

# Using LAMMPS with the Knowledgebase of Interatomic Models (KIM – <http://openKIM.org>)

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News item:

- Version 0.1.0 of the openKIM API was released yesterday, Aug. 8, 2011.  
(see <http://openKIM.org/resources> to download the source code.)

Funding:

National Science Foundation, Cyber-enabled Discovery and Innovation (CDI)  
grant

Program Manager: Beverly K. Berger

# Knowledgebase of Interatomic Models (KIM)

The *Knowledgebase of Interatomic Models (KIM)* project is based on a four-year NSF cyber-enabled discovery and innovation (CDI) grant.

KIM has the following main objectives:

- Development of an *online open resource* for standardized testing and long-term warehousing of interatomic models (potentials and force fields) and data.
- ❖ Development of an *application programming interface (API)* standard for atomistic simulations, which will allow any interatomic model to work seamlessly with any atomistic simulation code.
- Fostering the development of a quantitative theory of *transferability* of interatomic models to provide guidance for selecting application-appropriate models based on rigorous criteria, and error bounds on results.
- Striving for the permanence of the KIM project, including development of a sustainability plan, and establishment of a long-term home for its content.

More information on KIM is available at the project website: <http://openKIM.org>

# The KIM TEAM



## PIs

Ellad Tadmor (U. Minnesota)

Ryan Elliott (U. Minnesota)

James Sethna (Cornell)

## Developers

Valeriu Smirichinski (U. Minnesota)

Daniel Karls (U. Minnesota)

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Alex Alemi (Cornell)

John Crow (Silicon Life Sciences)

Trevor Wenblom (Silicon Life Sciences)

## Advisory Board

Graeme Ackland (U. Edinburgh)

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Ronald Miller (Carleton)

John Moriarty (LLNL)

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Adri van Duin (Penn State)

Gabriel Wainer (Carleton)

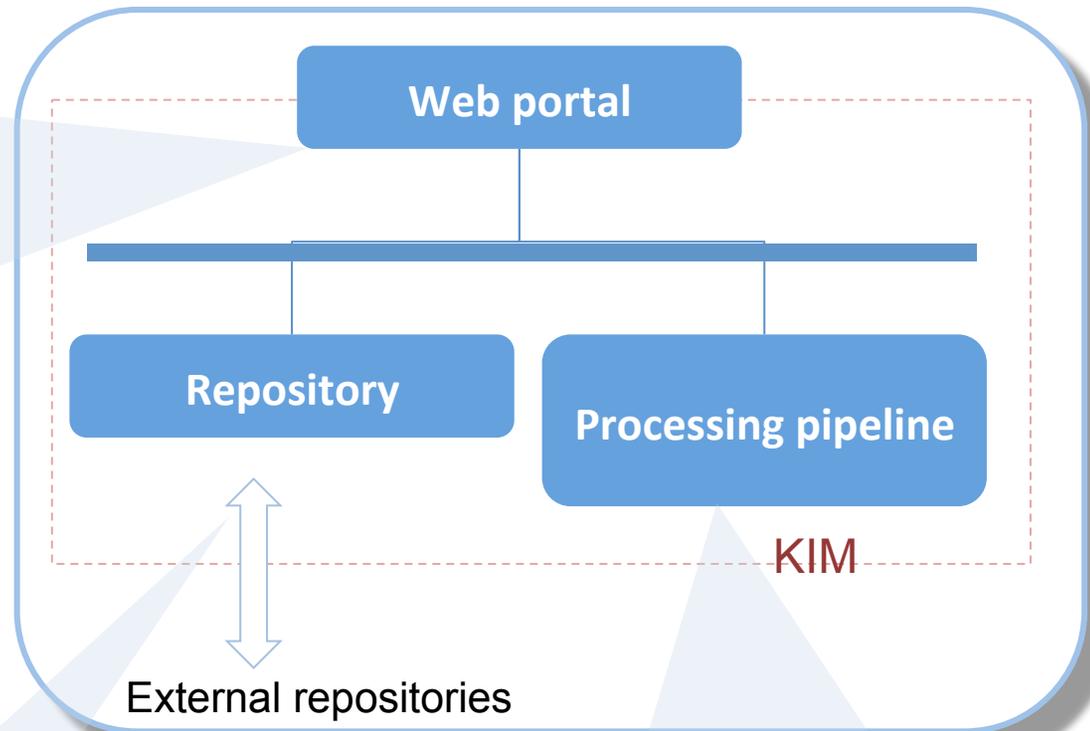
# The KIM framework

## A web interface that will facilitate:

- user **upload** and **download** of Tests, Models and Reference Data
- **searching** and querying the repository
- comparing and **visualizing** Predictions and Reference Data
- recording **user feedback** (ranking and discussion forums)

## A user-extendible database of

- interatomic **Models**
- standardized **Tests** (simulation codes)
- **Predictions** (results from Model-Test couplings)
- **Reference Data** (obtained from experiments and first principles calculations)

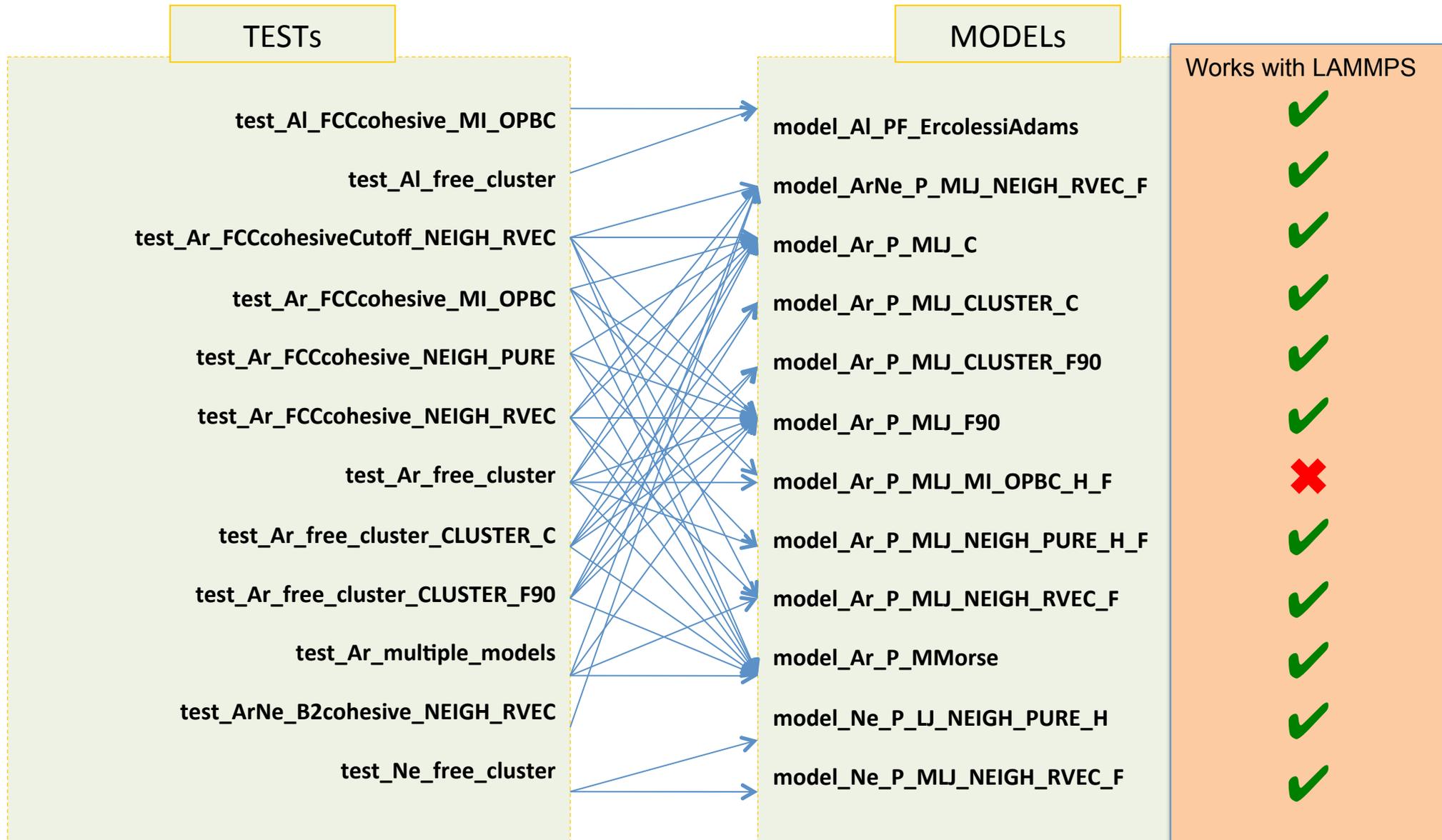


## Processing Pipeline:

**An automatic system for generating Predictions due to new Test or Model upload or changes:**

- detect viable **Test-Model couplings**
- assign **computational resources** based on priority and dependencies
- **store** results in Repository
- ❖ requires an application programming interface (**API**) to be defined

# Model and Test examples available in the current version of the openKIM API

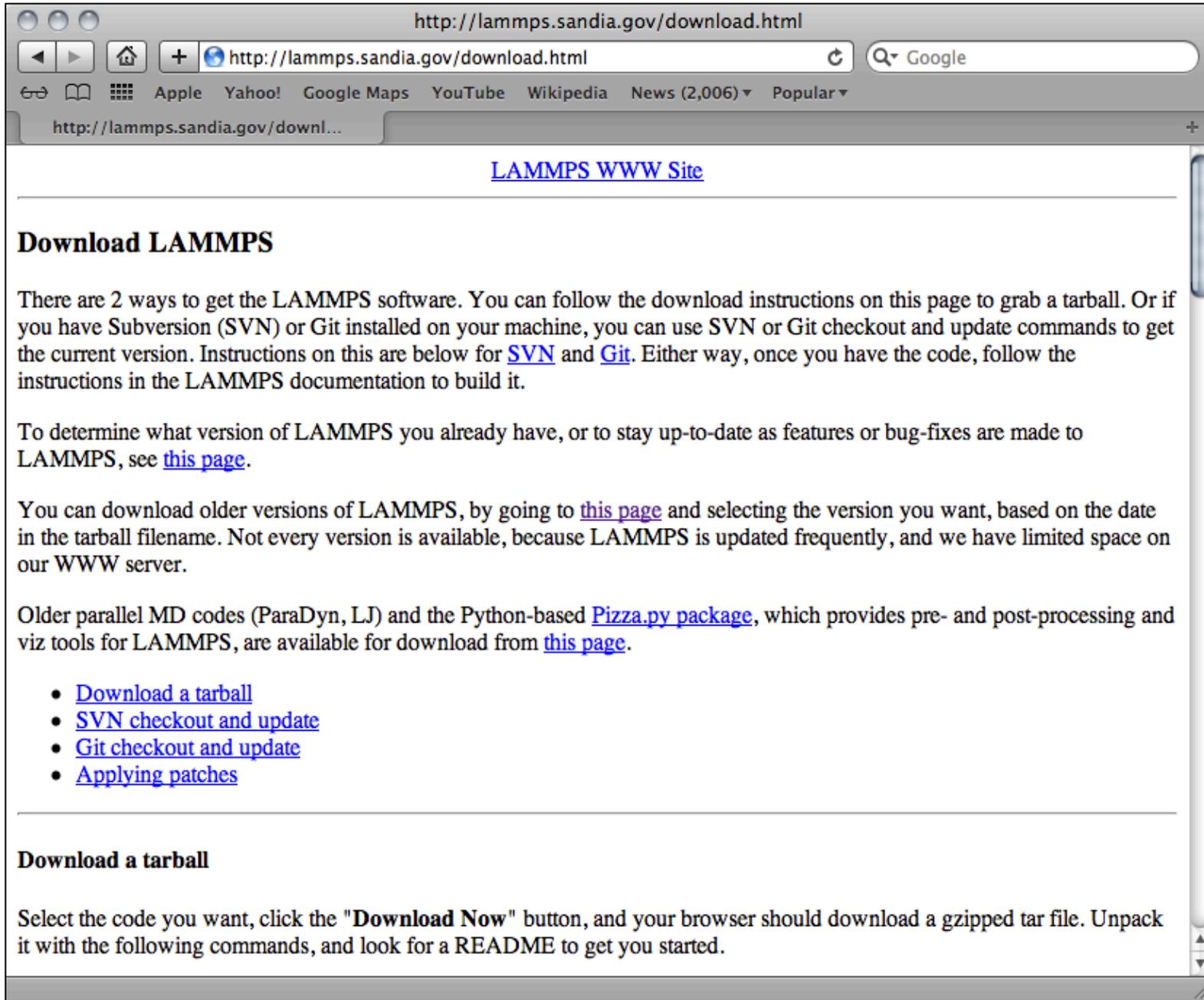


→ Indicates a **Test** can work (match) with a **Model** in the current KIM API version

Description of the Models and Tests provided with the KIM API package are given in the files MODELS/EXAMPLES.README and TESTs/EXAMPLES.README.

# Using the openKIM API with LAMMPS

## 1. Get LAMMPS: lammeps-27Mar11.tgz



The screenshot shows a web browser window with the address bar containing `http://lammeps.sandia.gov/download.html`. The page title is "LAMMPS WWW Site". The main heading is "Download LAMMPS". The text explains that there are two ways to get the software: following download instructions for a tarball, or using SVN or Git. It provides links for "SVN" and "Git" and refers to the LAMMPS documentation for building instructions. It also mentions that older versions can be downloaded from a specific page and that older parallel MD codes and the Python-based "Pizza.py package" are available for download. A bulleted list of links is provided: "Download a tarball", "SVN checkout and update", "Git checkout and update", and "Applying patches". The section "Download a tarball" is followed by instructions to click the "Download Now" button and unpack the resulting gzipped tar file.

<http://lammeps.sandia.gov/download.html>

<http://lammeps.sandia.gov/download.html> Google

Apple Yahoo! Google Maps YouTube Wikipedia News (2,006) Popular

<http://lammeps.sandia.gov/download.html>

[LAMMPS WWW Site](#)

### Download LAMMPS

There are 2 ways to get the LAMMPS software. You can follow the download instructions on this page to grab a tarball. Or if you have Subversion (SVN) or Git installed on your machine, you can use SVN or Git checkout and update commands to get the current version. Instructions on this are below for [SVN](#) and [Git](#). Either way, once you have the code, follow the instructions in the LAMMPS documentation to build it.

To determine what version of LAMMPS you already have, or to stay up-to-date as features or bug-fixes are made to LAMMPS, see [this page](#).

You can download older versions of LAMMPS, by going to [this page](#) and selecting the version you want, based on the date in the tarball filename. Not every version is available, because LAMMPS is updated frequently, and we have limited space on our WWW server.

Older parallel MD codes (ParaDyn, LJ) and the Python-based [Pizza.py package](#), which provides pre- and post-processing and viz tools for LAMMPS, are available for download from [this page](#).

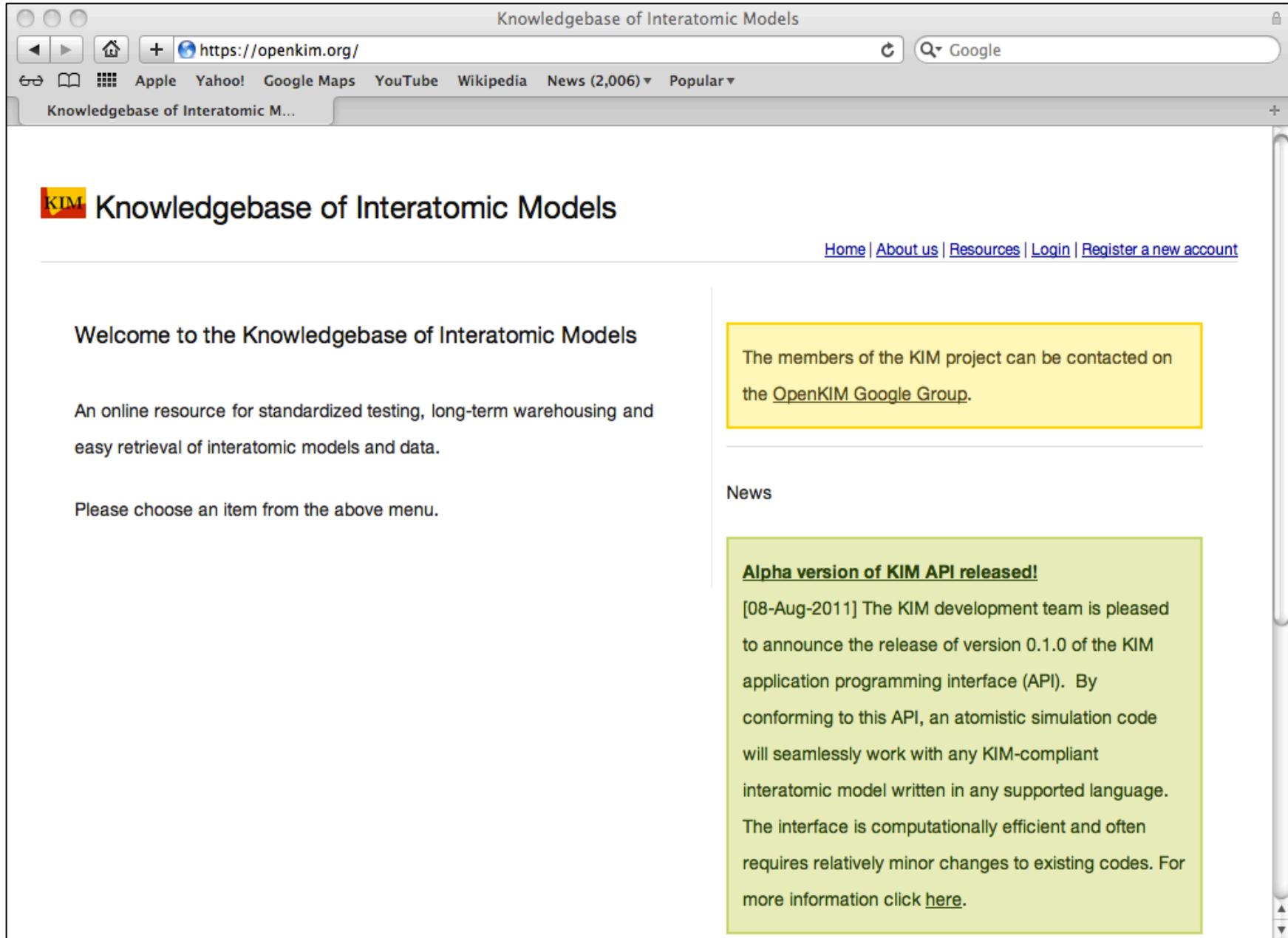
- [Download a tarball](#)
- [SVN checkout and update](#)
- [Git checkout and update](#)
- [Applying patches](#)

### Download a tarball

Select the code you want, click the "Download Now" button, and your browser should download a gzipped tar file. Unpack it with the following commands, and look for a README to get you started.

# Using the openKIM API with LAMMPS

## 2. Get the openkim-api package:



The screenshot shows a web browser window with the URL <https://openkim.org/>. The page title is "Knowledgebase of Interatomic Models". The main content area features a welcome message and a navigation menu. A yellow box highlights a contact link for the KIM project. A green box highlights a news item titled "Alpha version of KIM API released!" dated 08-Aug-2011, detailing the release of version 0.1.0 of the KIM application programming interface (API).

Knowledgebase of Interatomic Models

[Home](#) | [About us](#) | [Resources](#) | [Login](#) | [Register a new account](#)

**Welcome to the Knowledgebase of Interatomic Models**

An online resource for standardized testing, long-term warehousing and easy retrieval of interatomic models and data.

Please choose an item from the above menu.

The members of the KIM project can be contacted on the [OpenKIM Google Group](#).

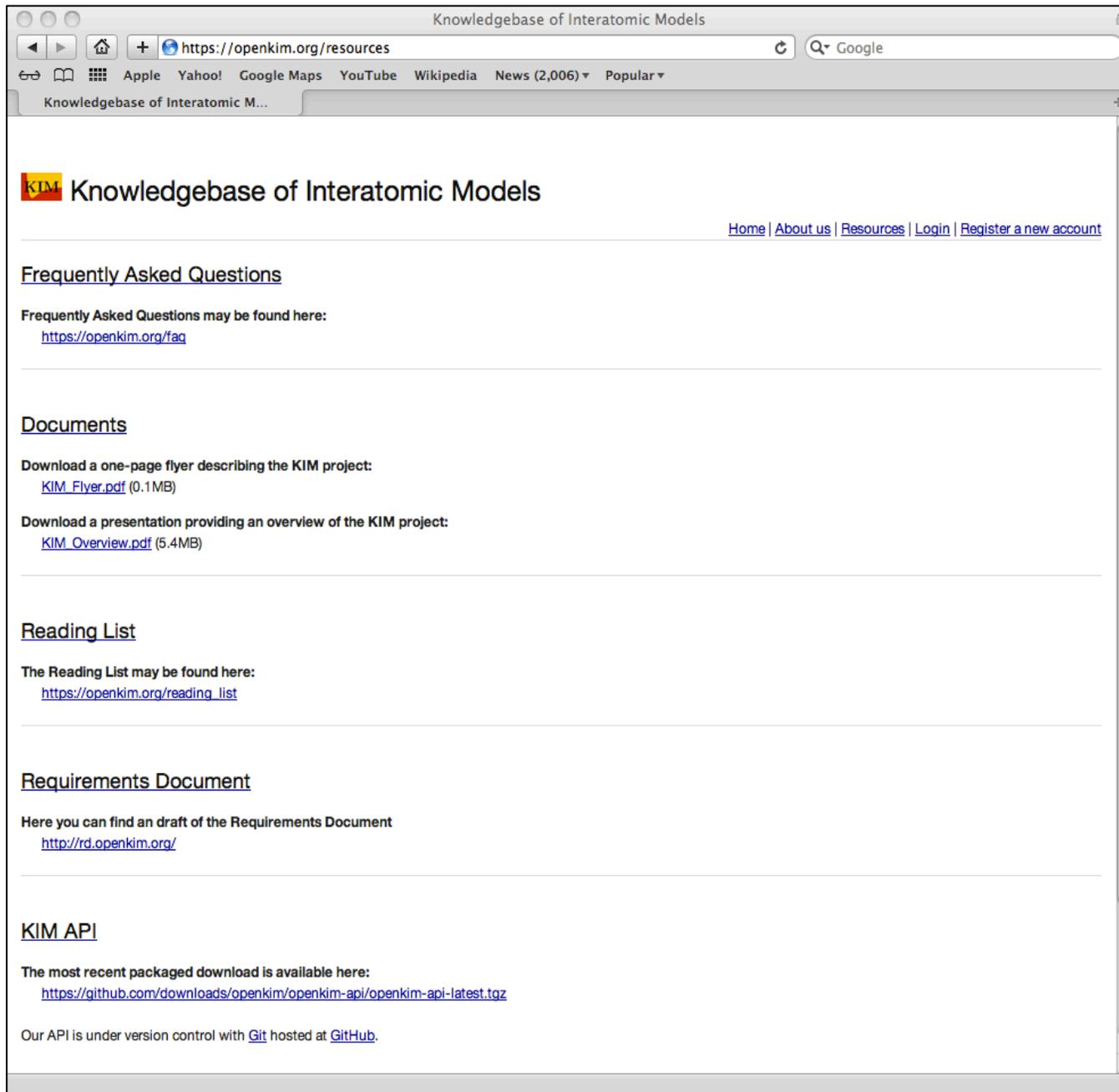
News

**Alpha version of KIM API released!**

[08-Aug-2011] The KIM development team is pleased to announce the release of version 0.1.0 of the KIM application programming interface (API). By conforming to this API, an atomistic simulation code will seamlessly work with any KIM-compliant interatomic model written in any supported language. The interface is computationally efficient and often requires relatively minor changes to existing codes. For more information click [here](#).

# Using the openKIM API with LAMMPS

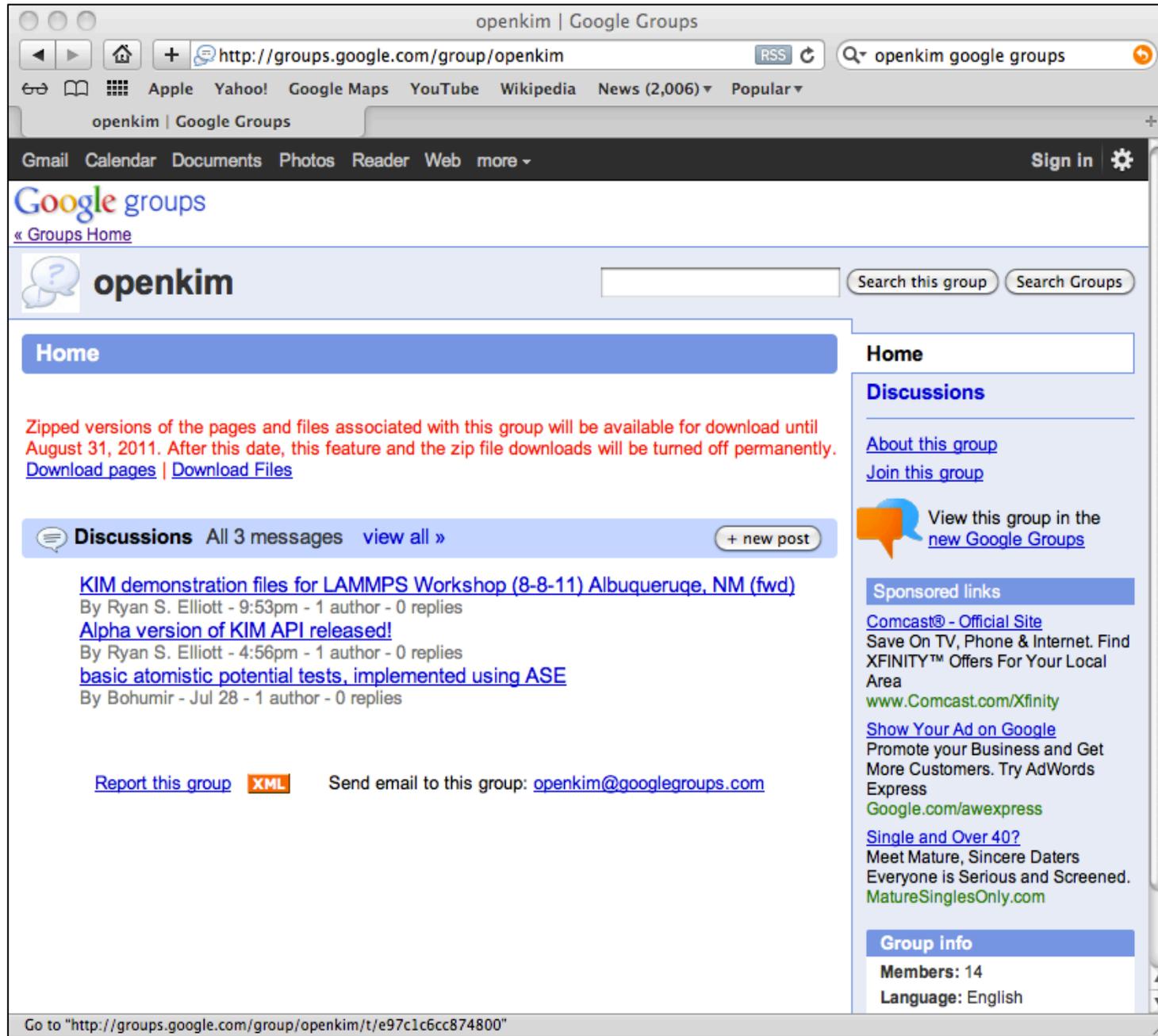
## 2. Get the openkim-api package:



The screenshot shows a web browser window with the URL <https://openkim.org/resources>. The page title is "Knowledgebase of Interatomic Models". The main content area includes a navigation menu with links for Home, About us, Resources, Login, and Register a new account. Below the navigation menu, there are several sections: "Frequently Asked Questions" with a link to <https://openkim.org/faq>; "Documents" with links to [KIM\\_Flyer.pdf](#) (0.1MB) and [KIM\\_Overview.pdf](#) (5.4MB); "Reading List" with a link to [https://openkim.org/reading\\_list](https://openkim.org/reading_list); "Requirements Document" with a link to <http://rd.openkim.org/>; and "KIM API" with a link to <https://github.com/downloads/openkim/openkim-api/openkim-api-latest.tgz>. The footer of the page states: "Our API is under version control with [Git](#) hosted at [GitHub](#)."

# Using the openKIM API with LAMMPS

## 3. Get the lammps/kim interface and example files:



The screenshot shows a web browser window displaying the Google Groups page for the 'openkim' group. The browser's address bar shows the URL 'http://groups.google.com/group/openkim'. The page features a search bar, a navigation menu with links like 'Home', 'Discussions', and 'About this group', and a list of recent discussions. The discussions include titles like 'KIM demonstration files for LAMMPS Workshop (8-8-11) Albuquerque, NM (fwd)' and 'Alpha version of KIM API released!'. The right sidebar contains sponsored links and group information, such as 'Members: 14' and 'Language: English'.

openkim | Google Groups

http://groups.google.com/group/openkim

openkim | Google Groups

Sign in

Google groups

« Groups Home

openkim

Search this group Search Groups

Home

Zipped versions of the pages and files associated with this group will be available for download until August 31, 2011. After this date, this feature and the zip file downloads will be turned off permanently. [Download pages](#) | [Download Files](#)

Discussions All 3 messages view all » + new post

[KIM demonstration files for LAMMPS Workshop \(8-8-11\) Albuquerque, NM \(fwd\)](#)  
By Ryan S. Elliott - 9:53pm - 1 author - 0 replies

[Alpha version of KIM API released!](#)  
By Ryan S. Elliott - 4:56pm - 1 author - 0 replies

[basic atomistic potential tests, implemented using ASE](#)  
By Bohumir - Jul 28 - 1 author - 0 replies

[Report this group](#) XML Send email to this group: [openkim@googlegroups.com](mailto:openkim@googlegroups.com)

Home

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Sponsored links

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Save On TV, Phone & Internet. Find XFINITY™ Offers For Your Local Area  
[www.Comcast.com/Xfinity](http://www.Comcast.com/Xfinity)

[Show Your Ad on Google](#)  
Promote your Business and Get More Customers. Try AdWords Express  
[Google.com/awexpress](http://Google.com/awexpress)

[Single and Over 40?](#)  
Meet Mature, Sincere Daters  
Everyone is Serious and Screened.  
[MatureSinglesOnly.com](http://MatureSinglesOnly.com)

Group info

Members: 14

Language: English

Go to "http://groups.google.com/group/openkim/t/e97c1c6cc874800"

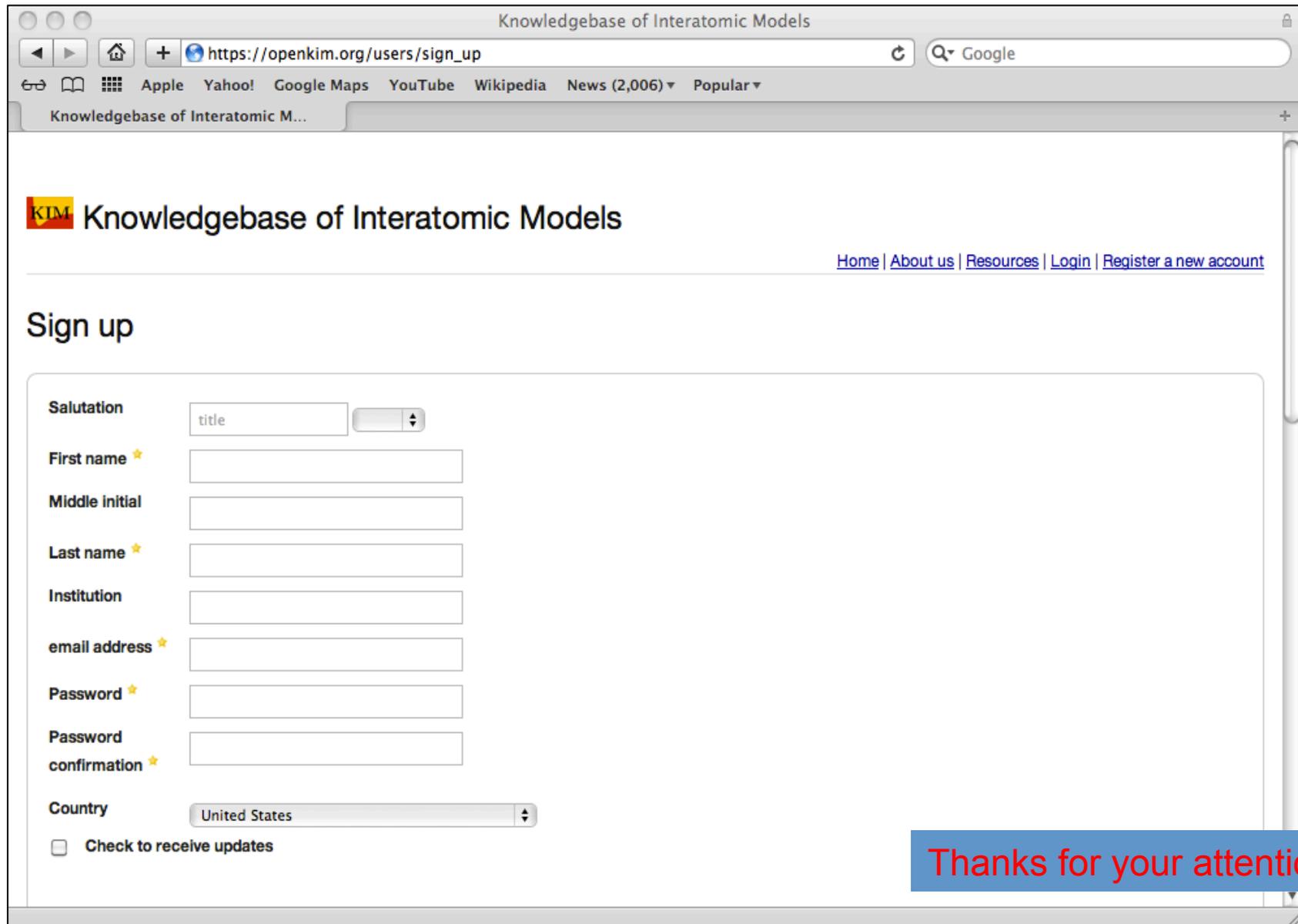
# Using the openKIM API with LAMMPS

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Go to command line window...

# Using the openKIM API with LAMMPS

## 4. Don't forget to sign up for updates!



The screenshot shows a web browser window with the URL `https://openkim.org/users/sign_up`. The page title is "Knowledgebase of Interatomic Models". The navigation menu includes links for Home, About us, Resources, Login, and Register a new account. The main heading is "Sign up". The form contains the following fields:

- Salutation: dropdown menu with "title" selected
- First name: text input field with a yellow star icon
- Middle initial: text input field
- Last name: text input field with a yellow star icon
- Institution: text input field
- email address: text input field with a yellow star icon
- Password: text input field with a yellow star icon
- Password confirmation: text input field with a yellow star icon
- Country: dropdown menu with "United States" selected
- Check to receive updates

A blue banner at the bottom right of the form area contains the text "Thanks for your attention!" in red.

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**The end**