A Class to Manage Large Ensembles and Batch Execution in Python

PyCon Canada

Andre R. Erler

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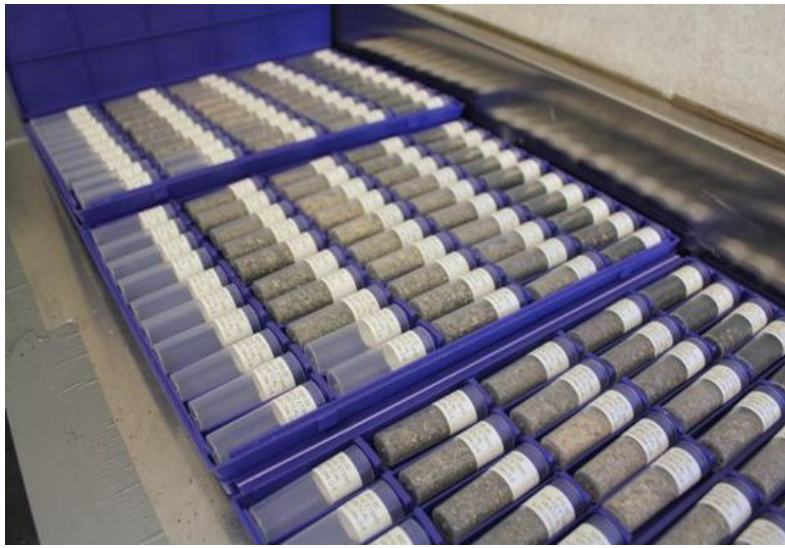
Outline

Science is Repetitive

To reach conclusive results, scientific experiments usually have to be repeated many times; either to establish statistical significance, or to test a range of parameter values for optimization.



Experiments are planned and conducted in large batches or so-called *ensembles*.

Automation

It is therefore desirable to automate the most repetitive tasks, and to create tools for this purpose.

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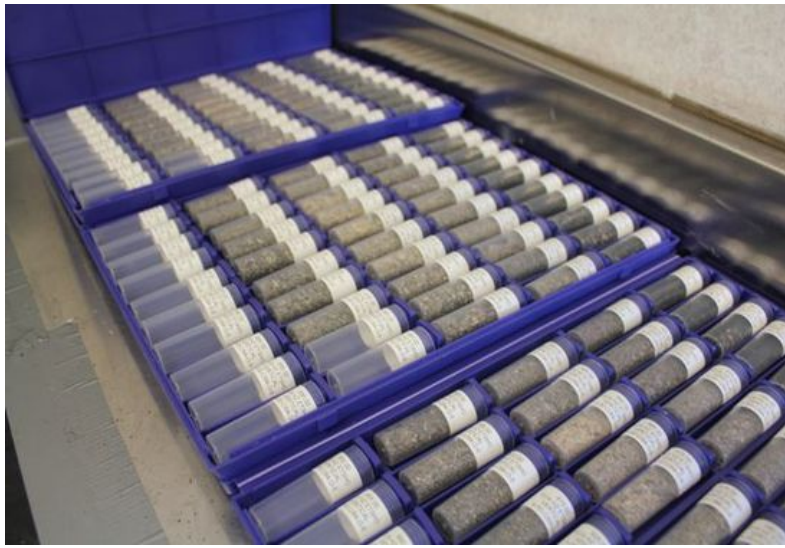

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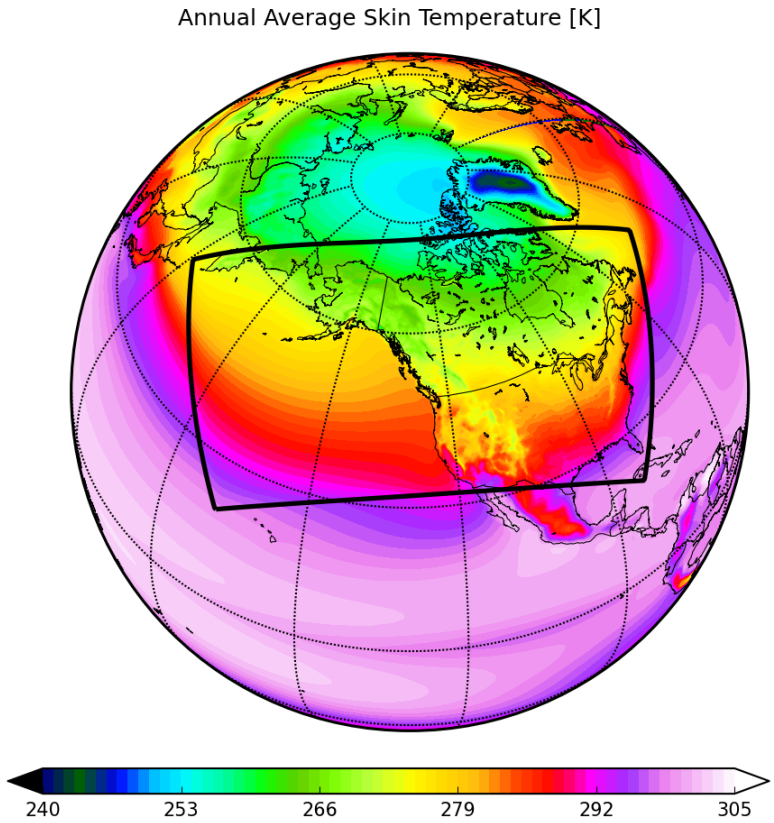
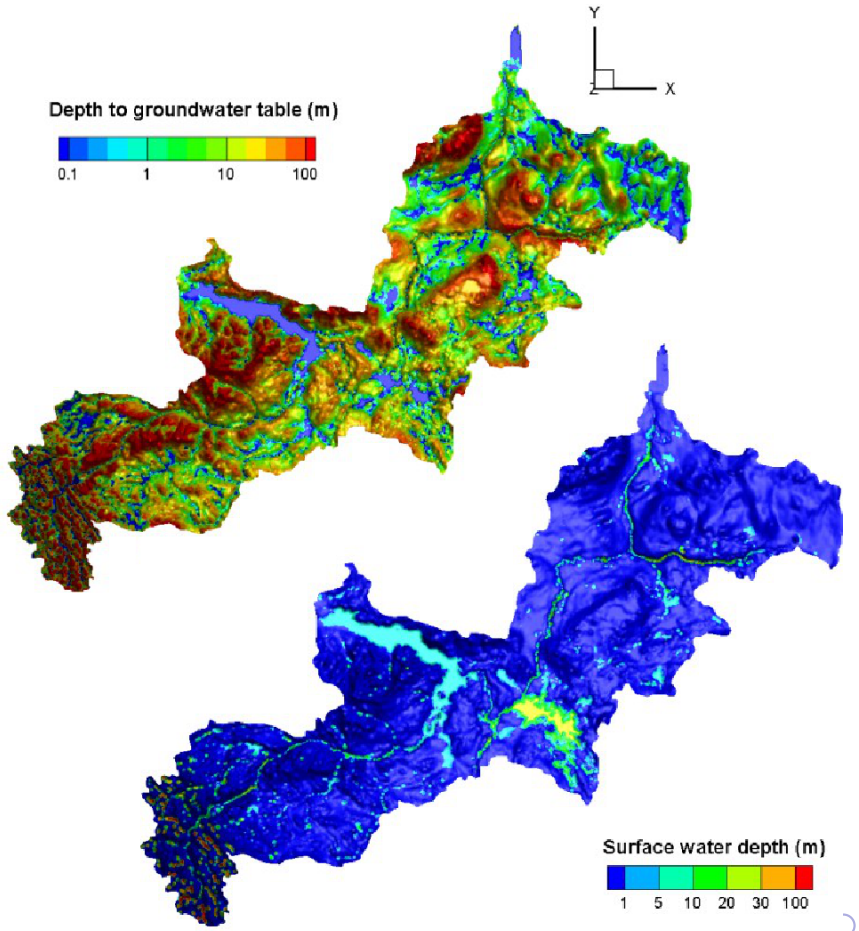


Surface Temperature in a Global and a nested Regional Climate Model

I run Climate and Hydrologic Models to study the impact of climate change on water resources and generate projections of future hydro-climate.

Coupling Climate Models with Hydrologic Models

Athabasca River watershed: groundwater depth (top) and surface water depth (bottom)



High Performance Computing

- High-resolution Climate simulations:
  - 4 days on 128 cores and 300GB of storage per model year
  - 36 ensemble members, 15 years each
- Surface-Subsurface Hydrologic Simulations:
  - 1 day on 2 cores per model year
  - also 15 years each, 100+ ensemble members

Motivation: Batch Processing

- In Computational Sciences repetitive tasks can be automated/scripted

Boilerplate Code

Python simplifies scripting a lot, but we still have a lot of boilerplate code! This can be simplified further.

Python is an Ideal Scripting Language

```
ensemble = [...] # a list of objects ''members''

# for loop iterating over list
tmp = [] # store results
for member in ensemble: # iterate over list
    tmp.append( result = member.operation(*args, **kwargs) )
ensemble = tmp

# list comprehension is already much shorter!
ensemble = [m.operation(*args, **kwargs) for m in ensemble]
```

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The Ensemble Class

- Emulate Container Type
- Redirect method calls to ensemble members

And Ideal Use-case Example

```
ensemble = Ensemble(*[...]) # create Ensemble object

# apply member methods to entire ensemble
ensemble = ensemble.operation_1(*args, **kwargs)
...
ensemble = ensemble.operation_N(*args, **kwargs)

member_N = ensemble[n] # access elements by index
member_key = ensemble[key] # .. or by name/key
...
```

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Implementation Snippet

```
class Ensemble(object):
  _members = None # members
  ...

  def __getitem__(self, i):
    # get individual members
    if isinstance(i, int):
      # access like list/tuple
      return self._members[i]
    elif isinstance(i, string):
      ...

  def __iter__(self):
    # iterate over members
    mm = self._members
    return mm.__iter__()
  ...
```

The Ensemble Class

Emulating the Python **Container Type**:

1. Support several built-in methods, such as `__len__`, `__contains__`, `__iter__`
2. Item assignment like `list` or `dict` using `__getitem__` and `__setitem__`

Return Values

Calls to member methods return a new container or Ensemble with the results

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Implementation of

Method Redirection:

1. Redirect calls to member methods/attributes by overloading `__getattr__`
2. Execute call on all Ensemble members
3. Return a new container or Ensemble with results

Ensemble Wrapper

Methods require helper Class `EnsWrap` to apply arguments

Implementation Snippet

```
class Ensemble(object):
  _members = None # members
  ...

  def __getattr__(self, attr):
    # check if callable
    mem0 = self._members[0]
    # assuming homogeneity...
    f = getattr(mem0,attr)
    if callable(f):
      # return Ensemble Wrapper
      v = EnsWrap(self,attr)
    else:
      # just return values
      v = [getattr(m,attr) \
          for m in self._members]
    return v
```

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```

Implementation Snippet

```
class EnsWrap(object):
  ...

  def __init__(self, ens, attr):
    _ensemble = ens # members
    _attr = attr # member method

  def __call__(self, **kwargs):
    # iterate over members
    new = Ensemble()
    for m in self._ensemble:
      f = getattr(m,self.attr)
      # execute member method
      new.append(f(**kwargs))
    # return new ensemble
    return new
  ...
```

A Helper Class

Implementation of the **Ensemble Wrapper**:

1. Initialize with ensemble members and the called attribute/method
2. Use `__call__` method to execute member method with arguments

Parallelization

Simple parallelization using `multiprocessing.Pool`'s `apply_async` can be applied

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How can we use Ensembles with Argument Lists

A Trivial Case

```
# this defeats the purpose
members = [member.operation(arg1=arg) for arg in arg_list]
Ensemble(*members) # initialize new ensemble

# a better solution: pass list directly
ensemble.operation(arg1=arg_list, inner_list=['arg1'])
```

Argument lists can easily be implemented in the __call__ method of the ensemble wrapper EnsWrap by creating a list of arguments for each member

```
# construct argument list
args_list = expandArgList(**kwargs)
# loop over lists
ens = self._ensemble
for m,args in zip(ens,args_list):
  f = getattr(m,self.attr)
  # execute member method with args
  new.append(f(**args))
```

How can we use Ensembles with Argument Lists

A More Complex Case: the Outer Product List

```
# again, this defeats the purpose
arg_list = []
for arg1 in arg_list1: # construct arg_list from two lists
  for arg2 in arg_list2: # i.e. all possible combinations
    arg_list.append(dict(arg1=arg1, arg2=arg2))
# apply list to ensemble
ensemble.operation(arg1=arg_list, inner_list=['arg1'])

# a better solution is to expand the lists internally
ensemble.operation(arg1=arg_list1, arg2=arg_list2,
                   outer_list=['arg1','arg2'])
```

The **Outer Product** expansion of multiple argument lists creates argument lists with all possible combinations of arguments. **Inner Product** expansion works like Python's `zip` function.

Argument Expansion via Outer Product

Recursive Implementation of **Outer Product**:

1. Separate expansion arguments from others
2. Recursively expand argument list
3. Generate argument set for each ensemble member

Decorator Class

Argument Expansion is most useful as a Decorator class

Implementation of Recursion

```
def expandArgsList(args_list,
                   exp_args, kwargs):
  # check recursion condition
  if len(exp_args) > 0:
    # expand arguments
    now_arg = exp_args.pop(0)
    new_list = [] # new arg list
    for narg in kwargs[now_arg]:
      for arg_list in args_list:
        arg_list.append(narg)
        new_list.append(arg_list)
    # next recursion level
    args_list = expandArgsList(
      new_list, exp_args, kwargs)
  ...
  # terminate: return arg lists
  return args_list
```

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Summary & Conclusion

The Ensemble Class

- Functions like a **container type** and redirects calls to (parallelized) **member methods**

Argument Expansion

- Systematic expansion of argument lists from **inner** or **outer product** (with decorator)

Sprint Project: Publish Ensemble Class

Create a stand-alone module with the Ensemble class and the argument expansion code for others to use, and add support for array-like item access/assignment

Thank You! ~ Questions?