = 1           ; transmission rate to IMD
IMD-version  = 3           ; version of IMD protocol
IMD-time     = yes         ; if time information should be
                           sent (time, dt, step)
IMD-box      = yes         ; if box dimensions should be sent
                           (lattice vectors a, b, c)
IMD-coords   = yes         ; if coordinates should be sent
IMD-unwrap   = no         ; if coordinates should be
                           unwrapped
IMD-vels     = yes         ; if velocities should be sent
IMD-forces   = yes         ; if forces should be sent
IMD-energies = yes         ; if energies should be sent
```

Availability of Source Codes and Docker containers





-  **lammps/lammps**
<https://github.com/lammps/lammps>

- *Part of official release*

-  **tcbgUIUC/namd**
<https://gitlab.com/tcbgUIUC/namd>

- *Part of official source code repo, will be part of release 3.1*

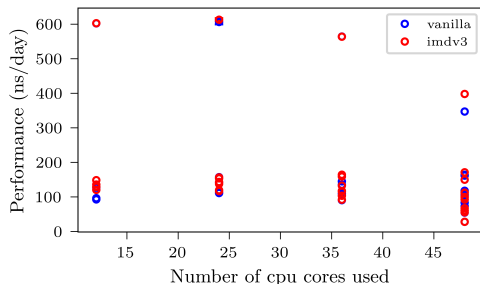
-  **heydenlabasu/streaming-md/gromacs**
https://gitlab.com/heydenlabasu/streaming-md/gromacs/-/tree/imd-v3?ref_type=heads

-  **Becksteinlab/streaming-md-docker**
<https://github.com/Becksteinlab/streaming-md-docker>

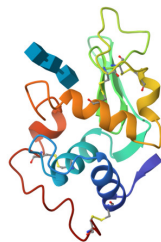


Does IMDv3 affect MD engine performance?

- We perform benchmarking analysis for IMDv3-modified version of our code with streaming
- Choose test system: HEWL in water (30,000 atom system)
- We limit our tests to certain computational resources – 1 exclusive node on ASU's SOL supercomputer - 1 A100 GPU and 48 CPU cores.
- First, test for optimized run setting for this system and compare with vanilla code.
- As an example, we show detailed results for GROMACS



GROMACS optimization results



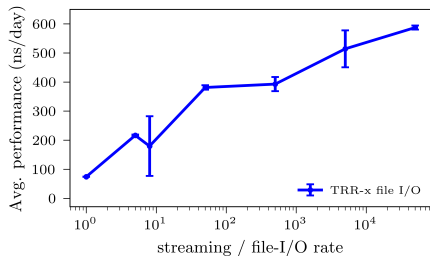
Hen Egg-White Lysozyme
(HEWL)

How good is IMDv3 streaming?

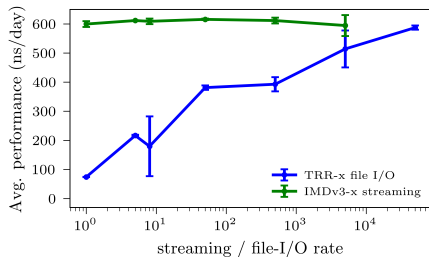
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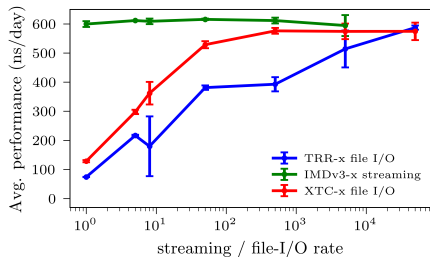


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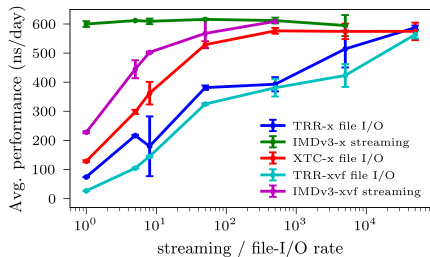
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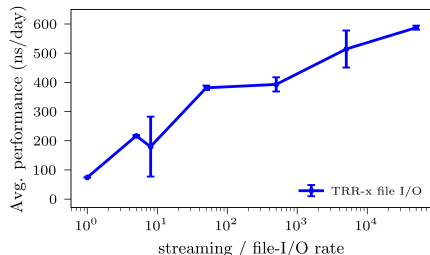
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- Writing to binary formats (.xtc) improves file I/O speeds
- When multiple data types are being streamed/written, streaming still outperforms file I/O
- Similar qualitative results when testing LAMMPS and NAMD

Conclusion

- We have successfully implemented and tested IMDv3 in 3 MD engines (GROMACS, LAMMPS, NAMD)
- The protocol allows enables various features, most importantly user-controlled flexible data streaming of various simulation properties
- Source code and Docker containers are available for easy adoption
- Tests show that IMDv3-modified MD engine code performs as well as the unmodified versions
- Benchmarks show IMDv3 streaming is efficient and outperforms file I/O
 - For certain scenarios streaming had negligible affect on performance of a running simulation
- IMDv3 can be used for many practical, high-performance molecular simulation based workflows

Questions?

Acknowledgements

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- Irfan Alibay

Thank you!
Happy to take any questions :)