Productivity-oriented software design for geoscientific modelling

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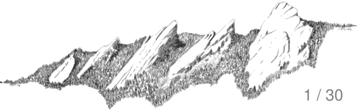

1. Introduction
2. Case study: **libmpdata++** & **libcloudph++** developed at the University of Warsaw
3. Future plans: (my upcoming 2-year **postdoc @NCAR)**

talk outline

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personal background

MSc theoretical elementary particle physics

PhD computational (F77) atmospheric physics

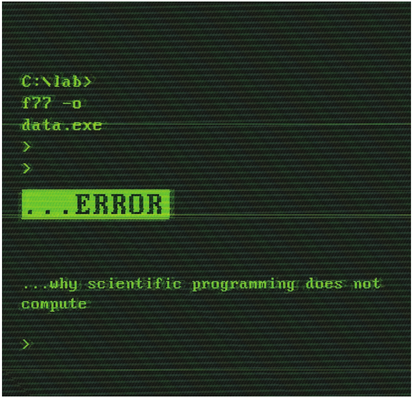
lessons learnt:

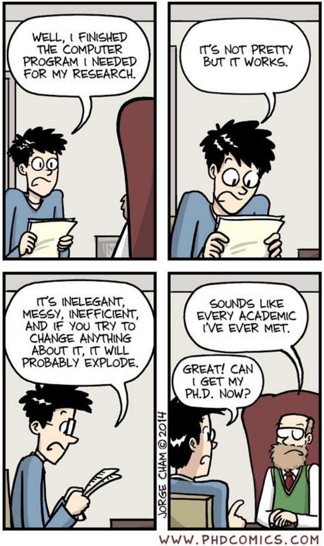
- prefer Python/NumPy to F77
- my research productivity can be improved!

  $\rightsquigarrow$ software design does matter!

lesson learnt - common perspective

Merali 2010 (Nature 467)





software design and researchers' productivity

users' perspective

- ease of use
- robustness
- result reproducibility

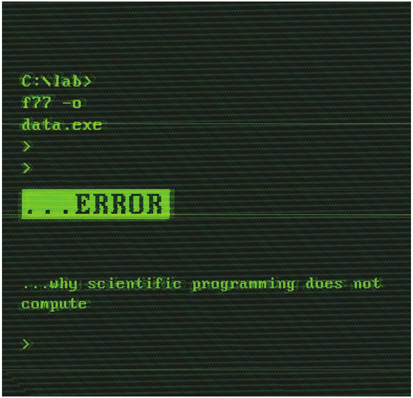
developers' perspective

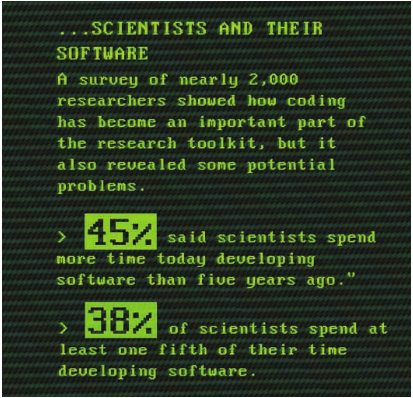
- extendability
- maintainability

researcher = user & developer

researcher = user & developer

Merali 2010 (Nature 467)





this talk: lessons learnt in a joint U. Warsaw/NCAR project

NCAR
NATIONAL CENTER FOR ATMOSPHERIC RESEARCH

UNIVERSITAS VARSOVIENSIS

funding (2011–2012 & 2013–2016)

NATIONAL SCIENCE CENTRE POLAND

the aim

develop a productivity-oriented open-source software suite for aerosol/cloud-microphysics research

the team

U. Warsaw: H. Pawłowska, S. Arabas, A. Jaruga, M. Waruszewski
NCAR: W. Grabowski & D. Jarecka
ECMWF: P. Smolarkiewicz (previously @NCAR)

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libmpdata++ & libcloudph++

libmpdata++ parallel solvers for systems of transport equations

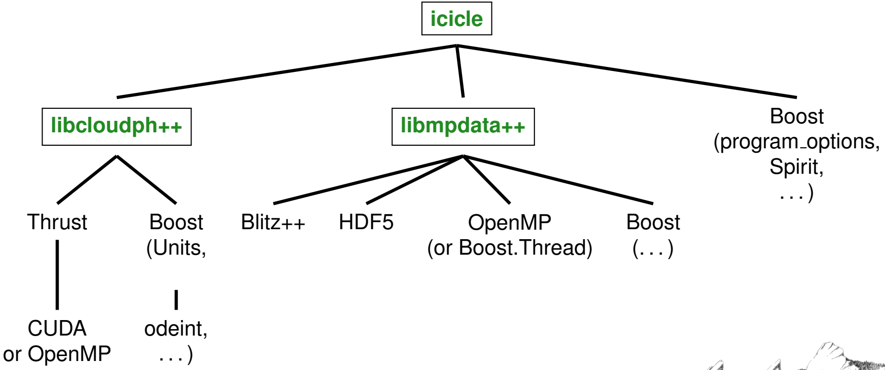
- http://libmpdataxx.igf.fuw.edu.pl/

libcloudph++ aerosol/cloud-microphysics algorithm collection

- http://libcloudphxx.igf.fuw.edu.pl/

a few words on first design choices

- structure the code into “standalone” libraries
  - ⇝ easier to document, to test and to contribute to
  - ⇝ easier to use in various contexts
- leverage existing **reusable** software
  - ⇝ save time, better test coverage



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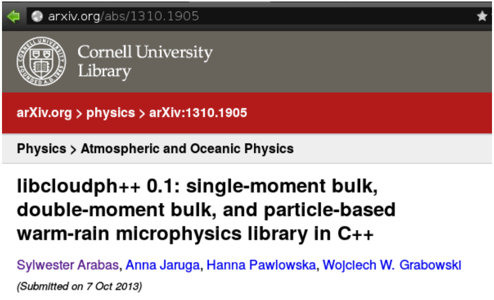
ease of use (and misuse) - model users' perspective

- understandable output
  $\rightsquigarrow$ docs, open data format
- easy way of providing input and "setup"
  (setups are much more than "parameters"!)
  $\rightsquigarrow$ docs, setup/solver separation!
  - setup implementation ***out of tree***
    (structuring into libraries helps!)
  - as few constraints as possible
    (e.g. dimensionality, data types $\rightsquigarrow$ C++ templates)
  - library API: flexible and documented

example: libcloudph++ docs @ arXiv

complete API docs on arXiv


arxiv.org/abs/1310.1905

Cornell University Library

arXiv.org > physics > arXiv:1310.1905

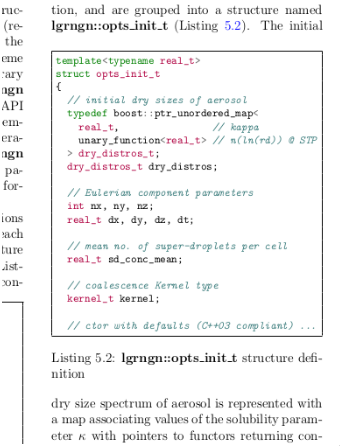
Physics > Atmospheric and Oceanic Physics

libcloudph++ 0.1: single-moment bulk, double-moment bulk, and particle-based warm-rain microphysics library in C++

Sylwester Arabas, Anna Jaruga, Hanna Pawlowska, Wojciech W. Grabowski

(Submitted on 7 Oct 2013)

code part of the paper!


tion, and are grouped into a structure named **lgrngn::opts_init_t** (Listing 5.2). The initial

```
template<typename real_t>
struct opts_init_t
{
  // initial dry sizes of aerosol
  typedef boost::ptr_unordered_map<
    real_t,                 // kappa
    unary_function<real_t> // n(ln(rd)) @ STP
  > dry_distros_t;
  dry_distros_t dry_distros;

  // Eulerian component parameters
  int nx, ny, nz;
  real_t dx, dy, dz, dt;

  // mean no. of super-droplets per cell
  real_t sd_conc_mean;

  // coalescence Kernel type
  kernel_t kernel;

  // ctor with defaults (C++03 compliant) ...
```

Listing 5.2: **lgrngn::opts_init_t** structure definition

dry size spectrum of aerosol is represented with a map associating values of the solubility parameter κ with pointers to functors returning con-

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robustness - model users' perspective

- detect and report out-of-range model parameters, e.g.
  - warm-rain microphysics below a freezing point
  - numerical stability criteria,
  - ill-posed initial conditions.

$\rightsquigarrow$ numerous asserts in ibmpdata++ & libcloudph++

(can be off for production runs - CMake's Release/Debug modes)

- sane error handling:
  - let the user choose what to ignore (do not ignore errors by default!),
  - propagate system/library errors (e.g. i/o, numerics),

$\rightsquigarrow$ take advantage of C++/Python exceptions

- mention all above in the docs...

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result reproducibility
- model users'/reviewers' perspective

Geosci. Model Dev. policy (doi: 10.5194/gmd-6-1233-2013)

- *...*
- *"paper must be accompanied by the code, or means of accessing the code, for the purpose of peer-review"*
- *"we strongly encourage referees to compile the code, and run test cases supplied by the authors"*
- *...*

result reproducibility - model users'/reviewers' perspective

- access to software and correct version of the code
  ⇝ free/libre & open code and version history

- avoid vendor-specific hardware requirements
  ⇝ e.g., use GPU/CUDA but offer a fallback option

libcloudph++

compile-time CUDA / OpenMP choice

99% common code ⇝ implemented using **Thrust**

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extendability - model developers' perspective

- language with a market of trained personnel
  (Python, C++, . . .)
- separation of concerns
  (cloud physicist does cloud physics, etc.)
  ⇝ structuring into libraries helps again!
- human-readable code
  (code vs. paper – they both describe the same algorithm)
  ⇝ dimensional analysis

Boost.units
zero-overhead dimensional analysis at compile time

```cpp
// Reynolds number for a particles falling with terminal velocity
// see e.g. section 4 in Smolik et al 2001, Aerosol Sci.
template <typename real_t>
BOOST_GPU_ENABLED
quantity<si::dimensionless, real_t> Re(
  const quantity<si::velocity, real_t> v_term,       // particle terminal velocity
  const quantity<si::length, real_t> r_w,            // particle wet radius
  const quantity<si::mass_density, real_t> rho,      // air density
  const quantity<si::dynamic_viscosity, real_t>  eta // air viscosity
)
{
  return v_term * (2 * r_w) * rho / eta;
}
```

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  (Python, C++, . . .)

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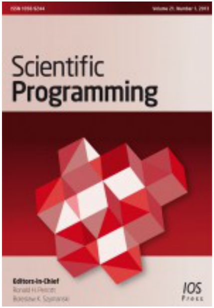
- human-readable code
  (code vs. paper – they both describe the same algorithm)
  $\rightsquigarrow$ dimensional analysis
  $\rightsquigarrow$ "blackboard abstractions"

OOP formula translation: C++, Fortran or Python?

Arabas, Jarecka et al. 2014



Formula translation in Blitz++, NumPy and modern Fortran: A case study of the language choice tradeoffs

Sylwester Arabas[1], Dorota Jarecka[1], Anna Jaruga[1], Maciej Fijałkowski[2]

[1]Institute of Geophysics, Faculty of Physics, University of Warsaw
[2]PyPy Team

Journal	Scientific Programming
DOI	10.3233/SPR-140379
Online Date	Monday, March 24, 2014

OOP formula translation: C++, Fortran or Python?

Arabas, Jarecka et al. 2014

$$\psi_i^{n+1} = \psi_i^n - \left(F\left[\psi_i^n, \psi_{i+1}^n, C_{i+1/2}\right] - F\left[\psi_{i-1}^n, \psi_i^n, C_{i-1/2}\right]\right)$$

$$F(\psi_L, \psi_R, C) = \frac{C + |C|}{2} \cdot \psi_L + \frac{C - |C|}{2} \cdot \psi_R$$

```python
def adv_op(psi, C, i):
    return (
        f(psi[i    ], psi[i+one], C[i+hlf]) -
        f(psi[i-one], psi[i    ], C[i-hlf])
        )

def scalar_advection(psi, n, C, i):
    psi[n+1][i] = psi[n][i] - adv_op(psi[n], C, i)


def f(psi_l, psi_r, C):
    return (C + abs(C))/2 * psi_l + (C - abs(C))/2 * psi_r
```

human-readable array expressions!

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maintainability - model developers' perspective

good test coverage

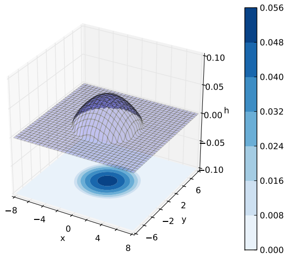
separations of concerns requires testing!

⇝ structuring into libraries helps again!

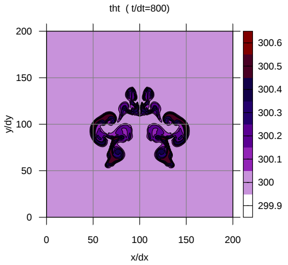
example: libmpdata++ tests

Jaruga et al. 2014 (in preparation)

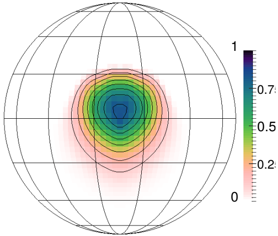
shallow-water system (vs. analytical)



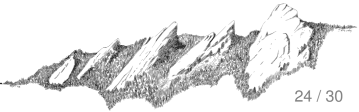
dry convection with interfacial instability



over-the-pole advection in spherical coord.



- unmodified code, out-of-tree setups
- but these are not unit tests...



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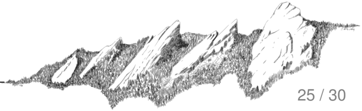

my upcoming 2-year postdoc @NCAR

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UNIVERSITAS VARSOVIENSIS

funding (2014–2016)

Ministry of Science and Higher Education
Republic of Poland

the aim

- development of a new parameterization of processes related to droplet growth and rain formation in numerical cloud models
- development of a testing protocol for microphysical schemes

collaboration with

U. Warsaw: H. Pawłowska, S. Arabas, A. Jaruga, M. Waruszewski
NCAR: W. Grabowski (MMM), D. Del Vento (CISL)

project's approach

- reuse reliable existing code whenever possible

- code in Python/NumPy whenever possible

  $\leadsto$ libmpdata++ and libcloudph++ do allow it!

project's methodology

- writing automated tests during code development
  ⇝ verify behaviors of schemes during the development
- using technics of object-oriented programming
  ⇝ help to maintain modularity and improve readability
- using the Python/Numpy language/library with solutions for improving the relatively poor performance
  ⇝ benefit from Python's ease of use

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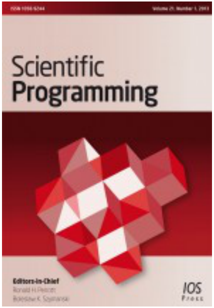
Arabas, Jarecka et al. 2014



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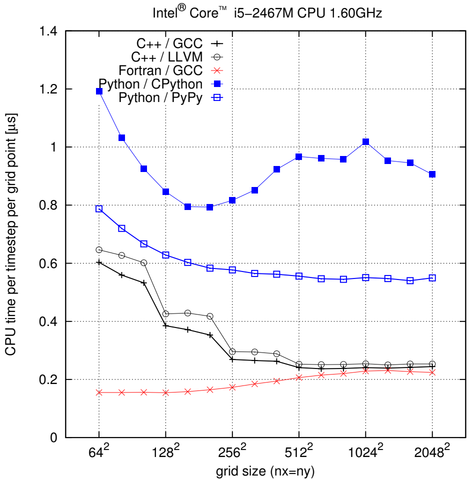
OOP formula translation: C++, Fortran or Python?

conclusions:

- Python is definitely the easiest language to use and debug among the three languages!
- PyPy performance is promising!



a take-home message

productivity-oriented design choices
$\rightsquigarrow$ investment that does pay back

further reading:

- **Arabas, Jarecka et al. 2014**:
  Formula translation in Blitz++, NumPy and modern Fortran: A case study of the language choice tradeoffs.
  Sci. Prog. (in press, doi: 10.3233/SPR-140379)
- **libcloudph++**: `http://libcloudphxx.igf.fuw.edu.pl/`
- **libmpdata++**: `http://libmpdataxx.igf.fuw.edu.pl/`

Thanks for your attention!

Suggestions are very welcome!