SCATTERING MEETING

2018-04-17

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TOPICS

1. Website
2. Shape conversions
3. Data availability
4. Support programs
5. May meeting scheduling

The last meeting was in November.

Not all of this will be covered today. Part will extend into the May meeting, part is to provide you with examples, and part is for reference.

Main goal: build the code, import some shapes, and discuss via the mailing list over the upcoming weeks.

WEBSITE https://rhoneyager.github.io/libicedb

icedb 0.4.2

Getting started with icedb

Summary: icedb is a toolkit for manipulating particle scattering databases. It is under heavy development, so this site doesn't have much content yet. The instructions here will help you quickly get started. The other topics listed in the sidebar will provide additional information and detail.

Edit me

There are now many published datasets on the scattering properties of realistically shaped snow and aerosol particles. These datasets represent increasingly sophisticated attempts to match the variability and detail of particles found in nature. Applications range from ground-based, airborne, and space-based retrievals to active and passive forward simulators and the assimilation of all-sky microwave observations into numerical weather prediction models.

The icedb toolkit provides the ability to manipulate both particle structural information and scattering information. It can be used to convert diverse sets of scattering databases into a common HDF5 / NetCDF file format. This format is an outgrowth of discussions at the 2017 International Summer Snowfall Workshop. Having a common format for storing scattering data is quite desirable, as it allows researchers to rapidly assess features of different particle models and use existing results in their own research. Different papers describe their particle models using different metrics, so icedb also provides functions to establish consistent definitions of quantities like particle size, aspect ratio, fractal dimension and projected area.

The library and the associated applications will build on Windows, OS X, many Linuxes and BSDs. It is written in C++, and will also eventually provide a C-style interface. This will allow end users to use the

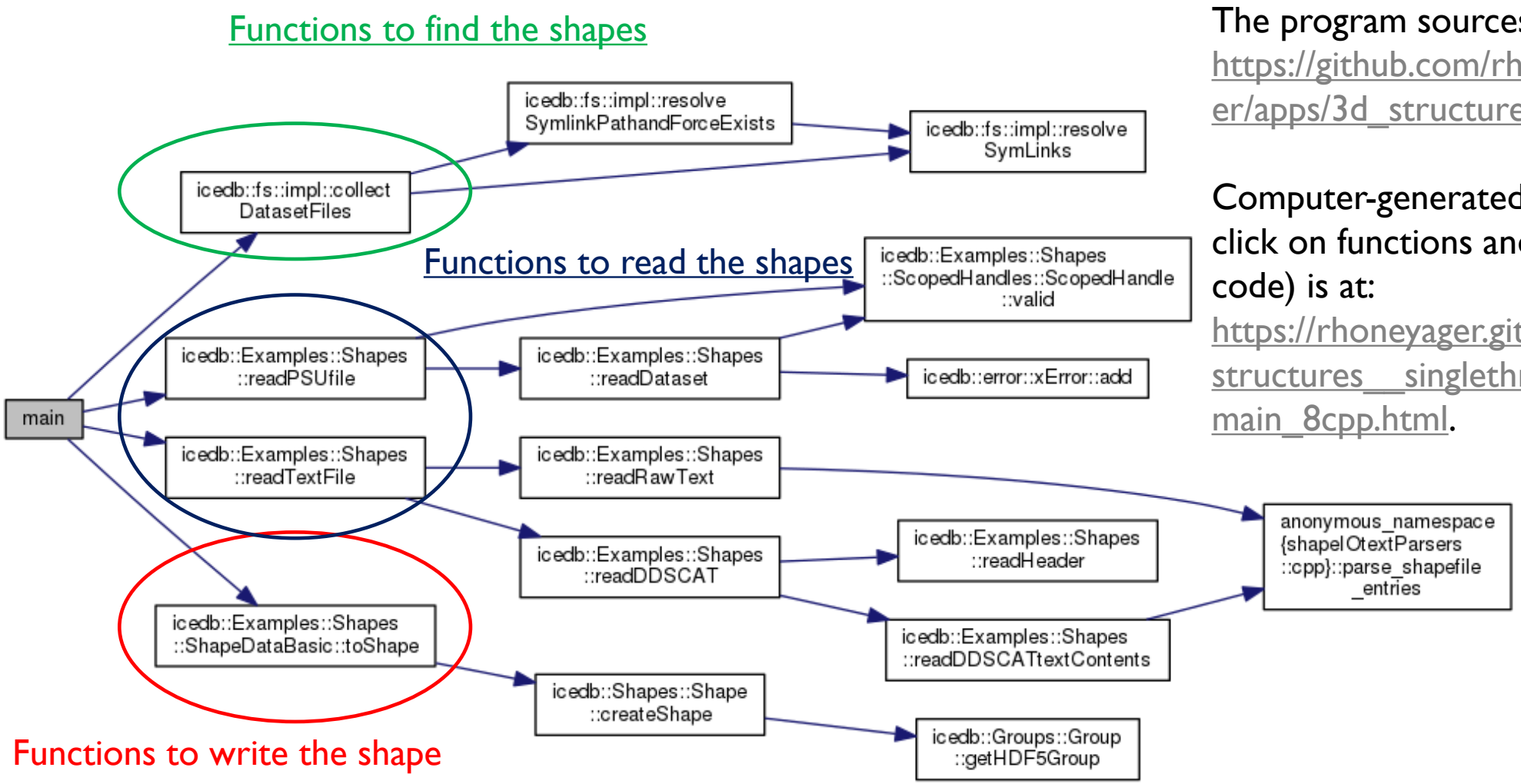
WEBSITE

- Supplements the source code site, which is still at https://www.github.com/rhoneyager/libicedb
- Will provide installation guide, links to download precompiled packages, manuals to all of the programs, description of the file structures, an API reference manual, tutorials, links to download the data.
- Lots of to-dos. Could anyone help with:
  - Adding meeting discussion notes
  - Adding discussions on how we host or share data? Links to papers describing databases, and download links.
  - Tutorials – building, running programs
  - Description of scattering theory, and need to document our conventions
  - Documented example programs, descriptions of algorithms that we want to implement (e.g. Jussi's example last year)

SHAPE CONVERSIONS

- Reference program to import 3d structures: 3d_structures_singlethreaded.
  1. It reads in user options. Which paths to be searched, how are the shapes formatted, what is their resolution, and where should the data be written?
  2. It finds the shapes to be read.
  3. It goes through a loop, reading the files.
  4. In the inner loop, each file's data is immediately converted to the new format and written.
- Initial example could import ADDA and DDSCAT shapes. Now can also import Penn State's aggregates.
- **Try it!**

SHAPE CONVERSIONS: THE IMPLEMENTATION DETAILS

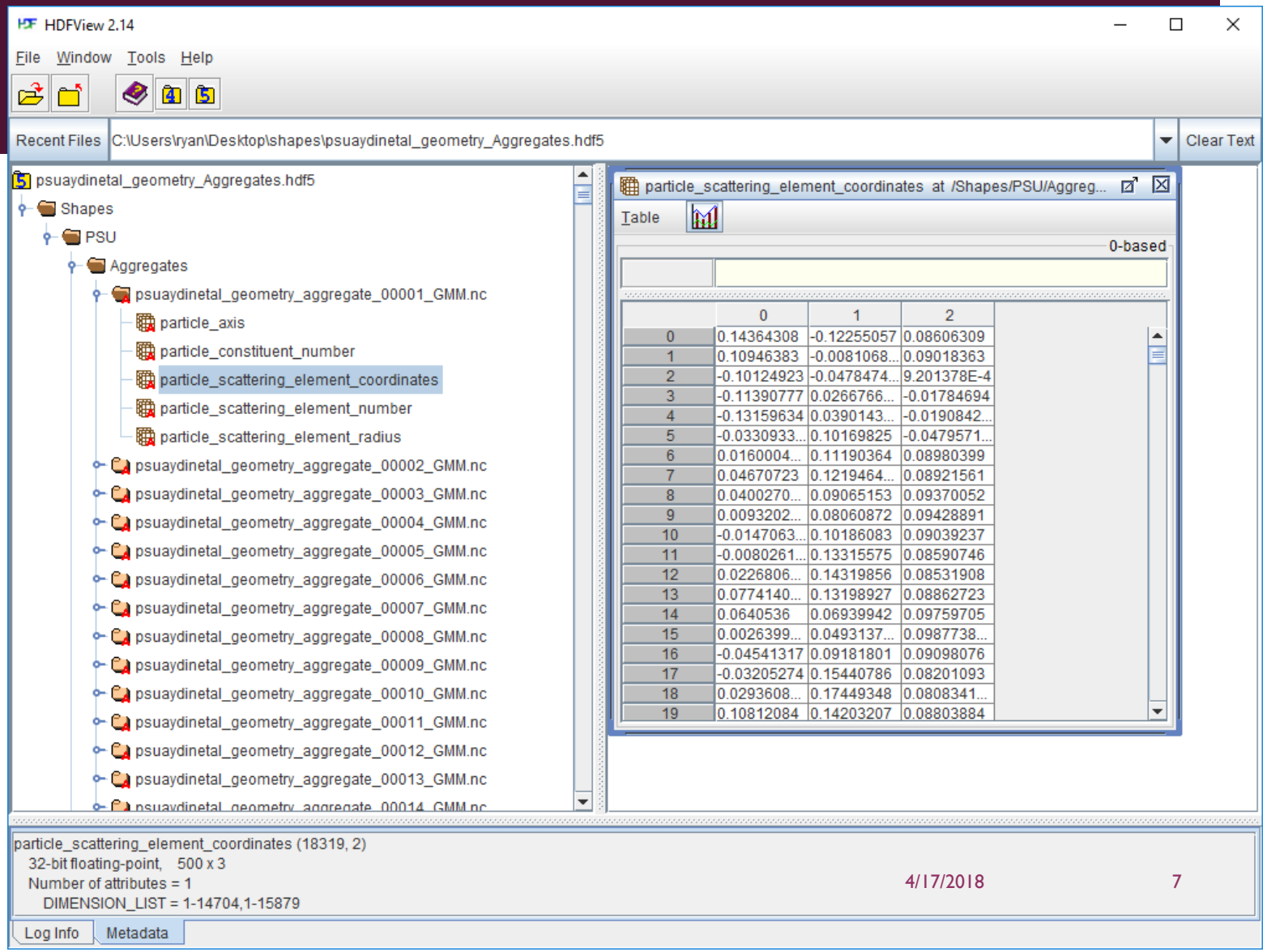


The program sources are at: https://github.com/rhoneyager/libicedb/blob/master/apps/3d_structures_singlethreaded/

Computer-generated documentation (you can click on functions and variables to explore the code) is at: https://rhoneyager.github.io/libicedb/api/cur/3d__structures__singlethreaded_2shapes-main_8cpp.html.

FUTURE STEP: STORING SCATTERING MATRICES

- For the next month, let's look at the shape conversion examples.
  - Do we like the structure?
  - Do we like the API for adding shapes?
- For the future: could anyone provide code examples to read scattering data?
  - I have code for DDSCAT, and need everything else.
  - Can everyone easily convert to the standard conventions (https://rhoneyager.github.io/libicedb/structs_exv.html)?
- Storage code for scattering matrices will be written pending low-level changes to how I handle HDF5 and netCDF files.

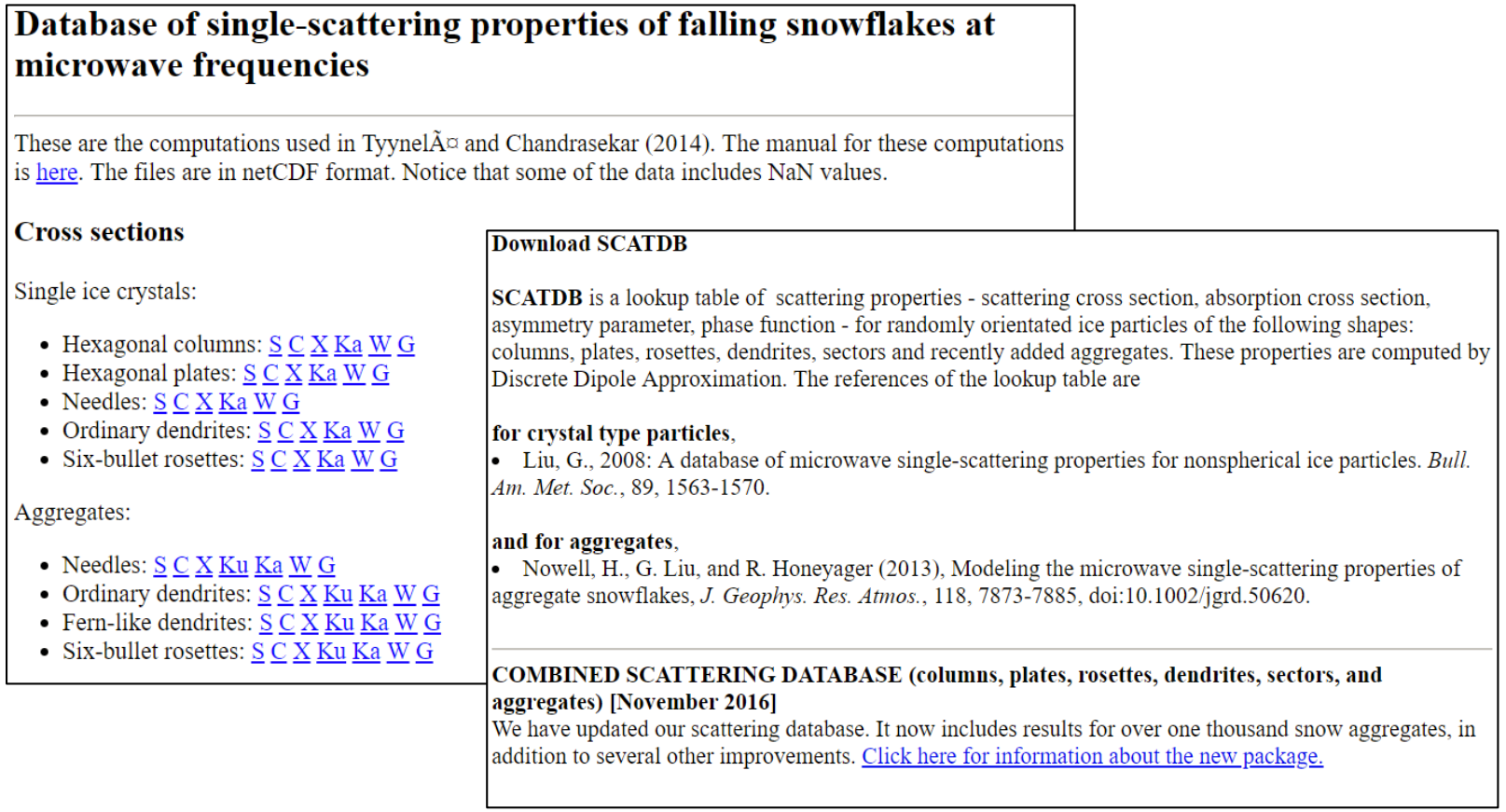


DATA DISTRIBUTION OPTION 1

- We can now compare results! But, how do we get the data?

Option 1:

- Individual websites
- Write a script to help users download data, or have them download from each hosting site.



Database of single-scattering properties of falling snowflakes at microwave frequencies

These are the computations used in TyynelÃ¤ and Chandrasekar (2014). The manual for these computations is here. The files are in netCDF format. Notice that some of the data includes NaN values.

Cross sections

Single ice crystals:

- Hexagonal columns: S C X Ka W G
- Hexagonal plates: S C X Ka W G
- Needles: S C X Ka W G
- Ordinary dendrites: S C X Ka W G
- Six-bullet rosettes: S C X Ka W G

Aggregates:

- Needles: S C X Ku Ka W G
- Ordinary dendrites: S C X Ku Ka W G
- Fern-like dendrites: S C X Ku Ka W G
- Six-bullet rosettes: S C X Ku Ka W G

Download SCATDB

SCATDB is a lookup table of scattering properties - scattering cross section, absorption cross section, asymmetry parameter, phase function - for randomly orientated ice particles of the following shapes: columns, plates, rosettes, dendrites, sectors and recently added aggregates. These properties are computed by Discrete Dipole Approximation. The references of the lookup table are

for crystal type particles,

- Liu, G., 2008: A database of microwave single-scattering properties for nonspherical ice particles. *Bull. Am. Met. Soc.*, 89, 1563-1570.

and for aggregates,

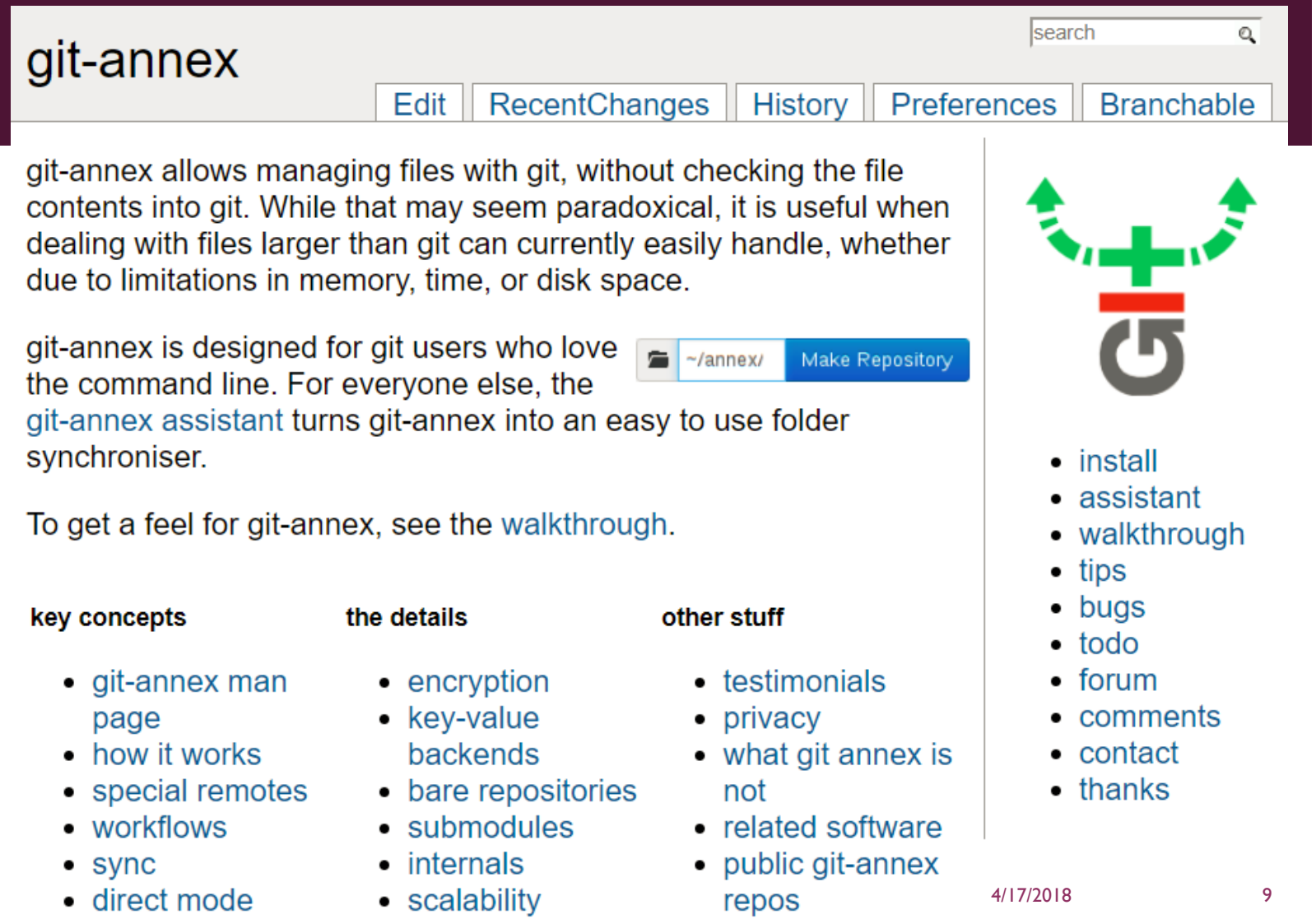
- Nowell, H., G. Liu, and R. Honeyager (2013), Modeling the microwave single-scattering properties of aggregate snowflakes, *J. Geophys. Res. Atmos.*, 118, 7873-7885, doi:10.1002/jgrd.50620.

COMBINED SCATTERING DATABASE (columns, plates, rosettes, dendrites, sectors, and aggregates) [November 2016]

We have updated our scattering database. It now includes results for over one thousand snow aggregates, in addition to several other improvements. Click here for information about the new package.

DATA DISTRIBUTION OPTION 2

- Use git. Git-LFS won't work. Not enough space. How about git-annex?
- https://git-annex.branchable.com/
- Can use regular websites, BitTorrent, rsync, Amazon S3, Box, Google Drive, Dropbox, OwnCloud, et cetera as backends to host data.
- Data can be spread across backends. Data can be replicated.
- Instead of end users having to go to each site to download data, they could just do:
  - git clone https://github.com/rhoneyager/libicedb.git
  - git annex get data/FSU data/PSU …
- Icedb's database routines are flexible enough to ignore unloaded data.



SUPPORT PROGRAMS

- These demonstrate the feasibility of using icedb as a toolbox for research
- icedb-units does unit conversions. It provides an example of how to use the library's unit conversion functions.
- icedb-refract's API allows us to "guess" at the temperature used in simulations, particularly during data import.
- Future work: icedb-onesphere and icedb-oneellip will add support for calculations of scattering by spheres and regular ellipsoids, using Rayleigh, Mie, Rayleigh-Gans and T-matrix theories.
  - Support for comparisons with database results.
  - They allow us to prototype and test new features, such as averaging over different distributions of particle orientation.
  - Later on, I can add another program to do Rayleigh-Gans (and SSRGA) modeling of more complex snowflakes.

SUPPORT PROGRAM AND API: ICEDB-UNITS UNIT CONVERSIONS

.\icedb-units.exe -h

Allowed options:

Command-line options:
```
  -h [ --help ]              produce help message
  -i [ --input ] arg         Input quantity
  -u [ --input-units ] arg   Input units
  -o [ --output-units ] arg  Output units
  --spec                     Perform spectral interconversion.
```

.\icedb-units.exe
Specify input number (without units): 94
Specify input units (terminate with 'enter'): GHz
Specify output units (terminate with 'enter'): mm
Is this an in-vacuo spectral unit conversion (i.e. GHz to mm) [yes]? yes
3.18928

.\icedb-units.exe -i 35 -u GHz -o Hz
3.5e+10

SUPPORT PROGRAM AND API: ICEDB-REFRACT REFRACTIVE INDEX CALCULATIONS

.\icedb-refract.exe

```
Command-line options:
  -h [ --help ]            produce help message
  --list-all               List all refractive index providers
  --list-subst arg         List all refractive index providers for a given
                           substance
  --list-substs            List all substances for which refractive indices can
                           be determined
  --list-provider arg      List information about a refractive index provider
                           (e.g. source paper, domain of validity)
  --subst arg              Substance of interest (ice, water)
  -f [ --freq ] arg        Frequency
  --freq-units arg (=GHz)  Frequency units
  -T [ --temp ] arg        Temperature
  --temp-units arg (=K)    Temperature units
```

.\icedb-refract.exe --list-substs

```
Substances:
        Dust
        NaCl
        Sand_E
        Sand_O
        SeaSalt
        ice
        water
```

SUPPORT PROGRAM AND API: ICEDB-REFRACT REFRACTIVE INDEX CALCULATIONS

```
.\icedb-refract.exe --list-subst ice
Providers enumerated: 3
Provider:       mIceMatzler
        Substance:      ice
        Source: Thermal Microwave Radiation: Applications for Remote Sensing,
Chapter 5, Microwave dielectric properties of ice, By Christian Matzler(2006)
        Notes:
        Requirements:
                Parameter:      spec            Range:  0 to 1000 GHz
                Parameter:      temp            Range:  0 to 273.15 K
Provider:       mIceWarren
        Substance:      ice
        Source: Stephen G. Warren, "Optical constants of ice from the ultraviolet
to the microwave, " Appl. Opt. 23, 1206-1225 (1984)
        Notes:
        Requirements:
                Parameter:      spec            Range:  0.167 to 8600 GHz
                Parameter:      temp            Range:  -60 to -1 degC
Provider:       mIceHanel
        Substance:      ice
        Source: Tables from Thomas Hanel. Not sure which paper.
        Notes:
        Requirements:
                Parameter:      spec            Range:  0.2 to 30000 um
```

```
.\icedb-refract.exe -f 183 --freq-units GHz -T 263 --temp-units K --subst
ice
(1.78306,-0.00385545)   was found using provider mIceMatzler.
(1.7837,-0.00012)       was found using provider mIceWarren.
(1.782,-0.00465122)     was found using provider mIceHanel.
```

```
.\icedb-refract.exe --subst water -f 35.6 -T 276
(4.21521,-2.49764)      was found using provider
mWaterFreshMeissnerWentz.
(4.53497,-2.58475)      was found using provider mWaterHanel.
```

MAY MEETING SCHEDULING

- Do we want to go back to meeting on Wednesdays? Has the university Spring schedule ended?