UFuncs and DTypes: New possibilities in NumPy

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NumPy

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Motivation

New DTypes:

- Physical units (e.g. meter)
- Modernized datetimes
- Strings with encodings
- Arbitrary precision
- …

Also:

- Cleaner NumPy DTypes
- Better ufuncs
- Bug fixes

NumPy DTypes: Example UnitDType


```
from unitdtype import UnitDType

# Array containing meters:
arr = np.zeros(
        3, dtype=UnitDType("m"))
#  ...
```

NumPy DTypes: Example UnitDType


```python
from unitdtype import UnitDType

# Array containing meters:
arr = np.zeros(
        3, dtype=UnitDType("m"))
#  ...
```

```python
class UnitDType(np.dtype):
    itemsize = 8

    def special_methods( ... ):
        pass
```

- Instance (also "descriptor" in C):
  `arr.dtype == UnitDType("m")`
- DType (class/type) defines behavior:
  `type(arr.dtype) is UnitDType`

NumPy DTypes: Example UnitDType

"Experimental" API outlined in NEP 41-43:

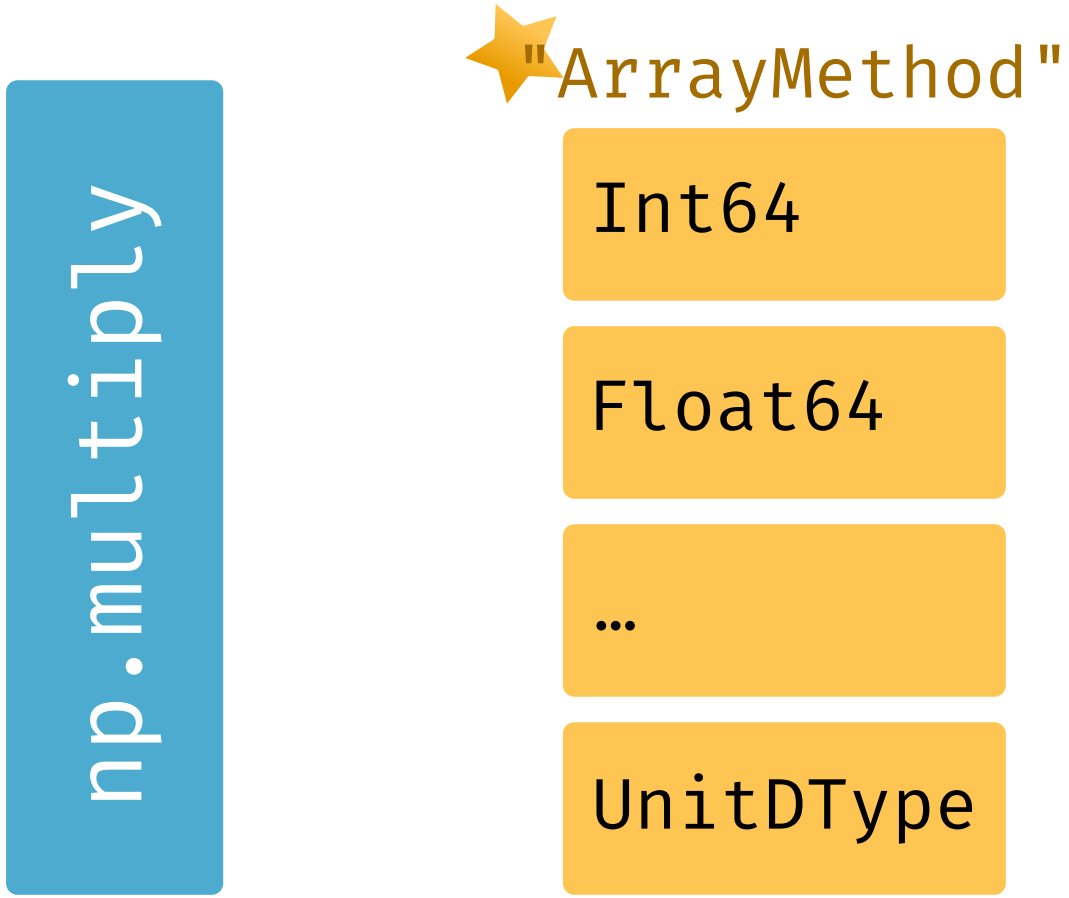
```
#include "numpy/experimental_dtype_api.h"

if (import_experimental_dtype_api(5) < 0) {
    return NULL;
}
```

- github.com/seberg/talk_unitdtype (NumPy main branch)
- github.com/seberg/unitdtype (currently own branch)

What is a UFunc?


```
arr1 = np.array([2*m])
arr2 = np.array([3*m])
res = np.multiply(arr1, arr2)
```



Whats New?

- encapsulation
- extensible

What is a UFunc?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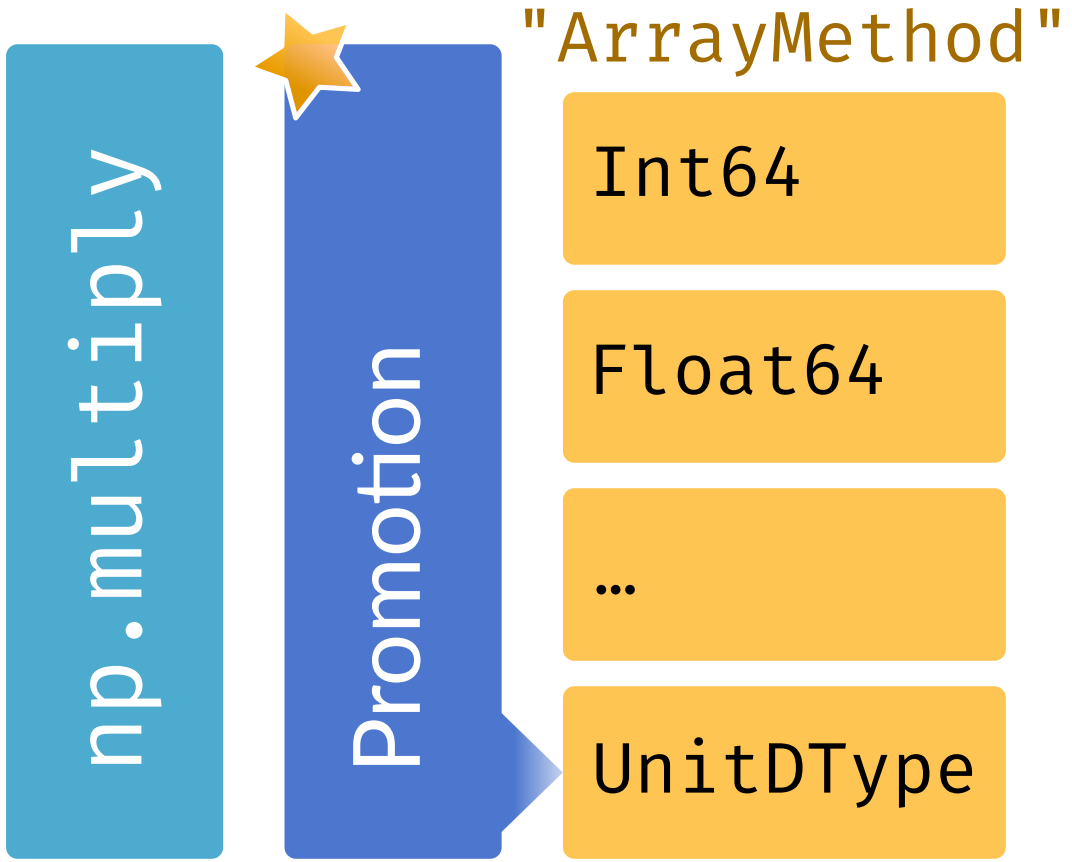
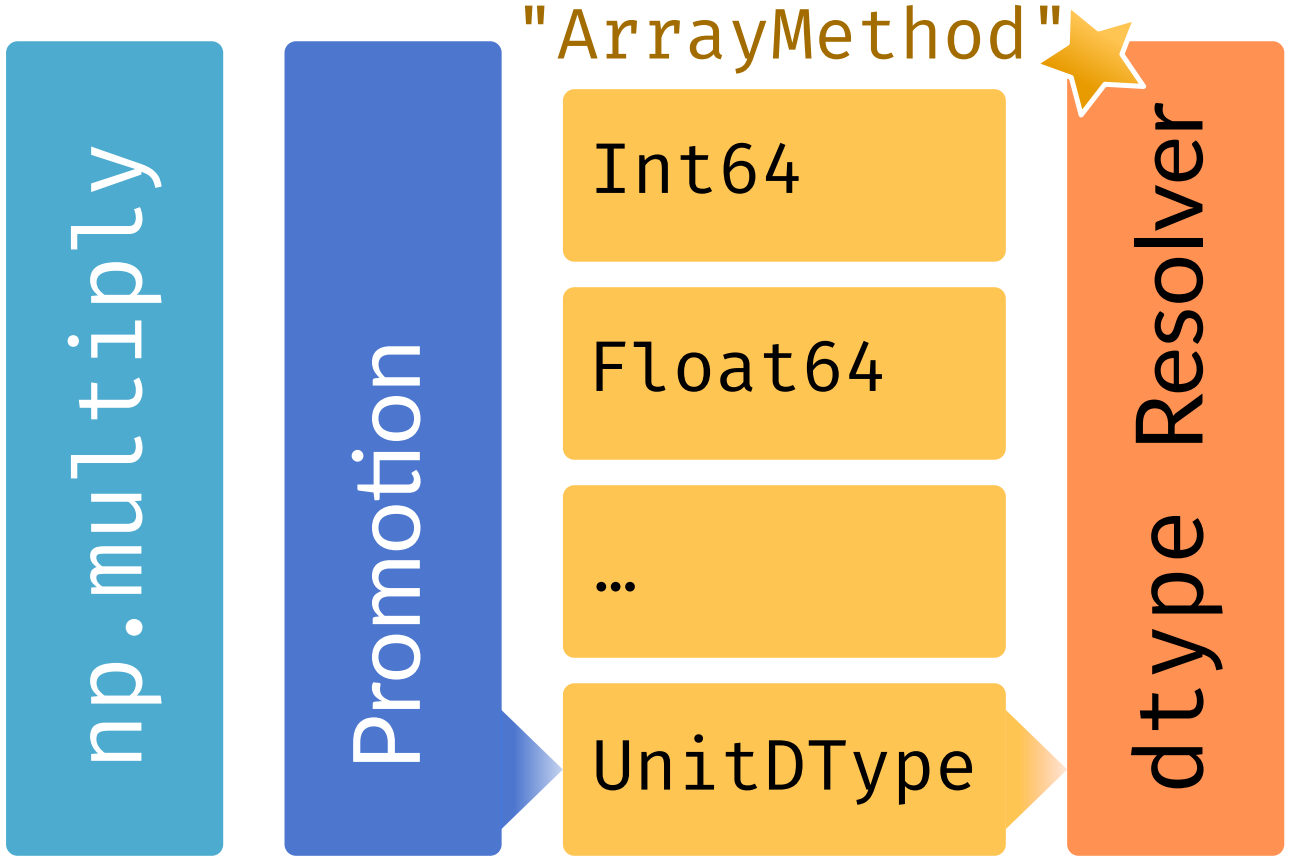


- Whats New?
  - Flexible
  - Customizable
  - useful for numba `DUfunc`

What is a UFunc?


```
arr1 = np.array([2*m])
arr2 = np.array([3*m])
res = np.multiply(arr1, arr2)
```

```
.dtype → "m"
       → "m"
       ← "m**2"
```



- Whats New?
  - on `ArrayMethod`
  - Customizable
  - …

What is a UFunc?


```
arr1 = np.array([2*m])
arr2 = np.array([3*m])
res = np.multiply(arr1, arr2)
```

```
.dtype → "m"
       → "m"
       ← "m**2"
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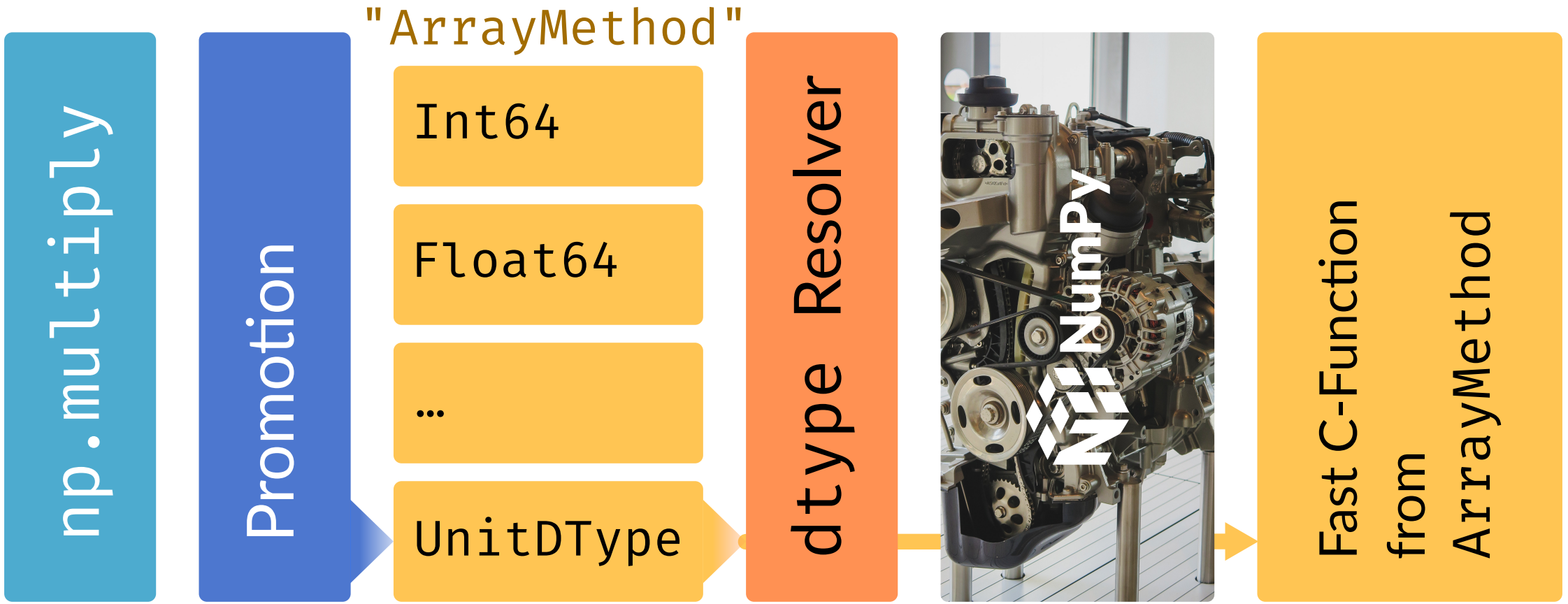
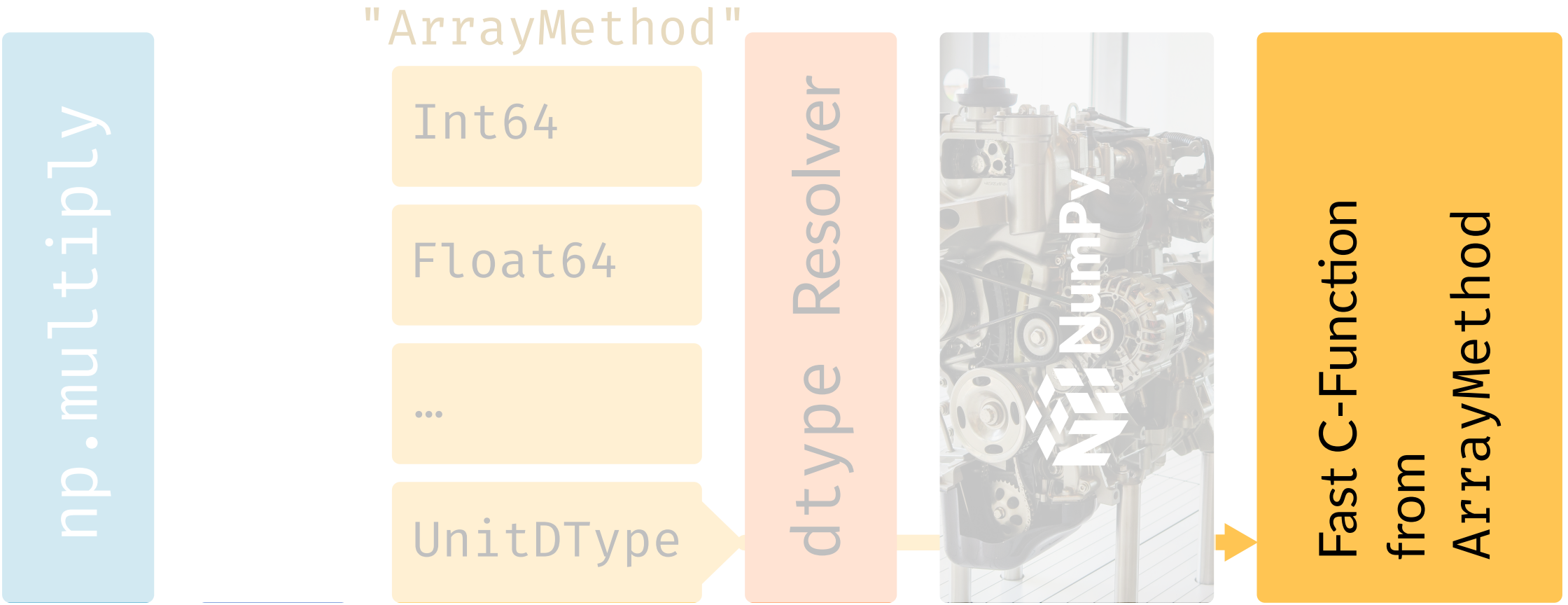


Lets make a UFunc: The "strided loop"



Lets make a UFunc: The "strided loop"


```c
static int
unit_multiply_strided_loop(PyArrayMethod_Context *context,
        char *const data[], npy_intp const dimensions[],
        npy_intp const strides[], NpyAuxData *auxdata)
{
    npy_intp N = dimensions[0];
    char *in1 = data[0], *in2 = data[1];
    char *out = data[2];
    npy_intp in1_stride = strides[0];
    npy_intp in2_stride = strides[1];
    npy_intp out_stride = strides[2];

    while (N--) {
        *(double *)out = *(double *)in1 * *(double *)in2;
        in1 += in1_stride;
        in2 += in2_stride;
        out += out_stride;
    }
    return 0;
}
```

Calculate result:

- 1-D loop
- no need for units

```
res[i] = arr1[i] * arr2[i]
```

Lets make a UFunc: The "strided loop"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        char *const data[], npy_intp const dimensions[],
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        in1 += in1_stride;
        in2 += in2_stride;
        out += out_stride;
    }
    return 0;
}
```

New "context" with info:

- caller (`np.multiply`)
- "`self`"
- dtypes/descriptors
- ... future additions

Lets make a UFunc: The "strided loop"


```c
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    while (N--) {
        *(double *)out = *(double *)in1 * *(double *)in2;
        in1 += in1_stride;
        in2 += in2_stride;
        out += out_stride;
    }
    return 0;
}
```

Array (current chunks) data:

- `arr1.data`
- `arr2.data`
- `res.data`

Lets make a UFunc: The "strided loop"


```c
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unit_multiply_strided_loop(PyArrayMethod_Context *context,
        char *const data[], npy_intp const dimensions[],
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    npy_intp in1_stride = strides[0];
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    while (N--) {
        *(double *)out = *(double *)in1 * *(double *)in2;
        in1 += in1_stride;
        in2 += in2_stride;
        out += out_stride;
    }
    return 0;
}
```

The length of the data:

```
N = dimensions[0]
for i in range(N):
    …
```

(more info for generalized UFuncs)

Lets make a UFunc: The "strided loop"


```c
static int
unit_multiply_strided_loop(PyArrayMethod_Context *context,
        char *const data[], npy_intp const dimensions[],
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{
    npy_intp N = dimensions[0];
    char *in1 = data[0], *in2 = data[1];
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    while (N--) {
        *(double *)out = *(double *)in1 * *(double *)in2;
        in1 += in1_stride;
        in2 += in2_stride;
        out += out_stride;
    }
    return 0;
}
```

The "`arr.strides[-1]`":

- how to iterate the data

Lets make a UFunc: The "strided loop"


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        in1 += in1_stride;
        in2 += in2_stride;
        out += out_stride;
    }
    return 0;
}
```

Return:

- success: `0`
- error: `-1`

Important API addition!

Lets make a UFunc: The "strided loop"


```c
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        in2 += in2_stride;
        out += out_stride;
    }
    return 0;
}
```

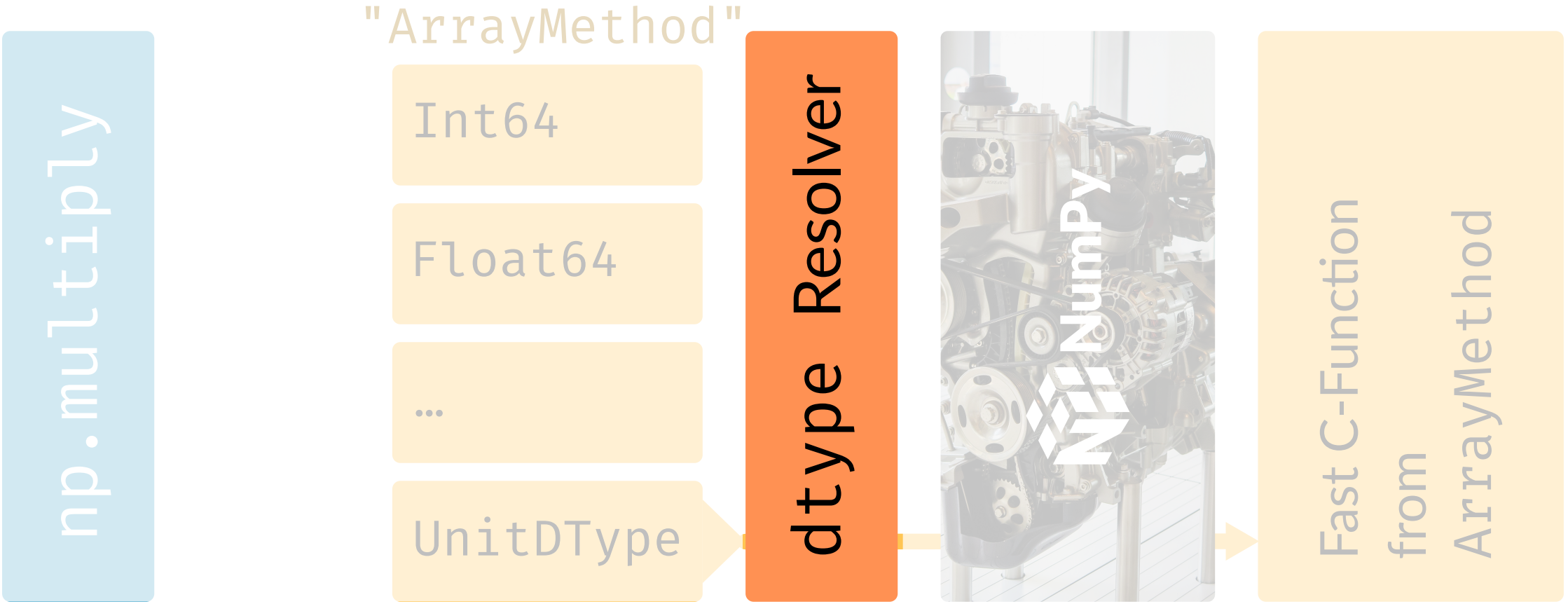
This is an Example!

Loop re-use possible!

`auxdata`:

- pass information
- scratch space

Lets make a UFunc: The "Resolver"



Lets make a UFunc: The "Resolver"


```c
static NPY_CASTING
unit_multiply_resolve_descriptors(PyObject *self,
        PyArray_DTypeMeta *dtypes[], PyArray_Descr *given_descrs[],
        PyArray_Descr *loop_descrs[], npy_intp *unused)
{
    /* Fetch the unyt based units: */
    PyObject *unit1 = ((UnitDTypeObject *)given_descrs[0])->unit;
    PyObject *unit2 = ((UnitDTypeObject *)given_descrs[1])->unit;
    /* Find the correct result unit: */
    PyObject *new_unit = PyNumber_Multiply(unit1, unit2);
    if (new_unit == NULL) {
        return -1;
    }
    /* Create new DType from the new unit: */
    loop_descrs[2] = new_unitdtype_instance(new_unit);
    if (loop_descrs[2] == NULL) {
        return -1;
    }
    /* The other operand units can be used as-is: */
    Py_INCREF(given_descrs[0]);
    loop_descrs[0] = given_descrs[0];
    Py_INCREF(given_descrs[1]);
    loop_descrs[1] = given_descrs[0];

    return NPY_NO_CASTING;
}
```

User code:

```
arr1 = np.array([2*m])
arr2 = np.array([3*m])
res = arr1 * arr2
```

Resolver finds:

```
dtype1 = arr1.dtype  # "m"
dtype2 = arr2.dtype  # "m"
res_dt = res.dtype   # "m**2"
```

Lets make a UFunc: The "Resolver"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    Py_INCREF(given_descrs[0]);
    loop_descrs[0] = given_descrs[0];
    Py_INCREF(given_descrs[1]);
    loop_descrs[1] = given_descrs[0];

    return NPY_NO_CASTING;
}
```

"self":

- fairly opaque currently
- Future information

Lets make a UFunc: The "Resolver"


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    loop_descrs[1] = given_descrs[0];

    return NPY_NO_CASTING;
}
```

The DTypes:

- just: `UnitDType`
- allows generic resolvers

Lets make a UFunc: The "Resolver"


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static NPY_CASTING
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    loop_descrs[1] = given_descrs[0];

    return NPY_NO_CASTING;
}
```

The dtypes / descriptors:

- `arr1.dtype`
- `arr2.dtype`
- `NULL` (or `out.dtype`)

Lets make a UFunc: The "Resolver"


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        PyArray_DTypeMeta *dtypes[], PyArray_Descr *given_descrs[],
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    return NPY_NO_CASTING;
}
```

Output the dtypes/descriptors to use in the C-loop:

- ?
- ?
- ?

Lets make a UFunc: The "Resolver"


```c
static NPY_CASTING
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    Py_INCREF(given_descrs[0]);
    loop_descrs[0] = given_descrs[0];
    Py_INCREF(given_descrs[1]);
    loop_descrs[1] = given_descrs[0];

    return NPY_NO_CASTING;
}
```

Find the result unit:

```
unit1 = arr1.dtype.unit
unit2 = arr2.dtype.unit

new_unit = unit1 * unit2
```

Lets make a UFunc: The "Resolver"


```c
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    return NPY_NO_CASTING;
}
```

Result dtype/descriptor:

```
res_dt = UnitDType(new_unit)
```

Lets make a UFunc: The "Resolver"


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    Py_INCREF(given_descrs[0]);
    loop_descrs[0] = given_descrs[0];
    Py_INCREF(given_descrs[1]);
    loop_descrs[1] = given_descrs[0];

    return NPY_NO_CASTING;
}
```

Output the dtypes/descriptors to use in the C-loop:

- `arr1.dtype`
- `arr2.dtype`
- `res_dt`

Lets make a UFunc: The "Resolver"


```c
static NPY_CASTING
unit_multiply_resolve_descriptors(PyObject *self,
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        PyArray_Descr *loop_descrs[], npy_intp *unused)
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    Py_INCREF(given_descrs[0]);
    loop_descrs[0] = given_descrs[0];
    Py_INCREF(given_descrs[1]);
    loop_descrs[1] = given_descrs[0];

    return NPY_NO_CASTING;
}
```
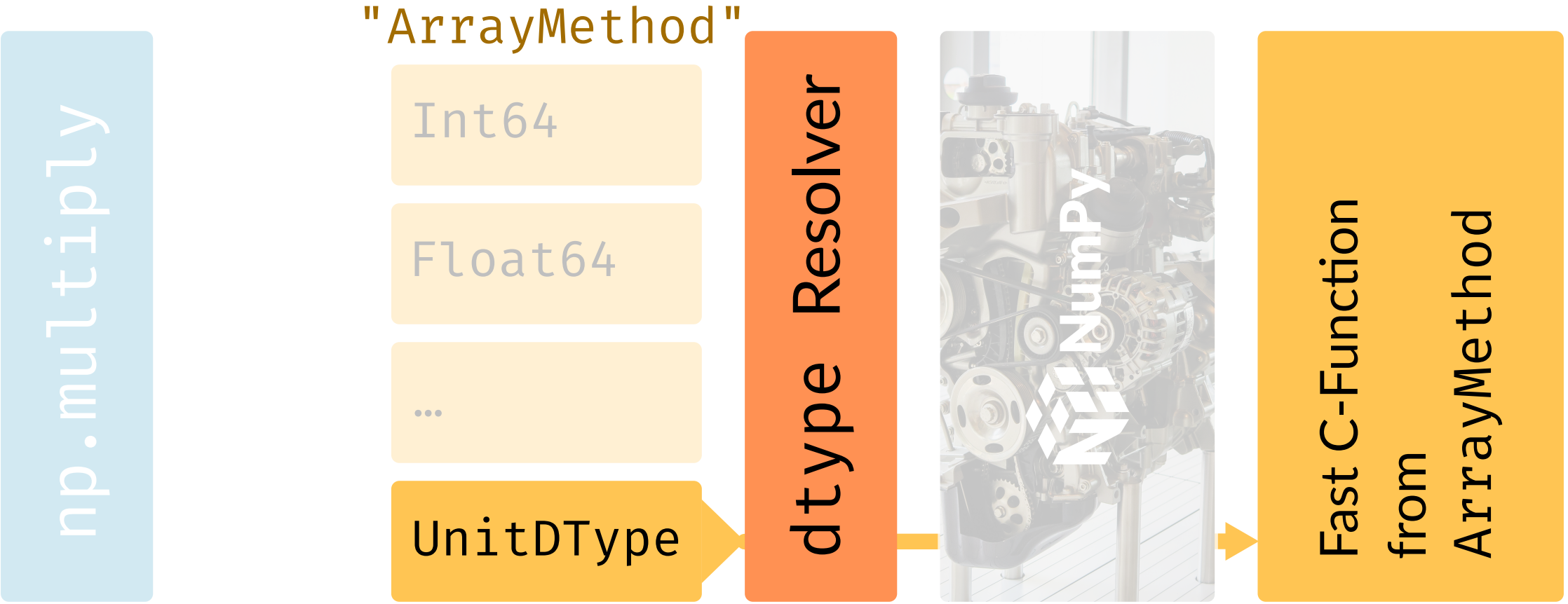

This UFunc does not cast!

- potential optimizations
- important for casts!

Lets make a UFunc: 🎁 Wrap it up!



Lets make a UFunc: 🎁 Wrap it up!


```
static PyArray_DTypeMeta *dtypes[3] = {
   &UnitDType, &UnitDType, &UnitDType};

static PyType_Slot slots[] = {
   {NPY_METH_resolve_descriptors,
        &unit_multiply_resolve_descriptors},
   {NPY_METH_strided_loop,
        &unit_multiply_strided_loop},
   {0, NULL}
};

PyArrayMethod_Spec MultiplySpec = {
    .name = "unit_multiply",
    .nin = 2,
    .nout = 1,
    .dtypes = dtypes,
    .slots = slots,
    .flags = 0,
    .casting = NPY_NO_CASTING,
};

/* Register */
PyUFunc_AddLoopFromSpec(multiply, &MultiplySpec);
```

Loop operates on `UnitDType`

Lets make a UFunc: 🎁 Wrap it up!


```
static PyArray_DTypeMeta *dtypes[3] = {
   &UnitDType, &UnitDType, &UnitDType};

static PyType_Slot slots[] = {
   {NPY_METH_resolve_descriptors,
        &unit_multiply_resolve_descriptors},
   {NPY_METH_strided_loop,
        &unit_multiply_strided_loop},
   {0, NULL}
};

PyArrayMethod_Spec MultiplySpec = {
    .name = "unit_multiply",
    .nin = 2,
    .nout = 1,
    .dtypes = dtypes,
    .slots = slots,
    .flags = 0,
    .casting = NPY_NO_CASTING,
};

/* Register */
PyUFunc_AddLoopFromSpec(multiply, &MultiplySpec);
```

List of "methods":

- Fill in what we defined
- Extensible

More options (not shown):

- Faster loops
- Set-up e.g. scratch space

Lets make a UFunc: 🎁 Wrap it up!


```c
static PyArray_DTypeMeta *dtypes[3] = {
   &UnitDType, &UnitDType, &UnitDType};

static PyType_Slot slots[] = {
   {NPY_METH_resolve_descriptors,
        &unit_multiply_resolve_descriptors},
   {NPY_METH_strided_loop,
        &unit_multiply_strided_loop},
   {0, NULL}
};

PyArrayMethod_Spec MultiplySpec = {
    .name = "unit_multiply",
    .nin = 2,
    .nout = 1,
    .dtypes = dtypes,
    .slots = slots,
    .flags = 0,
    .casting = NPY_NO_CASTING,
};

/* Register */
PyUFunc_AddLoopFromSpec(multiply, &MultiplySpec);
```

The "Spec" (C `struct`)

- name
- number of inputs/outputs
- DTypes (`UnitDType`)
- `slots`: "methods"
- ...

Lets make a UFunc: 🎁 Wrap it up!


```
static PyArray_DTypeMeta *dtypes[3] = {
   &UnitDType, &UnitDType, &UnitDType};

static PyType_Slot slots[] = {
   {NPY_METH_resolve_descriptors,
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    .flags = 0,
    .casting = NPY_NO_CASTING,
};

/* Register */
PyUFunc_AddLoopFromSpec(multiply, &MultiplySpec);
```
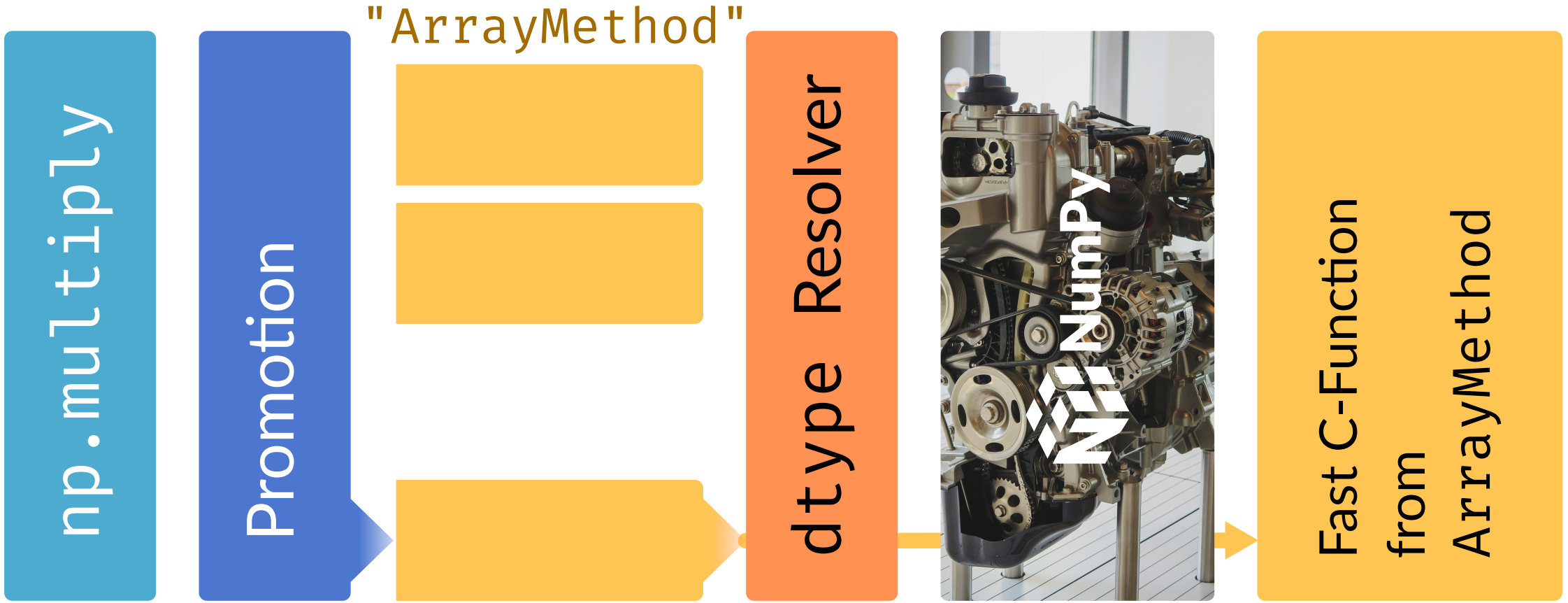

Add to multiply ufunc!

Done with UFunc!


```
arr1 = np.array([2*m])
arr2 = np.array([3*m])
res = np.multiply(arr1, arr2)
```



How do Casts work?


```
arr1 = np.array([2*m])

res = arr1.astype(UnitDType("cm"))
```

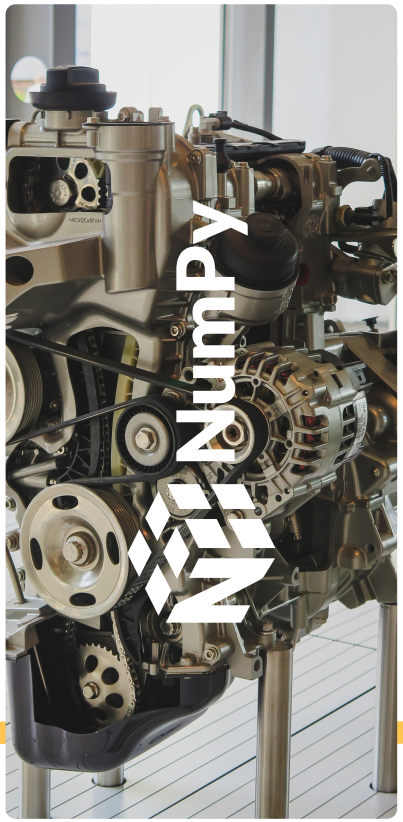
"ArrayMethod"

… → UnitDType

UnitDType → …

UnitDType → UnitDType

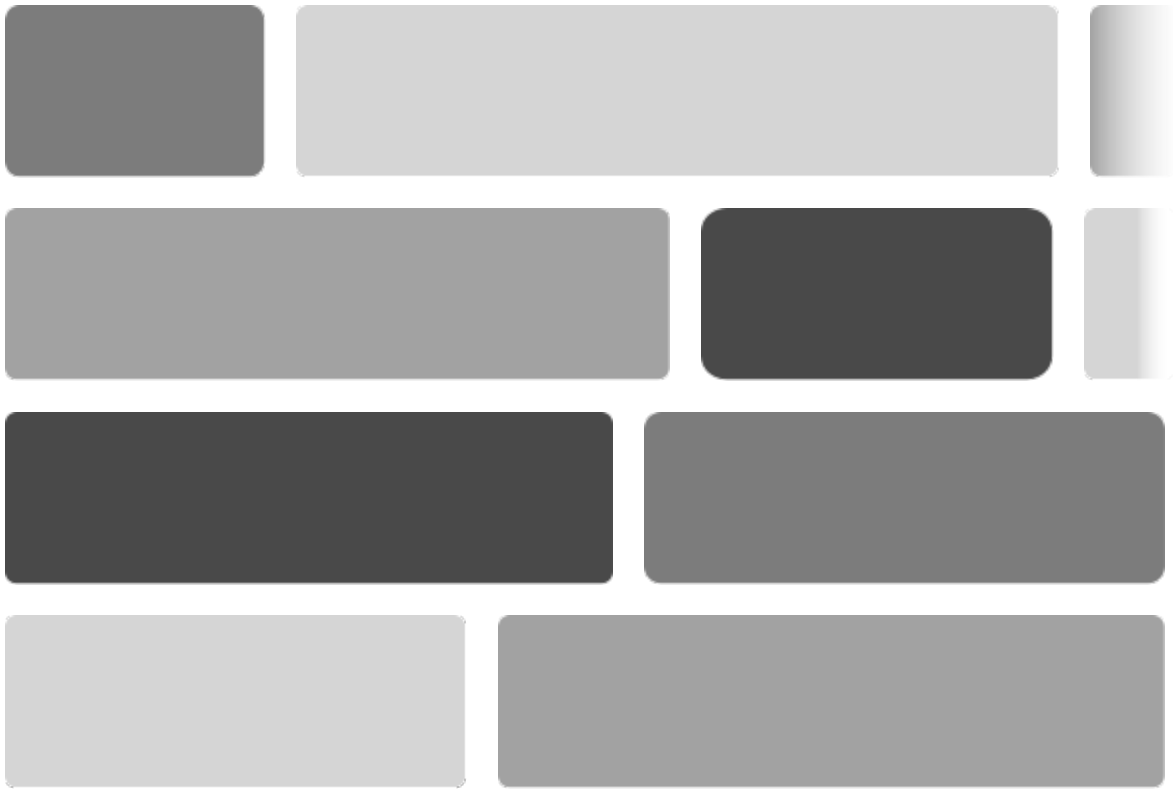
dtype Resolver



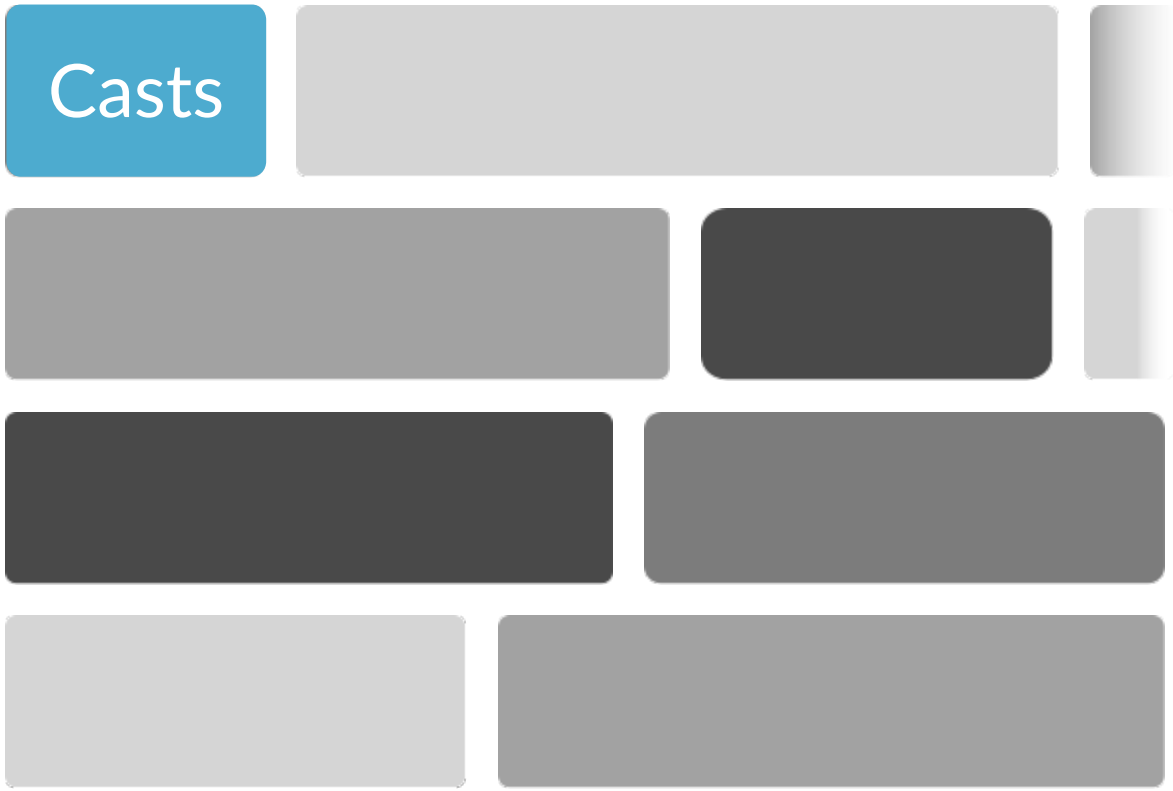
Fast C-Function from ArrayMethod

What makes the UnitDType?


```
class UnitDType(np.dtype):
    itemsize = 8

    def special_methods( ... ):
        pass
```



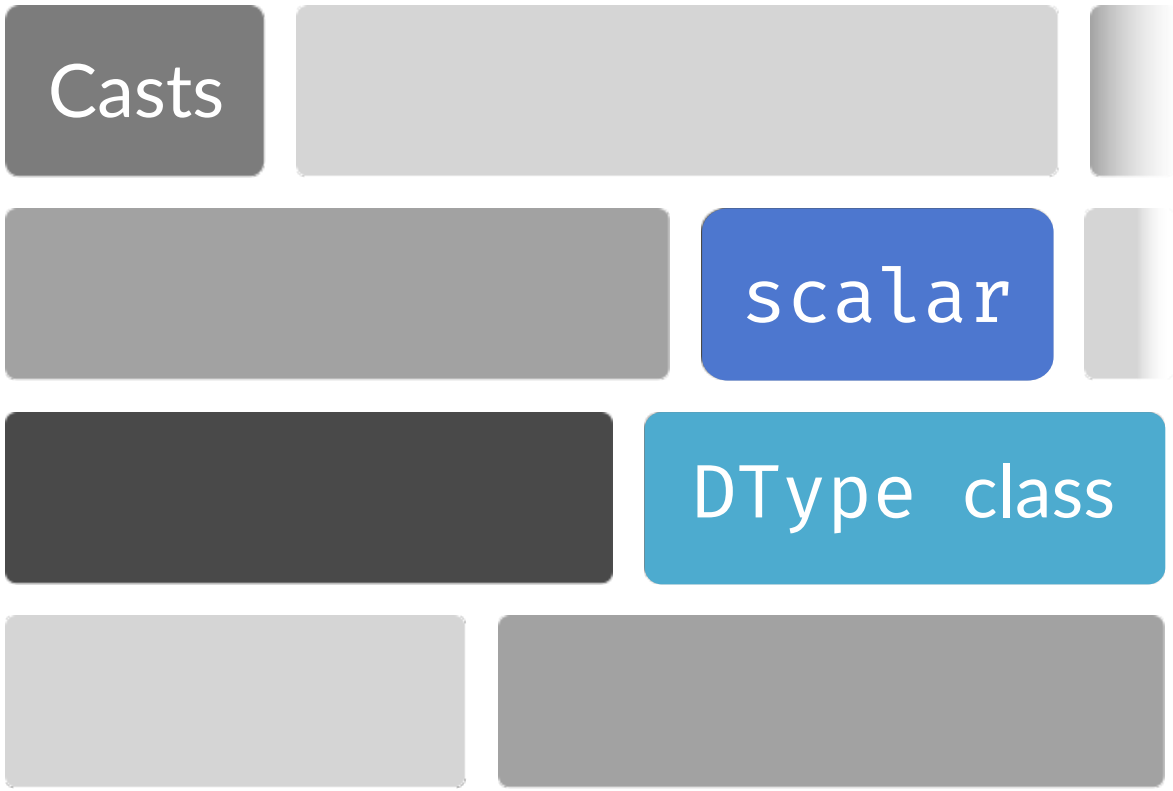
What makes the UnitDType?



What makes the UnitDType?

Type(s):

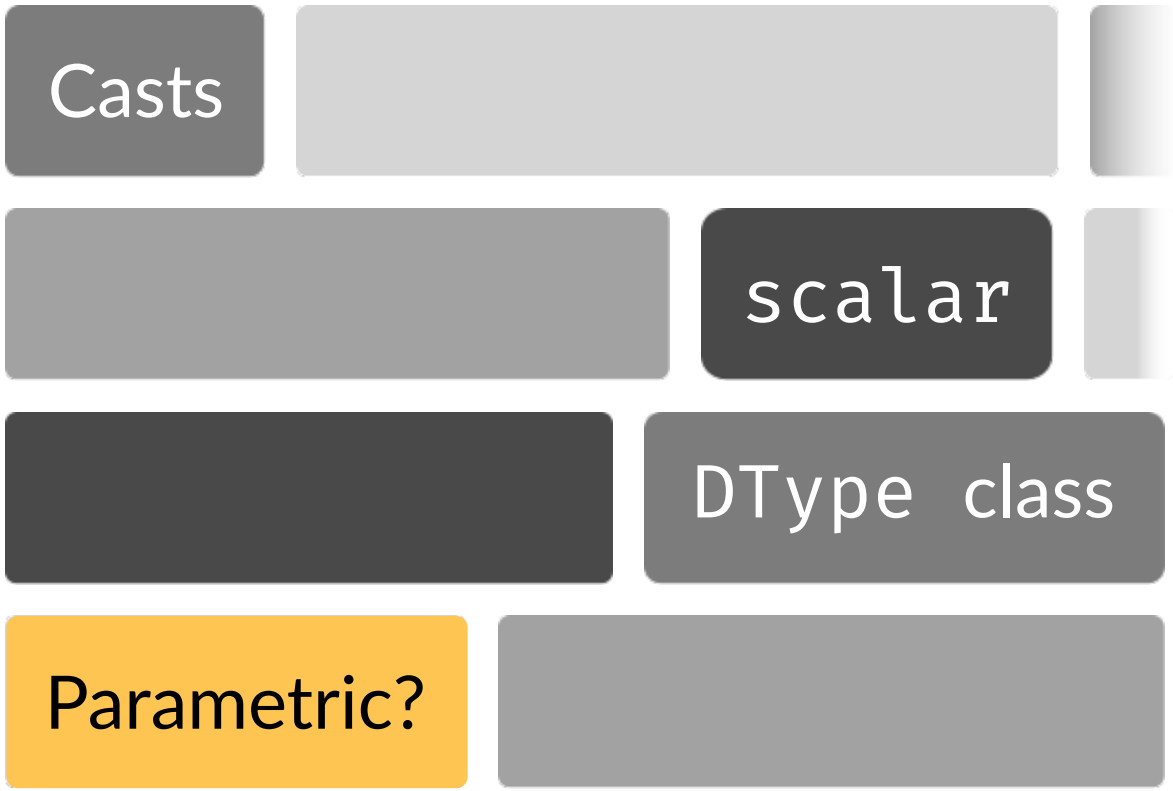
- Scalar Type (`2*m`)
- `UnitDType` class
- Future: no scalar?



What makes the UnitDType?

Flags:

- currently only one



What makes the UnitDType?

Set/Get element:

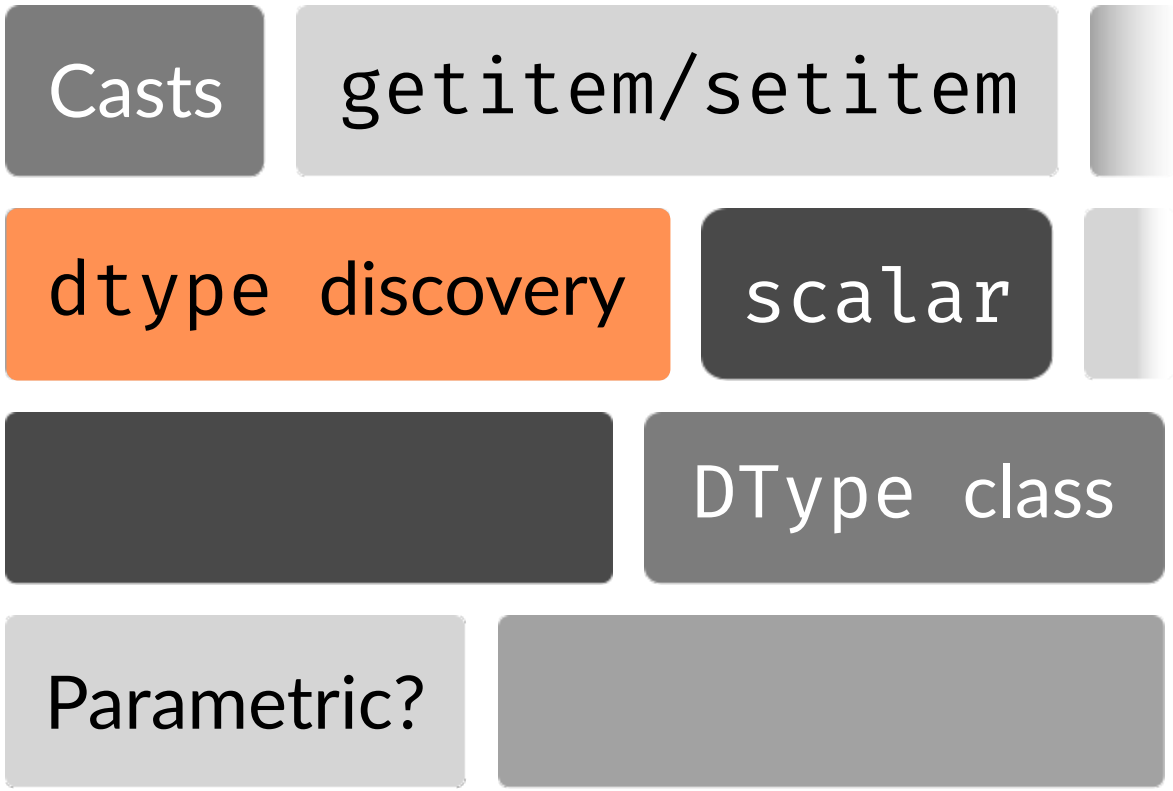
```
arr[i] = 2*m
scalar = arr[i]
```

What makes the UnitDType?

Discover dtype from scalar:

- only if parametric

```
scalar = 2*m
np.array([scalar])
```

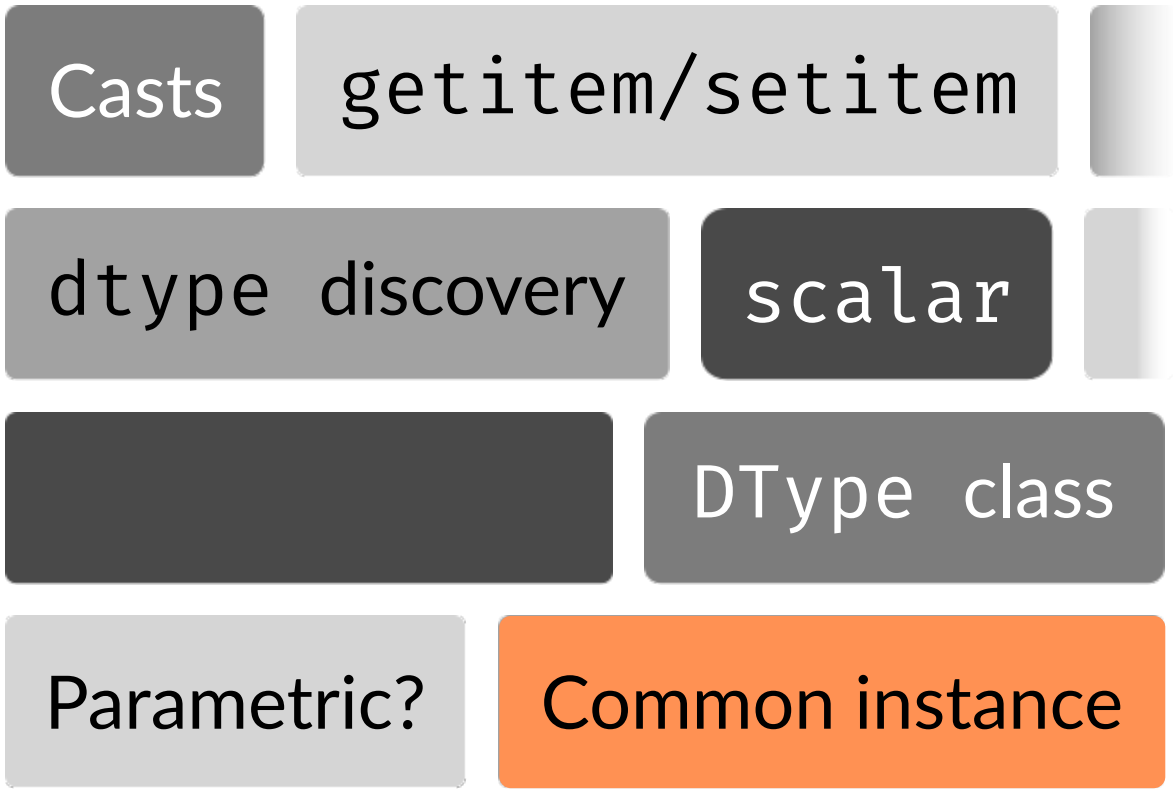


What makes the UnitDType?

Two `UnitDTypes`:

- Find "common" one
- only if parametric

```
np.array([1*m, 2*cm])
  → m
```

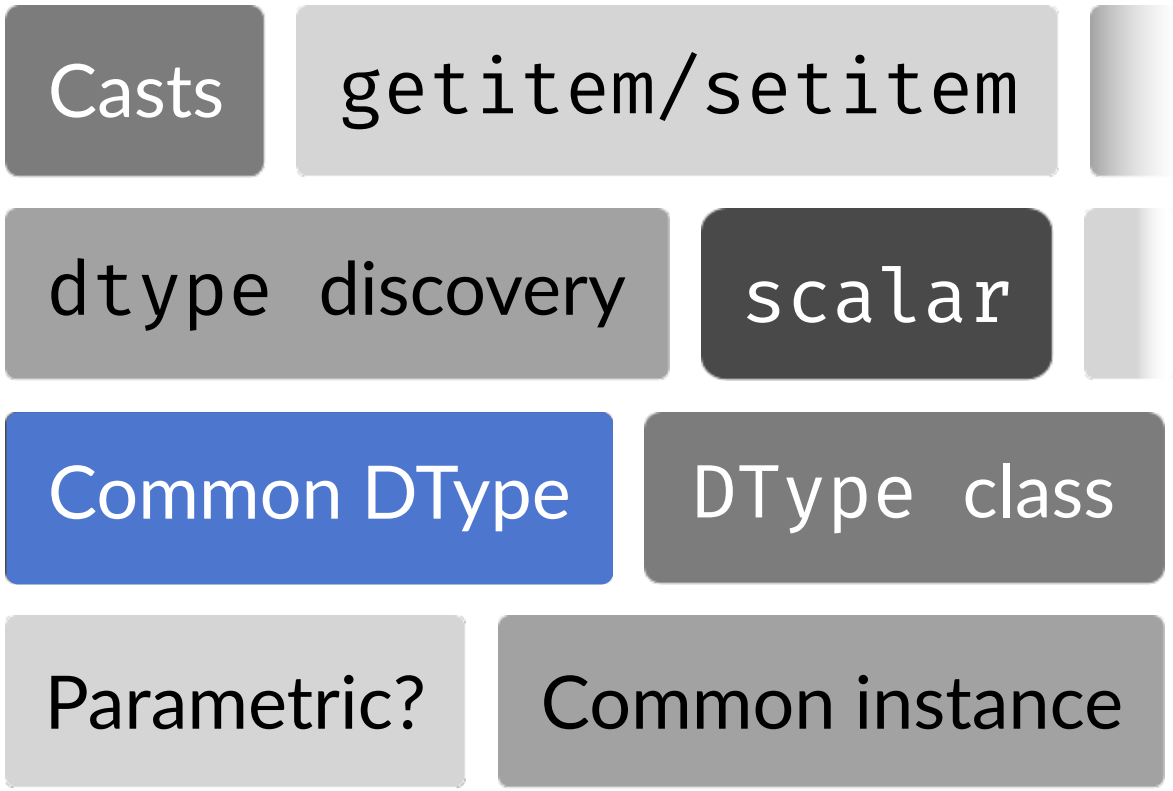


What makes the UnitDType?

Common `DType`:

- binary operator
- Promotion
- `concatenate()`

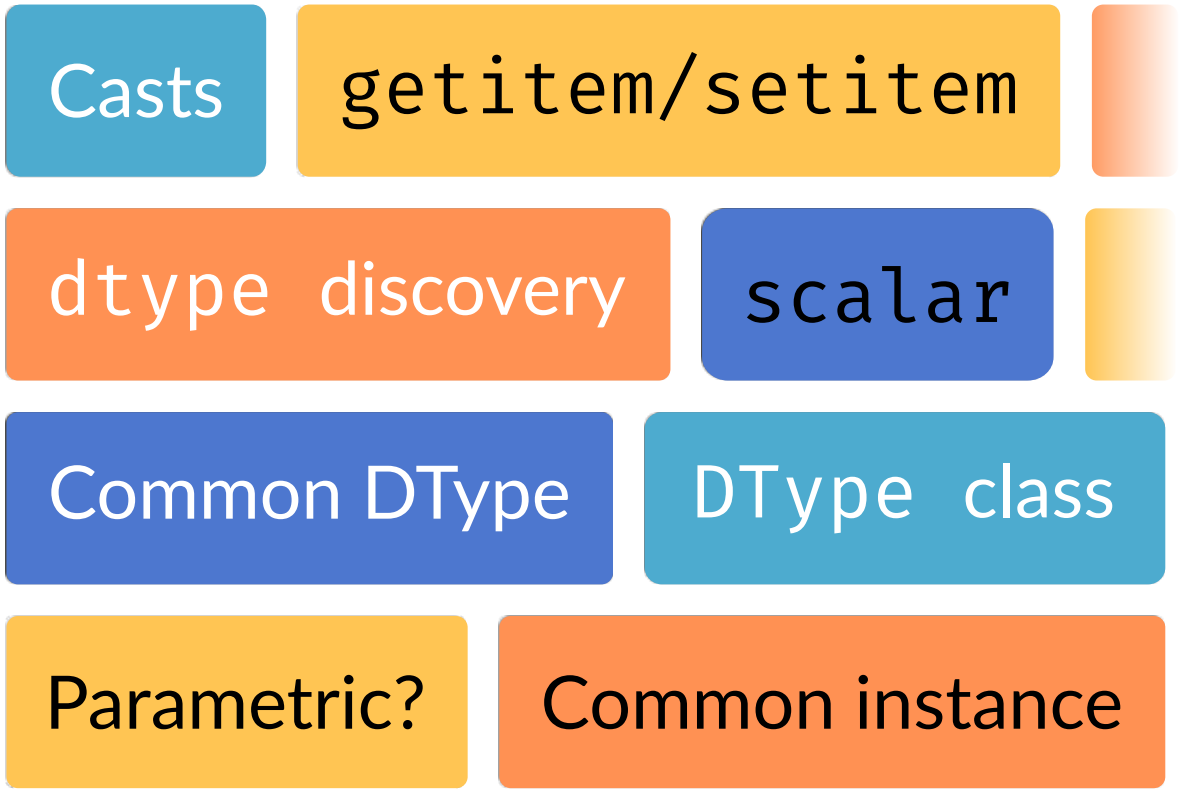
```
UnitDType & Float64
  → UnitDType
```



What makes the UnitDType?

Wrap it up:

- again: "`Spec`"
- extensible



Summary

- *First-class* user DTypes on the horizon
- Future extensibility easier
  - → e.g. new sorting methods
  - → string UFuncs
- experiment and help finalize API!

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Matti Picus, Marten van Kerkwijk, Ross Barnowsky, ...

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Summary

- *First-class* user DTypes on the horizon
- Future extensibility easier
  - → e.g. new sorting methods
  - → string UFuncs
- experiment and help finalize API!

```
numpy.org/neps  NEP 41-43
github.com/seberg/talk_unitdtype  (NumPy main)
github.com/seberg/unitdtype  (currently NumPy branch)
```

Thank You!