ares Documentation

Release 0.1

Jordan Mirocha

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The Accelerated Reionization Era Simulations (*ARES*) code was designed to rapidly generate models for the global 21-cm signal. It can also be used as a 1-D radiative transfer code, stand-alone non-equilibrium chemistry solver, or meta-galactic radiation background calculator. As of late 2016, it also contains a home-grown semi-analytic model of galaxy formation.

A few papers on how it works:

- 1-D radiative transfer: Mirocha et al. (2012).
- Uniform backgrounds & global 21-cm signal: Mirocha (2014).
- Galaxy luminosity functions: Mirocha, Furlanetto, & Sun (2017).
- Population III star formation: Mirocha et al. (2018)

Plus some more applications:

- First stars and early galaxies: Mirocha & Furlanetto (2019), Mebane, Mirocha, & Furlanetto (2019).
- Warm dark matter: Schneider (2018), Leo et al. (2019), Rudakovskyi et al. (2019).
- Parameter inference & forecasting: Mirocha, Harker, & Burns (2015), Tauscher et al. (2017), Sims & Pober (2019).

Be warned: this code is still under active development – use at your own risk! Correctness of results is not guaranteed. This documentation is as much of a work in progress as the code itself, so if you encounter gaps or errors please do let me know.

Current status:

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CHAPTER 1

Quick-Start

To make sure everything is working, a quick test is to generate a realization of the global 21-cm signal using all default parameter values:

```
import ares

sim = ares.simulations.Global21cm()
sim.run()
sim.GlobalSignature()
```

See example_gs_standard in *Examples* for a more thorough introduction to this type of calculation.

CHAPTER 2

Contents

2.1 Installation

ARES depends on:

- numpy
- scipy
- matplotlib

and optionally:

- progressbar2
- hmf
- emcee
- distpy
- mpi4py
- pymp
- h5py
- setuptools
- mpmath
- shapely
- descartes

If you have mercurial installed, you can clone ARES and its entire revision history via:

hg clone https://bitbucket.org/mirochaj/ares ares cd ares python setup.py install

If you do not have mercurial installed, and would rather just grab a tarball of the most recent version, select the Download repository option on bitbucket.

You'll need to set an environment variable which points to the ARES install directory, e.g. (in bash)

```
export ARES=/users/<yourusername>/ares
```

ARES will look in \$ARES/input for lookup tables of various kinds. To download said lookup tables, run

```
python remote.py
```

This might take a few minutes. If something goes wrong with the download, you can run

```
python remote.py fresh
```

to get fresh copies of everything. If you're concerned that a download may have been interrupted and/or the file appears to be corrupted (strange I/O errors may indicate this), you can also just download fresh copies of the particular file you want to replace. For example, to grab a fresh initial conditions file, simply do

```
python remote.py fresh inits
```

2.1.1 ARES branches

ARES has two main branches. The first, default, is meant to be stable, and will only be updated with critical bug fixes or upon arrival at major development milestones. The "bleeding edge" lives in the ares-dev branch, and while you are more likely to find bugs in ares-dev, you will also find the newest features.

By default after you clone ARES you'll be using the default branch. To switch, simply type:

```
hg update ares-dev
```

To switch back.

```
hq update default
```

For a discussion of the pros and cons of different branching techniques in mercurial, this article is a nice place to start.

2.1.2 ARES versions

The first stable release of *ARES* was used in Mirocha et al. (2015), and is tagged as v0.1 in the revision history. The tag v0.2 is associated with Mirocha, Furlanetto, & Sun (2017). Note that these tags are just shortcuts to specific revisions. You can switch between them just like you would switch between branches, e.g.,

```
hg update v0.2
```

If you're unsure which version is best for you, see the *Development History*.

2.1.3 Don't have Python already?

If you do *not* already have Python installed, you might consider downloading yt, which has a convenient installation script that will download and install Python and many commonly-used Python packages for you. Anaconda is also good for this.

2.1.4 Help

If you encounter problems with installation or running simple scripts, first check the *Troubleshooting* page in the documentation to see if you're dealing with a common problem. If you don't find your problem listed there, please let me know!

2.2 Examples

2.2.1 Running Individual Simulations

- Reionization & Global 21-cm Signal
 - example_gs_standard
 - example_gs_multipop
 - example_gs_phenomenological
- Uniform Radiation Backgrounds
 - example_crb_uv
 - example_crb_xr
- 1-D Radiative Transfer
 - example_rt06_1
 - example_rt06_2

2.2.2 Parameter Studies and Inference

- Running Large Suites of Models
 - example_grid
 - example_mc_sampling
- · Fitting and Forecasting
 - example_mcmc_gs
 - example_mcmc_lf
- Analyzing Sets of Models
 - example_inline_analysis
 - example_grid_analysis
 - example_mcmc_analysis

2.2.3 Extensions

- · Advanced physics
 - example_adv_RT_w_He
- · Advanced source populations
 - example_pop_galaxy

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- example_pop_sps
- example_popIII
- example_edges
- · Comparing to observational data
 - example_litdata
- Customization
 - example_embed_ares
 - uth_pq
 - uth_pop_new

2.3 Performance

The default parameter settings in ARES are not necessarily optimal for all applications. In this section, we detail some tricks that may be useful if one can tolerate a small hit in accuracy.

2.3.1 Time-stepping

For example_gs_standard, the main parameters that control the speed of the calculation are <code>epsilon_dt</code> and <code>max_timestep</code>, which are described a bit more in params_control. In short, <code>epsilon_dt</code> determines the largest fractional change allowed in any property of the intergalactic medium (IGM) – if a given timestep results in a larger fraction change than <code>epsilon_dt</code> allows, the iteration will be repeated with a smaller timestep. On the other hand, <code>max_timestep</code> governs the "global" timestep, i.e., the largest step we are allowed to take even in the limit where IGM quantities are evolving slowly, and thus are not restricted by <code>epsilon_dt</code>. This parameter is in some sense aesthetic, as it determines how frequently data is saved and as a result controls the smoothness in the time evolution of quantities of interest.

The default values for these parameters, <code>epsilon_dt=0.05</code> and <code>max_timestep=1</code> (the latter in Myr) are set so that they have no discernible impact on the evolution of the IGM. However, relaxing <code>epsilon_dt</code> by a factor of a few and increasing <code>max_timestep</code> to ~ 10 Myr can provide a factor of $\sim 2-3$ speed-up, with only a limited impact in the results (e.g., $\sim 5\%$ errors induced in global 21-cm signal). Their effects have not been studied exhaustively, so it is possible that for some combinations of parameters the impact of changing these parameters may be greater. Proceed with caution!

Time-stepping is controlled a little differently in models that properly solve for the evolution of the X-ray background (as in Mirocha (2014); see example_crb_xr). In this case, the time resolution is set to be logarithmic in 1+z, which accelerates solutions to the radiative transfer equation. The key parameter is tau_redshift_bins, which is 1000 by default in the mirocha2017:dpl models (see example_litdata). Reducing this to 400 or 500 can result in a factor of ~ 2 speed-up. Just note that you will need to re-generate a lookup table for the IGM optical depth of that resolution – see inits_tables for a few notes about how to do that (the relevant adjustment is re-setting Nz in the \$ARES/examples/generate_optical_depth_tables.py script).

2.3.2 Avoiding Overhead: Halo Mass Function and Stellar Population Synthesis Models

Most ARES calculations spend $\sim 10-30\%$ of the run-time simply reading in some necessary look-up tables – this sounds like a lot but is of course much faster than re-generating them on-the-fly. However, for most applications, these

tables are always the same, so you can read them into memory once and pass them along to subsequent calculations for a speed-up.

The two most common lookup tables are those for the halo mass function (HMF) and stellar population synthesis (SPS) models. The following example grabs instances of the HMF and SPS classes that are attached to an initial *ARES* simulation, and then supplies those objects to a subsequent model which then does not need to read them in for itself:

```
import ares
import time
# First, setup a UVLF-calibrated model for the global signal.
pars = ares.util.ParameterBundle('mirocha2017:base')
# Time it
t1 = time.time()
sim = ares.simulations.Global21cm(**pars)
sim.run()
t2 = time.time()
# Grab the HMF and SPS model instances from the first source population
# and pass them to the next model via parameters that exist solely for
# this purpose.
pars['hmf_instance'] = sim.pops[0].halos
pars['pop_src_instance{0}'] = sim.pops[0].src
# Time the new run.
t3 = time.time()
sim = ares.simulations.Global21cm(**pars)
sim.run()
t4 = time.time()
print("Sim 1 done in {} sec.".format(t2 - t1))
print("Sim 2 done in {} sec.".format(t4 - t3))
```

This should provide a $\sim 20\%$ speed-up.

Note: The HMF speed-up applies also to the simplest global signal models, but the pop_src_instance trick used above does not, as such models do not initialize stellar population synthesis models.

Note: These tricks are built-in to the ModelGrid and ModelFit machinery in *ARES*. Simply set the save_hmf and save_psm attributes of each class to True before running.

2.3.3 Turning off advanced solutions to radiative transfer

There are two main differences between the so-called $f_{\rm coll}$ models and the 'mirocha2017' UVLF-calibrated models relevant to the performance of the code: (i) the UVLF-calibrated models generate an entire population of galaxies, rather than linking the star formation rate density to $\dot{f}_{\rm coll}$, which is slightly slower, and (ii) by default, the 'mirocha2017:base' models will solve the cosmological radiative transfer equation in detail, as mentioned above in the "Time Stepping" section. The accuracy of this calculation can be reduced to achieve a speed-up (see above), but you can also just turn this off if you'd like – just beware that if performing inference, this will bias your constraints on any X-ray-related parameters.

To turn off the advanced RTE machinery, do the following:

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```
pars = ares.util.ParameterBundle('mirocha2017:base')

# X-rays are emitted by population #1: turn off RTE solution
pars['pop_solve_rte{1}'] = False

# Must also switch to a simpler, energy-independent scheme for
# depositing photo-electron energies in the IGM.
pars['secondary_ionization] = 1
```

Setting secondary_ionization=1 will revert to using the Shull & van Steenberg (1985) approach to secondary ionization and heating, which is an asymtoptic high-energy limit. By default, secondary_ionization=3, which corresponds to the energy-dependent results of Furlanetto & Johnson-Stoever (2010).

2.4 Under the Hood

Super incomplete, sorry!

2.4.1 Parameters, Fields, and Data Structures

- · params
- fields
- inits_tables
- uth_pq

2.4.2 Source Populations

- uth_pop_halo
- uth_pop_sfrd
- · uth_pop_radiation

2.4.3 Physics

• uth_physics_cosmo

2.4.4 Solvers

• uth_solver_chem

2.5 Troubleshooting

This page is an attempt to keep track of common errors and instructions for how to fix them. If you encounter a bug not listed below, fork ares on bitbucket and an issue a pull request to contribute your patch, if you have one. Otherwise, shoot me an email and I can try to help. It would be useful if you can send me the dictionary of parameters for a particular calculation. For example, if you ran a global 21-cm calculation via

```
import ares

pars = {'parameter_1': 1e6, 'parameter_2': 2} # or whatever

sim = ares.simulations.Global21cm(**pars)
sim.run()
```

and you get weird or erroneous results, pickle the parameters:

```
import pickle
f = open('problematic_model.pkl', 'wb')
pickle.dump(pars, f)
f.close()
```

and send them to me. Thanks!

Note: If you've got a set of problematic models that you encountered while running a model grid or some such thing, check out the section on "problem realizations" in example_grid_analysis.

2.5.1 Plots not showing up

If when running some *ARES* script the program runs to completion without errors but does not produce a figure, it may be due to your matplotlib settings. Most test scripts use draw to ultimately produce the figure because it is non-blocking and thus allows you to continue tinkering with the output if you'd like. One of two things is going on:

- You invoked the script with the standard Python interpreter (i.e., **not** iPython). Try running it with iPython, which will spit you back into an interactive session once the script is done, and thus keep the plot window open.
- Alternatively, your default matplotlib settings may have caused this. Check out your matplotlibrc file (in \$HOME/.matplotlibrc) and make sure interactive: True.

Future versions of *ARES* may use blocking commands to ensure that plot windows don't disappear immediately. Email me if you have strong opinions about this.

2.5.2 IOError: No such file or directory

There are a few different places in the code that will attempt to read-in lookup tables of various sorts. If you get any error that suggests a required input file has not been found, you should:

- Make sure you have set the \$ARES environment variable. See the *Installation* page for instructions.
- Make sure the required file is where it should be, i.e., nested under \$ARES/input.

In the event that a required file is missing, something has gone wrong. Run python remote.py fresh to download new copies of all files.

2.5.3 LinAlgError: singular matrix

This is known to occur in ares.physics.Hydrogen when using scipy.interpolate.interpld to compute the collisional coupling coefficients for spin-exchange. It is due to a bug in LAPACK version 3.4.2 (see this thread). One solution is to install a newer version of LAPACK. Alternatively, you could use linear interpolation, instead of a spline, by passing interp_cc='linear' as a keyword argument to whatever class you're instantiating, or more permanently by adding interp_cc='linear' to your custom defaults file (see params section for instructions).

2.5.4 21-cm Extrema-Finding Not Working

If the derivative of the signal is noisy (due to numerical artifacts, for example) then the extrema-finding can fail. If you can visually see three extrema in the global 21-cm signal but they are either absent or crazy in ares. simulations. Global21cm.turning_points, then this might be going on. Try setting the smooth_derivative parameter to a value of 0.1 or 0.2. This parameter will smooth the derivative with a boxcar of width $\Delta z = \text{smooth_derivative}$ before performing the extrema finding. Let me know if this happens (and under what circumstances), as it would be better to eliminate numerical artifacts than to smooth them out after the fact.

2.5.5 AttributeError: No attribute blobs.

This is a bit of a red herring. If you're running an MCMC fit and saving 2-D blobs, which always require you to pass the name of the function, this error occurs if you supply a function that does not exist. Check for typos and/or that the function exists where it should.

2.5.6 TypeError: __init__() got an unexpected keyword argument 'assume_sorted'

Turns out this parameter didn't exist prior to scipy version 0.14. If you update to scipy version >= 0.14, you should be set. If you're worried that upgrading scipy might break other codes of yours, you can also simply navigate to ares/physics/Hydrogen.py and delete each occurrence of assume_sorted=True, which should have no real effect (except for perhaps a very slight slowdown).

2.5.7 Failed to interpret file '<some-file>.npz' as a pickle

This is a strange one, which might arise due to differences in the Python and/or pickle version used to read/write lookup tables *ARES* uses. First, try to download new lookup tables via:

```
python remote.py fresh
```

If that doesn't magically fix it, please email me and I'll do what I can to help!

2.5.8 ERROR: Cannot generate halo mass function

This error generally occurs because lookup tables for the halo mass function are not being found, and when that happens, *ARES* tries to make new tables. This process is slow and so is not recommended! Instead you should check that (i) you have correctly set the \$ARES environment variable and (ii) that you have run the remote.py script (see *Installation*), which downloads the default HMF lookup table. If you have recently pulled changes, you may need to re-run remote.py since, e.g., the default HMF parameters may have been changed and corresponding tables may have been updated on the web. To save time, you can specify that you only want new HMF tables by executing python remote.py fresh hmf.

2.5.9 General Mysteriousness

• If you're running *ARES* from within an iPython (or Jupyter) notebook, be wary of initializing class instances in one notebook cell and modifying attributes in a separate cell. If you re-run the the second cell *without* re-running the first cell, this can cause problems because changes to attributes will not automatically propagate back up to any parent classes (should they exist). This is known to happen (at least) when using the ModelGrid and ModelSamples classes in the inference sub-module.

2.6 ARES Development: Staying Up To Date

Things are changing fast! To keep up with advancements, a working knowledge of mercurial will be very useful. If you're reading this, you may already be familiar with mercurial to some degree, as its clone command can be used to checkout a copy of the most-up-to-date version (the 'tip" of development) from bitbucket. For example (as in *Installation*),

```
hg clone https://bitbucket.org/mirochaj/ares ares
cd ares
python setup.py install
```

If you don't plan on making changes to the source code, but would like to make sure you have the most up-to-date version of ARES, you'll want to use the hg pull command regularly, i.e., simply type

```
hg pull
```

from anywhere within the ARES folder. After entering your bitbucket credentials, fresh copies of any files that have been changed will be downloaded. In order to accept those updates, you should then type:

```
hg update
```

or simply hg up for short. Then, to re-install ARES:

```
python setup.py install
```

If you plan on making changes to *ARES*, you should fork it so that your line of development can run in parallel with the "main line" of development. Once you've forked, you should clone a copy just as we did above. For example (note the hyperlink change),

```
hg clone https://bitbucket.org/mirochaj/ares-jordan ares-jordan cd ares-jordan python setup.py install
```

There are many good tutorials online, but in the following sections we'll go through the commands you'll likely be using all the time.

2.6.1 Checking the Status of your Fork

You'll typically want to know if, for example, you have changed any files recently and if so, what changes you have made. To do this, type:

```
hg status
```

This will print out a list of files in your fork that have either been modified (indicated with M), added (A), removed (R), or files that are not currently being tracked (?). If nothing is returned, it means that you have not made any changes to the code locally, i.e., you have no 'outstanding changes.'

If, however, some files have been changed and you'd like to see just exactly what changes were made, use the diff command. For example, if when you type hg status you see something like:

```
M tests/test_solver_chem_h.py
```

follow-up with:

```
hq diff tests/test_solver_chem_h.py
```

and you'll see a modified version of the file with + symbols indicating additions and - signs indicating removals. If there have been lots of changes, you may want to pipe the output of hg diff to, e.g., the UNIX program less:

```
hg diff tests/test_solver_chem_h.py | less
```

and use u and d to navigate up and down in the output.

2.6.2 Making Changes and Pushing them Upstream

If you convince yourself that the changes you've made are *good* changes, you should absolutely save them and beam them back up to the cloud. Your changes will either be:

- Modifications to a pre-existing file.
- Creation of an entirely new file.

If you've added new files to *ARES*, they should get an ? indicator when you type hg status, meaning they are untracked. To start tracking them, you need to add them to the repository. For example, if we made a new file tests/test_new_feature.py, we would do:

```
hg add tests/test_new_feature.py
```

Upon typing hg status again, that file should now have an A indicator to its left.

If you've modified pre-existing files, they will be marked M by hg status. Once you're happy with your changes, you must *commit* them, i.e.:

```
hg commit -m "Made some changes."
```

The -m indicates that what follows in quotes is the "commit message" describing what you've done. Commit messages should be descriptive but brief, i.e., try to limit yourself to a sentence (or maybe two), tops. You can see examples of this in the ares commit history.

Note that your changes are still *local*, meaning the *ARES* repository on bitbucket is unaware of them. To remedy that, go ahead and push:

```
hg push
```

You'll once again be prompted for your credentials, and then (hopefully) told how many files were updated etc.

If you get some sort of authorization error, have a look at the following file:

```
$ARES/.hg/hgrc
```

You should see something that looks like

```
[paths]
default = https://username@bitbucket.org/username/fork-name

[ui]
username = John Doe <johndoe@gmail.com>
```

If you got an authorization error, it is likely information in this file was either missing or incorrect. Remember that you won't have push access to the main *ARES* repository: just your fork (hence the use of 'fork-name" above).

2.6.3 Contributing your Changes to the main repository

If you've made changes, you should let us know! The most formal way of doing so is to issue a pull request (PR), which alerts the administrators of *ARES* to review your changes and pull them into the main line of *ARES* development.

2.6.4 Dealing with Conflicts

Will cross this bridge when we come to it!

2.7 ARES Development: Contributing!

If ARES lacks functionality you're interested in, but seems to exhibit some features you'd like to make use of, adapting it to suit your purpose should (in principle) be fairly straightforward. The following sections describe how you might go about doing this.

If you end up developing something that might be useful for others and are willing to share, you should absolutely fork ares on bitbucket. Feel free to shoot me an email if you need help getting started!

2.7.1 Adding new modules: general rules

There are a few basic rules to follow in adding new modules to ARES that should prevent major crashes. They are covered below.

Imports

First and foremost, when you write a new module you should follow the hierarchy that's already in place. Below, the pre-existing sub-modules within *ARES* are listed in an order representative of that hierarchy:

- inference
- simulations
- solvers
- static
- populations, sources
- · physics, util, analysis

It will hopefully be clear which sub-module your new code ought to be added to. For example, if you're writing code to fit a particular kind of dataset, you'll want to add your new module to ares.inference. If you're creating new kinds of source populations, ares.populations, and so on. If you're adding new physical constants, rate coefficients, etc., look at ares.physics.Constants and ares.physics.RateCoefficients.

Now, you'll (hopefully) be making use of at least some pre-existing capabilities of *ARES*, which means your module will need to import classes from other sub-modules. There is only one rule here:

When writing a new class, let's say within sub-module X, you cannot import classes from sub-modules Y that lie above X in the hierarchy.

This is to prevent circular imports (which result in recursion errors).

Inheritance

You might also want to inherit pre-existing classes rather than simply making new instances of them in your own. For example, if creating a class to represent a new type of source population, it would be wise to inherit the ares. populations. Population class, which has a slew of convenience routines. More on that later.

Again, there's only one rule, which is related to the hierarchy listed in the above section:

Parent Classes (i.e., those to be inherited) must be defined either at the same level in the hierarchy as the Child Classes or below.

This follows from the rule about imports, since a class must be either defined locally or imported before it can be inherited.

2.8 Development History

ARES used to exist as two separate codes: rt1d and glorb, which were introduced in Mirocha et al. (2012) and Mirocha (2014), respectively. Since then, the codes have been combined and restructured to provide a more unified framework for doing radiative transfer calculations, modeling of the global 21-cm signal, and exploring all types of parameter spaces using MCMC.

Here's an attempt to keep track of major changes to the code over time, which will be tagged in the bitbucket repository with version numbers. I haven't followed conventions for version numbering so far. Instead, I've simply tagged commits with a version number when a paper is submitted using that version of the code (e.g., v0.1 and v0.2), or when a series of noteworthy improvements or bug fixes have been made (v0.3).

2.8.1 v0.5

- This is the version of the code used in Mirocha & Furlanetto (2019).
- Note that several "litdata" modules have been updated so that the year is reflective of the year the paper was *published*, not *submitted*!

2.8.2 v0.4

• This is the version of the code used in Mirocha et al. (2018). The main addition is global Lyman-Werner feedback, which raises the minimum mass of star-forming halos self-consistently using an iterative technique.

2.8.3 v0.3

- Updated to work with hmf version 2.0.1.
- Bug fix in S_{α} calculation for Furlanetto & Pritchard (2006): sign error in higher order terms.
- Generalized *HaloProperty* objects from version 0.2 to allow dependence on any number of arbitrary quantities. Now called *ParameterizedQuantity* object.

2.8.4 v0.2

This is the version of the code used in Mirocha, Furlanetto, & Sun (submitted).

Main (new) features:

- Can model the star-formation efficiency as a mass- and redshift-dependent quantity using *HaloProperty* objects.
- This, coupled with the *GalaxyPopulation* class, allows one to generate models of the galaxy luminosity function. Also possible to fit real datasets (using ares.inference.FitLuminosityFunction module).
- Creation of a *litdata* module to facilitate use of data from the literature. At the moment, this includes recent measurements of the galaxy luminosity function and stellar population synthesis models (*starburst99* and *BPASS*).
- Creation of ParameterBundle objects to ease the initialization of calculations.

2.8.5 v0.1

This is the version of the code used in Mirocha et al. (2015).

Main features:

- Simple physical models for the global 21-cm signal available.
- Can use * emcee to fit these models to data.

2.9 Acknowledgements

Main developer(s):

· Jordan Mirocha

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