

MuPIF Reference manual Documentation

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CHAPTER 1

Introduction

Multi-Physics Integration Framework (MuPIF) is an integration framework, that will facilitate the implementation of multi-physic and multi-level simulations, built from independently developed components. The principal role of the framework is to steer individual components (applications) and to provide high-level data-exchange services. Each application should implement an interface that allows to steer application and execute data requests. The design supports various coupling strategies, discretization techniques, and also the distributed applications. The platform development is hosted on GitHub (https://github.com/mupif/mupif/).

The approach followed in this project is based on an object-oriented approach, consisting in designing a system of interacting objects for the purpose of solving a software problem. The identification of individual objects and their mutual interaction has been based on expertise of project partners, and later refined by analysis of simulation scenarios considered in the project. The main advantage of this approach lies in independence on particular data format(s), as the exchanged data (fields, properties) are represented as abstract classes. Therefore, the focus on services is provided by objects (object interfaces) and not on underlying data itself.

The integration framework is implemented in Python3. Python is an interpreted, interactive, object-oriented programming language. It runs on many Unix/Linux platforms, on the Mac, and on PCs under MS-DOS, Windows, Windows NT, and OS/2. The Python language is enriched by new objects/classes to describe and to represent complex simulation chains. Such approach allows profiting from the capabilities of established scripting environment, including numerical libraries, serialization/persistence support, VPN, and remote communication.

The proposed abstract classes are designed to represent the entities in a model space, including simulation tools, fields, discretizations, properties, etc. The purpose of these abstract classes is to define a common interface that needs to be implemented by any derived class. Such interface concept allows using any derived class on a very abstract level, using common interface for services, without being concerned with the implementation details of an individual software component.

To facilitate execution and development of the simulation workflows, the platform provides the transparent communication mechanism that will take care of the network communication between the objects. An important feature is the transparency, which hides the details of remote communication to the user and allows working with local and remote objects in the same way. The communication layer is built on Pyro4 library, which provides a transparent distributed object system fully integrated into Python. It takes care of the network communication between the objects when they are distributed over different machines on the network. The platform is designed to work on virtually any distributed platform, including grid and cloud infrastructure.

In addition to this MuPIF reference manual, a user manual from https://github.com/mupif/mupif/tree/master/mupif/doc/userManual can be obtained, showing details on API implementation, installation, networking and providing several examples in local/distributed setups.

CHAPTER 2

mupif package

2.1 Subpackages

2.1.1 mupif.Physics package

2.1.1.1 Submodules

2.1.1.2 mupif.Physics.NumberDict module

Dictionary storing numerical values

class mupif.Physics.NumberDict.NumberDict

Bases: dict

Dictionary storing numerical values

Constructor: NumberDict()

An instance of this class acts like an array of number with generalized (non-integer) indices. A value of zero is assumed for undefined entries. NumberDict instances support addition, and subtraction with other NumberDict instances, and multiplication and division by scalars.

2.1.1.3 mupif.Physics.PhysicalQuantities module

Physical quantities with units.

This module provides a data type that represents a physical quantity together with its unit. It is possible to add and subtract these quantities if the units are compatible, and a quantity can be converted to another compatible unit. Multiplication, subtraction, and raising to integer powers is allowed without restriction, and the result will have the correct unit. A quantity can be raised to a non-integer power only if the result can be represented by integer powers of the base units.

The values of physical constants are taken from the 1986 recommended values from CODATA. Other conversion factors (e.g. for British units) come from various sources. I can't guarantee for the correctness of all entries in the unit table, so use this at your own risk.

SI derived units; these automatically get prefixes: Y (1E+24), Z (1E+21), E (1E+18), P (1E+15), T (1E+12), G (1E+09), M (1E+06), k (1E+03), h (1E+02), da (1E+01), d (1E-01), c (1E-02), m (1E-03), mu (1E-06), n (1E-09), p (1E-12), f (1E-15), a (1E-18), z (1E-21), y (1E-24)

Hz Hertz 1/s N Newton m*kg/s**2 Pa Pascal N/m**2 J Joule N*m W Watt J/s C Coulomb s*A V Volt W/A F Farad C/V ohm Ohm V/A S Siemens A/V Wb Weber V*s T Tesla Wb/m**2 H Henry Wb/A lm Lumen cd*sr lx Lux lm/m**2 Bq Becquerel 1/s Gy Gray J/kg Sv Sievert J/kg

Prefixed units for m:

Ym, Zm, Em, Pm, Tm, Gm, Mm, km, hm, dam, dm, cm, mm, mum, nm, pm, fm, am, zm, ym

Prefixed units for g:

Yg, Zg, Eg, Pg, Tg, Gg, Mg, kg, hg, dag, dg, cg, mg, mug, ng, pg, fg, ag, zg, yg

Prefixed units for s:

Ys, Zs, Es, Ps, Ts, Gs, Ms, ks, hs, das, ds, cs, ms, mus, ns, ps, fs, as, zs, ys

Prefixed units for A:

YA, ZA, EA, PA, TA, GA, MA, kA, hA, daA, dA, cA, mA, muA, nA, pA, fA, aA, zA, yA

Prefixed units for K:

YK, ZK, EK, PK, TK, GK, MK, kK, hK, daK, dK, cK, mK, muK, nK, pK, fK, aK, zK, yK

Prefixed units for mol:

Ymol, Zmol, Emol, Pmol, Tmol, Gmol, Mmol, kmol, hmol, damol, dmol, cmol, mmol, mumol, nmol, pmol, fmol, amol, zmol, ymol

Prefixed units for cd:

Ycd, Zcd, Ecd, Pcd, Tcd, Gcd, Mcd, kcd, hcd, dacd, dcd, ccd, mcd, mucd, ncd, pcd, fcd, acd, zcd, ycd

Prefixed units for rad:

Yrad, Zrad, Erad, Prad, Trad, Grad, Mrad, krad, hrad, darad, drad, crad, mrad, murad, nrad, prad, frad, arad, zrad, yrad

Prefixed units for sr:

Ysr, Zsr, Esr, Psr, Tsr, Gsr, Msr, ksr, hsr, dasr, dsr, csr, msr, musr, nsr, psr, fsr, asr, zsr, ysr

Prefixed units for none:

Ynone, Znone, Enone, Pnone, Tnone, Gnone, Mnone, knone, hnone, danone, dnone, cnone, mnone, munone, mnone, pnone, fnone, anone, znone, ynone

Prefixed units for Hz:

YHz, ZHz, EHz, PHz, THz, GHz, MHz, kHz, hHz, daHz, dHz, cHz, mHz, muHz, nHz, pHz, fHz, aHz, zHz, yHz

Prefixed units for N:

YN, ZN, EN, PN, TN, GN, MN, kN, hN, daN, dN, cN, mN, muN, nN, pN, fN, aN, zN, yN

Prefixed units for Pa:

YPa, ZPa, EPa, PPa, TPa, GPa, MPa, kPa, hPa, daPa, dPa, cPa, mPa, muPa, nPa, pPa, fPa, aPa, zPa, yPa

Prefixed units for J:

YJ, ZJ, EJ, PJ, TJ, GJ, MJ, kJ, hJ, daJ, dJ, cJ, mJ, muJ, nJ, pJ, fJ, aJ, zJ, yJ

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Prefixed units for W:

YW, ZW, EW, PW, TW, GW, MW, kW, hW, daW, dW, cW, mW, muW, nW, pW, fW, aW, zW, yW

Prefixed units for C:

YC, ZC, EC, PC, TC, GC, MC, kC, hC, daC, dC, cC, mC, muC, nC, pC, fC, aC, zC, yC

Prefixed units for V:

YV, ZV, EV, PV, TV, GV, MV, kV, hV, daV, dV, cV, mV, muV, nV, pV, fV, aV, zV, yV

Prefixed units for F:

YF, ZF, EF, PF, TF, GF, MF, kF, hF, daF, dF, cF, mF, muF, nF, pF, fF, aF, zF, yF

Prefixed units for ohm:

Yohm, Zohm, Eohm, Pohm, Tohm, Gohm, Mohm, kohm, hohm, daohm, dohm, cohm, mohm, muohm, nohm, pohm, fohm, aohm, zohm, yohm

Prefixed units for S:

YS, ZS, ES, PS, TS, GS, MS, kS, hS, daS, dS, cS, mS, muS, nS, pS, fS, aS, zS, yS

Prefixed units for Wb:

YWb, ZWb, EWb, PWb, TWb, GWb, MWb, kWb, hWb, daWb, dWb, cWb, mWb, muWb, nWb, pWb, fWb, aWb, zWb, yWb

Prefixed units for T:

YT, ZT, ET, PT, TT, GT, MT, kT, hT, daT, dT, cT, mT, muT, nT, pT, fT, aT, zT, yT

Prefixed units for H:

YH, ZH, EH, PH, TH, GH, MH, kH, hH, daH, dH, cH, mH, muH, nH, pH, fH, aH, zH, yH

Prefixed units for lm:

Ylm, Zlm, Elm, Plm, Tlm, Glm, Mlm, klm, hlm, dalm, dlm, clm, mlm, mulm, nlm, plm, flm, alm, zlm, ylm

Prefixed units for lx:

Ylx, Zlx, Elx, Plx, Tlx, Glx, Mlx, klx, hlx, dalx, dlx, clx, mlx, mulx, nlx, plx, flx, alx, zlx, ylx

Prefixed units for Bq:

YBq, ZBq, EBq, PBq, TBq, GBq, MBq, kBq, hBq, daBq, dBq, cBq, mBq, muBq, nBq, pBq, fBq, aBq, zBq, yBq

Prefixed units for Gy:

YGy, ZGy, EGy, PGy, TGy, GGy, MGy, kGy, hGy, daGy, dGy, cGy, mGy, muGy, nGy, pGy, fGy, aGy, zGy, yGy

Prefixed units for Sv:

YSv, ZSv, ESv, PSv, TSv, GSv, MSv, kSv, hSv, daSv, dSv, cSv, mSv, muSv, nSv, pSv, fSv, aSv, zSv, ySv

Fundamental constants: c speed of light 299792458.*m/s mu0 permeability of vacuum 4.e-7*pi*N/A**2 eps0 permittivity of vacuum 1/mu0/c**2 Grav gravitational constant 6.67259e-11*m**3/kg/s**2 hplanck Planck constant 6.6260755e-34*J*s hbar Planck constant / 2pi hplanck/(2*pi) e elementary charge 1.60217733e-19*C me electron mass 9.1093897e-31*kg mp proton mass 1.6726231e-27*kg Nav Avogadro number 6.0221367e23/mol k Boltzmann constant 1.380658e-23*J/K

Time units: min minute 60*s h hour 60*min d day 24*h wk week 7*d yr year 365.25*d

Length units: inch inch 2.54*cm ft foot 12*inch yd yard 3*ft mi (British) mile 5280.*ft nmi Nautical mile 1852.*m Ang Angstrom 1.e-10*m lyr light year c*yr Bohr Bohr radius 4*pi*eps0*hbar**2/me/e**2

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Area units: ha hectare 10000*m**2 acres acre mi**2/640 b barn 1.e-28*m**2

Volume units: 1 liter dm**3 dl deci liter 0.1*l cl centi liter 0.01*l ml milli liter 0.001*l tsp teaspoon 4.92892159375*ml tbsp tablespoon 3*tsp floz fluid ounce 2*tbsp cup cup 8*floz pt pint 16*floz qt quart 2*pt galUS US gallon 4*qt galUK British gallon 4.54609*l

Mass units: amu atomic mass units 1.6605402e-27*kg oz ounce 28.349523125*g lb pound 16*oz ton ton 2000*lb

Force units: dyn dyne (cgs unit) 1.e-5*N

Energy units: erg erg (cgs unit) 1.e-7*J eV electron volt e*V Hartree Wavenumbers/inverse cm me*e**4/16/pi**2/eps0**2/hbar**2 Ken Kelvin as energy unit k*K cal thermochemical calorie 4.184*J kcal thermochemical kilocalorie 1000*cal cali international calorie 4.1868*J kcali international kilocalorie 1000*cali Btu British thermal unit 1055.05585262*J

Prefixed units for eV:

```
YeV, ZeV, EeV, PeV, TeV, GeV, MeV, keV, heV, daeV, deV, ceV, meV, mueV, neV, peV, feV, aeV, zeV, yeV
```

Power units: hp horsepower 745.7*W

Pressure units: bar bar (cgs unit) 1.e5*Pa atm standard atmosphere 101325.*Pa torr torr = mm of mercury atm/760 psi pounds per square inch 6894.75729317*Pa

Angle units: deg degrees pi*rad/180

Temperature units: degR degrees Rankine (5./9.)*K degC degrees Celcius <PhysicalUnit degC> degF degree Fahrenheit <PhysicalUnit degF>

```
class mupif.Physics.PhysicalQuantities.PhysicalQuantity(*args)
    Bases: object
```

Physical quantity with units

PhysicalQuantity instances allow addition, subtraction, multiplication, and division with each other as well as multiplication, division, and exponentiation with numbers. Addition and subtraction check that the units of the two operands are compatible and return the result in the units of the first operand. A limited set of mathematical functions (from module Numeric) is applicable as well:

- sqrt: equivalent to exponentiation with 0.5.
- sin, cos, tan: applicable only to objects whose unit is compatible with 'rad'.

See the documentation of the PhysicalQuantities module for a list of the available units.

Here is an example on usage:

```
>>> from PhysicalQuantities import PhysicalQuantity as p # short hand
>>> distance1 = p('10 m')
>>> distance2 = p('10 km')
>>> total = distance1 + distance2
>>> total
PhysicalQuantity(10010.0,'m')
>>> total.convertToUnit('km')
>>> total.getValue()
10.01
>>> total.getUnitName()
'km'
>>> total = total.inBaseUnits()
>>> total
PhysicalQuantity(10010.0,'m')
>>> total
PhysicalQuantity(10010.0,'m')
>>> total
```

```
>>> t2 = t.inUnitsOf('d','h','min','s')
>>> t2_print = ' '.join([str(i) for i in t2])
>>> t2_print
'3.0 d 15.0 h 15.0 min 59.0 s'
>>> e = p('2.7 Hartree*Nav')
>>> e.convertToUnit('kcal/mol')
PhysicalQuantity (1694.2757596034764, 'kcal/mol')
>>> e = e.inBaseUnits()
>>> str(e)
'7088849.77818 kg*m**2/s**2/mol'
>>> freeze = p('0 degC')
>>> freeze = freeze.inUnitsOf ('degF')
>>> str(freeze)
'32.0 degF'
>>>
m = PQ(12, 'kg')
a = PQ('0.88 \text{ km/s**2'})
F = m*a
print F
#vector valued quantities: a = PQ((1,2,3),m') scalar = PQ(2.0, s') a.convertToUnit('km') a.inUnitsOf('dm')
```

a*3.0 a*scalar

#F = F.inBaseUnits() print F

print F.isCompatible('MN') print F.isCompatible('m')

F.convertToUnit('MN') # convert to Mega Newton print F F = F + PQ(0.1, 'kPa*m**2') # kilo Pascal m^2 print F print str(F)

value = float(str(F).split()[0]) print value

convertToUnit (unit)

Change the unit and adjust the value such that the combination is equivalent to the original one. The new unit must be compatible with the previous unit of the object.

```
Parameters unit (C{str}) - a unit
```

Raises TypeError – if the unit string is not a know unit or a unit incompatible with the current one

cos()

getUnitName()

Return unit (string) of physical quantity.

getValue()

Return value (float) of physical quantity (no unit).

inBaseUnits()

Returns the same quantity converted to base units, i.e. SI units in most cases

Return type L{PhysicalQuantity}

inUnitsOf (*units)

Express the quantity in different units. If one unit is specified, a new PhysicalQuantity object is returned that expresses the quantity in that unit. If several units are specified, the return value is a tuple of PhysicalObject instances with with one element per unit such that the sum of all quantities in the tuple equals

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the the original quantity and all the values except for the last one are integers. This is used to convert to irregular unit systems like hour/minute/second. **Parameters units** $(C\{str\})$ or sequence of $C\{str\}$) – one or several units **Returns** one or more physical quantities **Return type** L{PhysicalQuantity} or C{tuple} of L{PhysicalQuantity} Raises TypeError – if any of the specified units are not compatible with the original unit isCompatible (unit) Parameters unit $(C\{str\})$ – a unit **Returns** C{True} if the specified unit is compatible with the one of the quantity **Return type** C{bool} sin() sqrt() tan() **class** mupif.Physics.PhysicalQuantities.**PhysicalUnit** (names, factor, powers, offset=0) Bases: object Physical unit A physical unit is defined by a name (possibly composite), a scaling factor, and the exponentials of each of the SI base units that enter into it. Units can be multiplied, divided, and raised to integer powers. conversionFactorTo(other) **Parameters** other (L{PhysicalUnit}) – another unit **Returns** the conversion factor from this unit to another unit **Return type** C{float} Raises TypeError – if the units are not compatible conversionTupleTo(other)**Parameters other** (L{PhysicalUnit}) – another unit **Returns** the conversion factor and offset from this unit to another unit **Return type** (C{float}, C{float}) **Raises** TypeError – if the units are not compatible isAngle() $\verb|isCompatible| (other)$ **Parameters** other (L{PhysicalUnit}) – another unit **Returns** C{True} if the units are compatible, i.e. if the powers of the base units are the same Return type C{bool} isDimensionless() name() setName (name)

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mupif.Physics.PhysicalQuantities.assertPhysicalUnitEqual (first, second, msg=None)

```
mupif.Physics.PhysicalQuantities.cmp(a, b)
mupif.Physics.PhysicalQuantities.description()
    Return a string describing all available units.
mupif.Physics.PhysicalQuantities.findUnit(unit)
mupif.Physics.PhysicalQuantities.getDimensionlessUnit()
    return dimensionless unit
mupif.Physics.PhysicalQuantities.isPhysicalQuantity(x)
    Parameters x(any) - an object
    Returns C{True} if x is a L{PhysicalQuantity}
    Return type C{bool}
mupif.Physics.PhysicalQuantities.isPhysicalUnit(x)
    Parameters x(any) - an object
    Returns C{True} if x is a L{PhysicalUnit}
Return type C{bool}
```

2.1.1.4 Module contents

2.2 Submodules

2.3 mupif.APIError module

```
exception mupif.APIError.APIError Bases: Exception
```

This class serves as a base class for exceptions thrown by the framework. Raising an exception is a way to signal that a routine could not execute normally - for example, when an input argument is invalid (e.g. value is outside of the domain of a function) or when a resource it relies on is unavailable (like a missing file, a hard disk error, or out-of-memory errors)

Exceptions provide a way to react to exceptional circumstances (like runtime errors) in programs by transferring control to special functions called handlers. To catch exceptions, a portion of code is placed under exception inspection. This is done by enclosing that portion of code in a try-block. When an exceptional circumstance arises within that block, an exception is thrown that transfers the control to the exception handler. If no exception is thrown, the code continues normally and all handlers are ignored.

An exception is thrown by using the throw keyword from inside the "try" block. Exception handlers are declared with the keyword "except", which must be placed immediately after the try block.

2.4 mupif.Application module

```
class mupif.Application.Application(metaData={})
    Bases: mupif.Model.Model
Fully derived from Model.Model. Only kept for backward compatibility.
```

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```
class mupif.Application.RemoteApplication(decoratee, jobMan=None, jobID=None, app-
Tunnel=None)
```

Bases: mupif.Model.RemoteModel

Fully derived from Model.RemoteModel. Only kept for backward compatibility.

2.5 mupif.BBox module

```
class mupif.BBox.BBox (coords_ll, coords_ur)
    Bases: object
```

Represents a bounding box - a rectange in 2D and prism in 3D. Its geometry is described using two points - lover left and upper right corners. The bounding box class provides fast and efficient methods for testing whether point is inside it and whether intersection with other BBox exist.

```
__init__ (coords_ll, coords_ur)
Constructor.
```

Parameters

- coords_11 (tuple) Tuple with coordinates of lower left corner
- coords_ur (tuple) Tuple with coordinates of uper right corner

```
__str__()
```

Returns Returns lower left and upper right coordinate of the bounding box

Return type str

containsPoint (point)

Check whether a point lies within a receiver.

Parameters point (tuple) – 1D/2D/3D position vector

Returns Returns True if point is inside receiver, otherwise False

Return type bool

intersects(bbox)

Check intersection of a receiver with a bounding box

Parameters bbox (BBox) – an instance of BBox class

Returns Returns True if receiver intersects given bounding box, otherwise False

Return type bool

merge (entity)

Merges receiver with given entity (position vector or a BBox).

Parameters

- entity (BBox) 1D/2D/3D position vector or
- entity an instance of BBox class

2.6 mupif.Cell module

```
class mupif.Cell.Brick_3d_lin (mesh, number, label, vertices)
    Bases: mupif.Cell.Cell
```

Unstructured 3d tetrahedral element with linear interpolation

```
oldsymbol{\_evalN}\left(lc
ight)
```

Evaluates shape functions at given point (given in parametric coordinates) :param tuple lc: A local coordinate :return: shape function :rtype: tuple of float

containsPoint (point)

Check if a cell contains a point.

Parameters point (tuple) - 1D/2D/3D position vector

Returns True if cell contains a given point

Return type bool

copy()

This will copy the receiver, making a deep copy of all atributes EXCEPT mesh attribute.

Returns A deep copy of a receiver

Return type Cell

classmethod getGeometryType()

Returns geometry type of receiver.

Returns Returns geometry type of receiver

Return type *CellGeometryType*

getTransformationJacobian (coords)

Returns the transformation jacobian (the determinant of jacobian) of the receiver

Parameters coords (tuple) - local (parametric) coordinates of the point

Returns jacobian

Return type float

glob2loc(coords)

Converts global coordinate to local (area) coordinate.

Parameters coords (tuple) - A coordinate in global system

Returns local (area) coordinate

Return type tuple

interpolate (point, vertexValues)

Interpolates given vertex values to a given point.

Parameters

- point (tuple) 1D/2D/3D position vector
- **vertexValues** (tuple) A tuple containing vertex values

Returns Interpolated value at a given point

Return type tuple

loc2glob(lc)

Converts local (parametric) coordinates to global ones

Parameters 1c (tuple) - A local coordinate

Returns global coordinate

Return type tuple

```
class mupif.Cell.Cell (mesh, number, label, vertices)
```

Bases: object

Representation of a computational cell.

The solution domain is composed of cells (e.g. finite element), whose geometry is defined using vertices (e.g. nodes). Cells provide interpolation over their associated volume, based on given vertex values. Derived classes will be implemented to support common interpolation cells (finite elements, FD stencils, etc.)

```
__init__ (mesh, number, label, vertices)
```

Initializes the cell.

Parameters

- mesh (Mesh. Mesh) The mesh to which a cell belongs to
- **number** (*int*) A local cell number. Local numbering should start from 0 and should be continuous.
- label (int) A cell label. Arbitrary unique number.
- **vertices** (tuple) A cell vertices (local numbers)

containsPoint (point)

Check if a cell contains a point.

Parameters point (tuple) – 1D/2D/3D position vector

Returns Returns True if cell contains a given point

Return type bool

copy()

This will copy the receiver, making a deep copy of all attributes EXCEPT a mesh attribute

Returns A deep copy of a receiver

Return type Cell

getBBox (relPad=1e-05)

Return bounding box. The box is by default slightly enlarged via *relPad* to avoid finite-precision issues when testing for a boundary point being inside the box.

Parameters relPad (float) – relative padding of the box; tight (geometrical) bbox will be enlarged along each axis by *relPad* times size along that axis, in both directions.

Returns Returns a bounding box of the receiver

Return type BBox

static getClassForCellGeometryType (cgt)

Return class object (not instance) for given cell geometry type. Does introspection of all subclasses of Cell caches the result.

classmethod getGeometryType()

Returns geometry type of receiver.

Returns Returns geometry type of receiver

Return type *CellGeometryType*

getNumberOfVertices()

Returns Number of vertices

Return type int

```
Returns the transformation jacobian (the determinant of jacobian) of the receiver
               Parameters coords (tuple) – local (parametric) coordinates of the point
               Returns jacobian
               Return type float
     getVertices()
               Returns The list of cell vertices
               Return type tuple
     interpolate (point, vertexValues)
          Interpolates given vertex values to a given point.
               Parameters
                   • point (tuple) – 1D/2D/3D position vector
                   • vertexValues (tuple) – A tuple containing vertex values
               Returns Interpolated value at a given point
               Return type tuple
class mupif.Cell.Quad_2d_lin (mesh, number, label, vertices)
     Bases: mupif.Cell.Cell
     Unstructured 2d quad element with linear interpolation
     containsPoint (point)
          Check if a cell contains a point.
               Parameters point (tuple) – 1D/2D/3D position vector
               Returns Returns True if cell contains a given point
               Return type bool
     copy()
          This will copy the receiver, making deep copy of all atributes EXCEPT mesh attribute.
               Returns A deep copy of a receiver
               Return type Cell
     classmethod getGeometryType()
          Returns geometry type of receiver.
               Returns Returns geometry type of receiver
               Return type CellGeometryType
     getTransformationJacobian (coords)
          Returns the transformation jacobian (the determinant of jacobian) of the receiver
               Parameters coords (tuple) – local (parametric) coordinates of the point
               Returns jacobian
               Return type float
     glob2loc (coords)
          Converts global coordinate to local (area) coordinate.
               Parameters coords (tuple) – A coordinate in global system
```

getTransformationJacobian (coords)

```
Returns local (area) coordinate
               Return type tuple
     interpolate (point, vertexValues)
          Interpolates given vertex values to a given point.
               Parameters
                   • point (tuple) – 1D/2D/3D position vector
                   • vertexValues (tuple) - A tuple containing vertex values
               Returns Interpolated value at a given point
               Return type tuple
     loc2glob(lc)
          Converts local (parametric) coordinates to global ones.
               Parameters 1c (tuple) - A local coordinate
               Returns global coordinate
               Return type tuple
class mupif.Cell.Tetrahedron_3d_lin (mesh, number, label, vertices)
     Bases: mupif.Cell.Cell
     Unstructured 3d tetrahedral element with linear interpolation.
     containsPoint(point)
          Check if a cell contains a point.
               Parameters point (tuple) - 1D/2D/3D position vector
               Returns Returns True if cell contains a given point
               Return type bool
     copy()
          This will copy the receiver, making a deep copy of all atributes EXCEPT mesh attribute.
               Returns A deep copy of a receiver
               Return type Cell
     classmethod getGeometryType()
          Returns geometry type of receiver.
               Returns Returns geometry type of receiver
               Return type CellGeometryType
     getTransformationJacobian (coords)
          Returns the transformation jacobian (the determinant of jacobian) of the receiver
               Parameters coords (tuple) - local (parametric) coordinates of the point
               Returns jacobian
               Return type float
     glob2loc (coords)
          Converts global coordinate to local (area) coordinate.
```

Parameters coords (tuple) - A coordinate in global system

Returns local (area) coordinate

Return type tuple

interpolate (point, vertexValues)

Interpolates given vertex values to a given point.

Parameters

- point (tuple) 1D/2D/3D position vector
- **vertexValues** (tuple) A tuple containing vertex values

Returns Interpolated value at a given point

Return type tuple

loc2glob(lc)

Converts local (parametric) coordinates to global ones

Parameters 1c (tuple) - A local coordinate

Returns global coordinate

Return type tuple

class mupif.Cell.Triangle_2d_lin (mesh, number, label, vertices)

Bases: mupif.Cell.Cell

Unstructured 2D triangular element with linear interpolation Node numbering convention:

2 | | | | 0 ---- 1

containsPoint (point)

Check if a cell contains a point.

Parameters point (tuple) – 1D/2D/3D position vector

Returns Returns True if cell contains a given point

Return type bool

copy()

This will copy the receiver, making a deep copy of all atributes EXCEPT mesh attribute.

Returns A deep copy of a receiver

Return type Cell

classmethod getGeometryType()

Returns geometry type of receiver.

Returns Returns geometry type of receiver

Return type *CellGeometryType*

getTransformationJacobian (coords)

Returns the transformation jacobian (the determinant of jacobian) of the receiver

Parameters coords (tuple) - local (parametric) coordinates of the point

Returns jacobian

Return type float

glob2loc (coords)

Converts global coordinate to local (area) coordinate.

Parameters coords (tuple) - A coordinate in global system

Returns local (area) coordinate

Return type tuple

interpolate (point, vertexValues)

Interpolates given vertex values to a given point.

Parameters

- point (tuple) 1D/2D/3D position vector
- **vertexValues** (tuple) A tuple containing vertex values

Returns Interpolated value at a given point

Return type tuple

loc2glob(lc)

Converts local (parametric) coordinates to global ones.

Parameters 1c (tuple) - A local coordinate

Returns global coordinate

Return type tuple

class mupif.Cell.Triangle_2d_quad (mesh, number, label, vertices)

Bases: mupif.Cell.Cell

Unstructured 2D triangular element with quadratic interpolation Node numbering convention:

2 | | 5 4 | | 0-3-1

containsPoint (point)

Check if a cell contains a point.

Parameters point (tuple) – 1D/2D/3D position vector

Returns Returns True if cell contains a given point

Return type bool

copy()

This will copy the receiver, making a deep copy of all atributes EXCEPT mesh attribute.

Returns A deep copy of a receiver

Return type Cell

classmethod getGeometryType()

Returns geometry type of receiver.

Returns Returns geometry type of receiver

Return type *CellGeometryType*

getTransformationJacobian (coords)

Returns the transformation jacobian (the determinant of jacobian) of the receiver

Parameters coords (tuple) - local (parametric) coordinates of the point

Returns jacobian

Return type float

glob2loc (coords)

Converts global coordinate to local (area) coordinate.

Parameters coords (tuple) - A coordinate in global system

Returns local (area) coordinate

Return type tuple

interpolate (point, vertexValues)

Interpolates given vertex values to a given point.

Parameters

- point (tuple) 1D/2D/3D position vector
- vertexValues (tuple) A tuple containing vertex values

Returns Interpolated value at a given point

Return type tuple

loc2glob(lc)

Converts local (parametric) coordinates to global ones.

Parameters 1c (tuple) - A local coordinate

Returns global coordinate

Return type tuple

2.7 mupif.CellGeometryType module

Enumeration defining the supported cell geometries

2.8 mupif.EnsightReader2 module

mupif.EnsightReader2.readEnsightField (name, parts, partRec, type, fieldID, mesh, units, time)
Reads either Per-node or Per-element variable file and returns corresponding Field representation.

Parameters

- name (str) Input field name with variable data
- parts (tuple) Only parts with id contained in partFiler will be imported
- partRec (list) A list containing info about individual parts (number of elements per each element type).
- type (int) Determines type of field values: type = 1 scalar, type = 3 vector, type = 6 tensor
- **fieldID** (FieldID) Field type (displacement, strain, temperature ...)
- mesh (Mesh.Mesh) Corresponding mesh
- units (PhysicalUnit) field units
- time (Physical Quantity) time

Returns FieldID for unknowns

Return type Field

mupif.EnsightReader2.readEnsightGeo(name, partFilter, partRec)

Reads Ensight geometry file (Ensight6 format) and returns corresponding Mesh object instance. Supports only unstructured meshes.

Parameters

- name (str) Path to Ensight geometry file (*.geo)
- partFilter (tuple) Only parts with id contained in partFiler will be imported
- partRec (list) A list containing info about individual parts (number of elements). Needed by readEnsightField

Returns mesh

Return type Mesh.Mesh

mupif.EnsightReader2.readEnsightGeo_Part (f, line, mesh, enum, cells, vertexMapping, partnum, partdesc, partRec)

Reads single cell part geometry from an Ensight file.

Parameters

- f (File) File object
- **line** (str) Current line to process (should contain element type)
- mesh (Mesh.Mesh) Mupif mesh object to accommodate new cells
- enum (int) Accumulated cell number
- **cells** (*list*) List of individual Cells
- vertexMapping (dict) Map from vertex label (as given in Ensight file) to local number
- partnum (int) Part number
- partdesc (list) Partition description record
- partRec (list) Output agrument (list) containing info about individual parts (number of elements). Needed by readEnsightField

Returns tuple (line, cell number)

Return type tuple (line, enum)

2.9 mupif.Field module

Representation of field. Field is a scalar, vector, or tensorial quantity defined on a spatial domain. The field, however is assumed to be fixed at certain time. The field can be evaluated in any spatial point belonging to underlying domain.

Derived classes will implement fields defined on common discretizations, like fields defined on structured/unstructured FE meshes, FD grids, etc.

Parameters

- mesh (Mesh. Mesh) Instance of a Mesh class representing the underlying discretization
- **fieldID** (FieldID) Field type (displacement, strain, temperature ...)

- **valueType** (ValueType) Type of field values (scalar, vector, tensor). Tensor is a tuple of 9 values. It is changed to 3x3 for VTK output automatically.
- units (Physics.PhysicalUnits) Field value units
- time (Physics.PhysicalQuantity) Time associated with field values
- **values** (list of tuples representing individual values) Field values (format dependent on a particular field type, however each individual value should be stored as tuple, even scalar value)
- **fieldType** (FieldType) Optional, determines field type (values specified as vertex or cell values), default is FT_vertexBased
- objectID (int) Optional ID of problem object/subdomain to which field is related, default = 0

_evaluate(position, eps)

Evaluates the receiver at a single spatial position.

Parameters

- position (tuple) 1D/2D/3D position vector
- **eps** (*float*) Optional tolerance

Returns field value

Return type tuple of doubles

Note: This method has some issues related to https://sourceforge.net/p/mupif/tickets/22/.

commit()

Commits the recorded changes (via setValue method) to a primary field.

dumpToLocalFile (fileName, protocol=4)

Dump Field to a file using a Pickle serialization module.

Parameters

- **fileName** (str) File name
- protocol (int) Used protocol 0=ASCII, 1=old binary, 2=new binary

evaluate (positions, eps=0.0)

Evaluates the receiver at given spatial position(s).

Parameters

- positions (tuple, a list of tuples) 1D/2D/3D position vectors
- **eps** (float) Optional tolerance for probing whether the point belongs to a cell (should really not be used)

Returns field value(s)

Return type Physics. Physical Quantity with given value or tuple of values

field2Image2D (plane='xy', elevation=(-1e-06, 1e-06), numX=10, numY=20, interp='linear', fieldComponent=0, vertex=True, colorBar='horizontal', colorBarLegend=", bar-Range=(None, None), barFormatNum='%.3g', title=", xlabel=", ylabel=", file-Name=", show=True, figsize=(8, 4), matPlotFig=None)

Plots and/or saves 2D image using a matplotlib library. Works for structured and unstructured 2D/3D fields. 2D/3D fields need to define plane. This method gives only basic viewing options, for aesthetic and

more elaborated output use e.g. VTK field export with postprocessors such as ParaView or Mayavi. Idea from https://docs.scipy.org/doc/scipy/reference/tutorial/interpolate.html#id1

Parameters

- plane (str) what plane to extract from field, valid values are 'xy', 'xz', 'yz'
- **elevation** (tuple) range of third coordinate. For example, in plane='xy' is grabs z coordinates in the range
- numX (int) number of divisions on x graph axis
- numY (int) number of divisions on y graph axis
- interp (str) interpolation type when transferring to a grid. Valid values 'linear', 'nearest' or 'cubic'
- **fieldComponent** (*int*) component of the field
- **vertex** (bool) if vertices should be plot as points
- colorBar (str) color bar details. Valid values "for no colorbar, 'vertical' or 'horizontal'
- **colorBarLegend** (*str*) Legend for color bar. If '', current field name and units are printed. None prints nothing.
- barRange (tuple) min and max bar range. If barRange=('NaN','NaN'), it is adjusted automatically
- barFormatNum (str) format of color bar numbers
- title (str) title
- xlabel (str) x axis label
- ylabel (str) y axis label
- **fileName** (str) if nonempty, a filename is written to the disk, usually png, pdf, ps, eps and svg are supported
- **show** (bool) if the plot should be showed
- **figsize** (tuple) size of canvas in inches. Affects only showing a figure. Image to a file adjust one side automatically.
- matPlotFig (obj) False means plot window remains in separate thread, True waits until a plot window becomes closed

Returns handle to matPlotFig

Return type matPlotFig

field2Image2DBlock()

Block an open window from matPlotLib. Waits until closed.

${\tt field2VTKData}~(name = None, lookupTable = None)$

Creates VTK representation of the receiver. Useful for visualization. Requires pyvtk module.

Parameters

- name (str) human-readable name of the field
- lookupTable (pyvtk.LookupTable) color lookup table

Returns Instance of pyvtk

Return type pyvtk.VtkData

```
getCellValue (cellID)
     Returns the value associated with a given cell.
         Parameters cellID (int) - Cell identifier
         Returns The value
         Return type Physics.PhysicalQuantity
getFieldID()
     Returns FieldID, e.g. FID_Displacement, FID_Temperature.
         Returns Returns field ID
         Return type FieldID
getFieldIDName()
     Returns name of the field.
         Returns Returns fieldID name
         Return type string
getFieldType()
     Returns receiver field type (values specified as vertex or cell values)
         Returns Returns fieldType id
         Return type FieldType
getMartixForTensor(values)
     Reshape values to a list with 3x3 arrays. Usable for VTK export.
         Parameters values (list) – List containing tuples of 9 values, e.g. [(1,2,3,4,5,6,7,8,9),
             (1,2,3,4,5,6,7,8,9),\ldots
         Returns List containing 3x3 matrices for each tensor
         Return type list
getMesh()
     Obtain mesh.
         Returns Returns a mesh of underlying discretization
         Return type Mesh.Mesh
getObjectID()
     Returns field objectID.
         Returns Object's ID
         Return type int
getRecordSize()
     Return the number of scalars per value, depending on valueType passed when constructing the instance.
         Returns number of scalars (1,3,9 respectively for scalar, vector, tensor)
         Return type int
getTime()
     Get time of the field.
         Returns Time of field data
         Return type Physics. Physical Quantity
```

getUnits()

Returns Returns units of the receiver

Return type Physics.PhysicalUnits

getValueType()

Returns ValueType of the field, e.g. scalar, vector, tensor.

Returns Returns value type of the receiver

Return type ValueType

getVertexValue (vertexID)

Returns the value associated with a given vertex.

Parameters vertexID (int) - Vertex identifier

Returns The value

Return type Physics.PhysicalQuantity

giveValue (componentID)

Returns the value associated with a given component (vertex or cell).

Parameters componentID (int) - An identifier of a component: vertexID or cellID

Returns The value

Return type tuple

inUnitsOf (*units)

Should return a new instance. As deep copy is expensive, this operation should be avoided. Better to use convertToUnits method performing in place conversion.

classmethod loadFromLocalFile (fileName)

Alternative constructor which loads instance directly from a Pickle module.

Parameters fileName (str) - File name

Returns Field instance

Return type Field

static makeFromHdf5 (fileName, group='component1/part1')

Restore Fields from HDF5 file.

Parameters

- **fileName** (str) HDF5 file
- **group** (str) HDF5 group the data will be read from (IOError is raised if the group does not exist).

Returns list of new Field instances

Return type [Field,Field,...]

Note: This method has not been tested yet.

static makeFromVTK2 (fileName, unit, time=0, skip=['coolwarm'])

Return fields stored in *fileName* in the VTK2 (.vtk) format.

Parameters

• **fileName** (str) – filename to load from

- unit (PhysicalUnit) physical unit of filed values
- **time** (*float*) time value for created fields (time is not saved in VTK2, thus cannot be recovered)
- **skip** ([string,]) file names to be skipped when reading the input file; the default value skips the default coolwarm colormap.

Returns one field from VTK

Return type Field

static makeFromVTK3 (fileName, units, time=0, forceVersion2=False)

Create fields from a VTK unstructured grid file (.vtu, format version 3, or .vtp with *forceVersion2*); the mesh is shared between fields.

vtk.vtkXMLGenericDataObjectReader is used to open the file (unless *forceVersion2* is set), but it is checked that contained dataset is a vtk.vtkUnstructuredGrid and an error is raised if not.

Note: Units are not supported when loading from VTK, all fields will have None unit assigned.

Parameters

- fileName (str) VTK (*.vtu) file
- units (PhysicalUnit) units of read values
- **time** (*float*) time value for created fields (time is not saved in VTK3, thus cannot be recovered)
- forceVersion2 (bool) if True, vtk.vtkGenericDataObjectReader (for VTK version 2) will be used to open the file, isntead of vtk. vtkXMLGenericDataObjectReader; this also supposes fileName ends with .vtk (not checked, but may cause an error).

Returns list of new Field instances

Return type [Field,Field,..]

static manyToVTK3 (fields, fileName, ascii=False, compress=True)

Save all fields passed as argument into VTK3 Unstructured Grid file (*.vtu).

All *fields* must be defined on the same mesh object; exception will be raised if this is not the case.

Parameters

- of Field fields (list) -
- **fileName** output file name
- ascii(bool) write numbers are ASCII in the XML-based VTU file (rather than base64-encoded binary in XML)
- compress (bool) apply compression to the data

merge (field)

Merges the receiver with given field together. Both fields should be on different parts of the domain (can also overlap), but should refer to same underlying discretization, otherwise unpredictable results can occur.

Parameters field (Field) – given field to merge with.

$\verb"setValue" (component ID, value")$

Sets the value associated with a given component (vertex or cell).

Parameters

- component ID (int) An identifier of a component: vertexID or cellID
- **value** (tuple) Value to be set for a given component, should have the same units as receiver

Note: If a mesh has mapping attached (a mesh view) then we have to remember value locally and record change. The source field values are updated after commit() method is invoked.

toHdf5 (fileName, group='component1/part1')

Dump field to HDF5, in a simple format suitable for interoperability (TODO: document).

Parameters

- fileName (str) HDF5 file
- **group** (str) HDF5 group the data will be saved under.

The HDF hierarchy is like this:

```
group
  +--- mesh_01 {hash=25aa0aa04457}
       +--- [vertex_coords]
        +--- [cell_types]
        \--- [cell_vertices]
  +--- mesh_02 {hash=17809e2b86ea}
        +--- [vertex_coords]
        +--- [cell_types]
        \--- [cell_vertices]
  +--- field_01
        +--- -> mesh_01
        \--- [vertex_values]
  +--- field_02
        +--- -> mesh_01
        \--- [vertex_values]
  +--- field 03
        +--- -> mesh_02
        \--- [cell_values]
```

where plain names are HDF (sub)groups, [bracketed] names are datasets, {name=value} are HDF attributes, -> prefix indicated HDF5 hardlink (transparent to the user); numerical suffixes (_01, ...) are auto-allocated. Mesh objects are hardlinked using HDF5 hardlinks if an identical mesh is already stored in the group, based on hexdigest of its full data.

Note: This method has not been tested yet. The format is subject to future changes.

```
toVTK2 (fileName, format='ascii')
```

Save the instance as Unstructured Grid in VTK2 format (.vtk).

Parameters

- **fileName** (str) where to save
- **format** (str) one of ascii or binary

```
toVTK3 (fileName, **kw)
```

Save the instance as Unstructured Grid in VTK3 format (.vtu). This is a simple proxy for calling manyToVTK3 with the instance as the only field to be saved. If multiple fields with identical mesh are to be saved in VTK3, use manyToVTK3 directly.

Parameters

- fileName output file name
- **kw passed to manyToVTK3

class mupif.Field.FieldType

Bases: enum. IntEnum

Represent the supported values of FieldType, i.e. FT_vertexBased or FT_cellBased.

```
FT_cellBased = 2
FT_vertexBased = 1
```

2.10 mupif.Function module

```
class mupif.Function.Function (funcID, objectID=0)
```

Bases: object

Represents a function.

Usage of class Function for data transfers between codes as with Field or Property is deprecated. It is not supposed for data transfers any more, thus becomes an auxiliary class.

Function is an object defined by mathematical expression. Function can depend on spatial position and time. Derived classes should implement evaluate service by providing a corresponding expression.

```
Example: f(x,t)=\sin(2*3.14159265*x(1)/10.)
```

```
__init__ (funcID, objectID=0)
```

Initializes the function.

Parameters

- funcID (FunctionID) function ID, e.g. FuncID_ProbabilityDistribution
- objectID (int) Optional ID of associated subdomain, default 0

evaluate (d)

Evaluates the function for given parameters packed as a dictionary.

A dictionary is container type that can store any number of Python objects, including other container types. Dictionaries consist of pairs (called items) of keys and their corresponding values.

Example: $d=\{'x':(1,2,3), 't':0.005\}$ initializes dictionary containing tuple (vector) under 'x' key, double value 0.005 under 't' key. Some common keys: 'x': position vector 't': time

Parameters d (dictionary) – Dictionaty containing function arguments (number and type depends on particular function)

Returns Function value evaluated at given position and time

Return type int, float, tuple

getID()

Obtain function's ID.

Returns Returns receiver's ID.

Return type int

getObjectID()

Get optional ID of associated subdomain.

Returns Returns receiver's object ID,

Return type int

2.11 mupif.IntegrationRule module

```
class mupif.IntegrationRule.GaussIntegrationRule
    Bases: mupif.IntegrationRule.IntegrationRule
```

Gauss integration rule.

```
getIntegrationPoints(cgt, npt)
```

See IntegrationRule.getIntegrationPoints().

getRequiredNumberOfPoints(cgt, order)

See IntegrationRule.getRequiredNumberOfPoints().

class mupif.IntegrationRule.IntegrationRule

Bases: object

Represent integration rule to be used on cells.

```
___init___()
```

getIntegrationPoints(cgt, npt)

Returns a list of integration points and corresponding weights.

Parameters

- cgt (CellGeometryType) Type of underlying cell geometry (e.g. linear triangle CGT_TRIANGLE_1)
- **npt** (*int*) Number of desired integration points

Returns A list of tuples containing natural coordinates of integration point and weights, i.e. [((c1_ksi, c1_eta), weight1), ((c2_ksi, c2_eta), weight2)]

Return type a list of tuples

getRequiredNumberOfPoints (cgt, order)

Returns required number of integration points to exactly integrate polynomial of order approxOrder on a given cell type.

Parameters

- cgt (CellGeometryType) Type of underlying cell geometry (e.g. linear triangle CGT_TRIANGLE_1)
- order (int) Target polynomial order

2.12 mupif.JobManager module

exception mupif.JobManager.JobManException

Bases: Exception

This class serves as a base class for exceptions thrown by the job manager.

exception mupif.JobManager.JobManNoResourcesException

Bases: mupif.JobManager.JobManException

This class is thrown when there are no more available resources.

class mupif.JobManager(appName, jobManWorkDir, maxJobs=1)

Bases: object

An abstract (base) class representing a job manager. The purpose of the job manager is the following:

- To allocate and register the new instance of application (called job)
- To query the status of job
- To cancel the given job
- To register its interface to pyro name server

```
__init__(appName, jobManWorkDir, maxJobs=1)
```

Constructor. Initializes the receiver.

Parameters

- appName (str) Name of receiver (used also by NS)
- jobManWorkDir (str) Absolute path for storing data, if necessary
- maxJobs (int) Maximum number of jobs to run simultaneously

allocateJob (user, natPort)

Allocates a new job.

Parameters

- user(str) user name
- natPort (int) NAT port used in ssh tunnel

Returns tuple (error code, None). errCode = (JOBMAN_OK, JOBMAN_ERR, JOBMAN_NO_RESOURCES). JOBMAN_OK indicates successfull allocation and JobID contains the PYRO name, under which the new instance is registered (composed of application name and a job number (allocated by jobmanager), ie, Miccress23). JOBMAN_ERR indicates an internal error, JOBMAN_NO_RESOURCES means that job manager is not able to allocate new instance of application (no more recources available)

Return type tuple

Except JobManException when allocation of new job failed

```
getJobStatus (jobID)
```

Returns the status of the job.

```
Parameters jobID (str) - jobID
```

```
getJobWorkDir(jobID)
```

Returns working directory of a job with given ID.

```
Parameters jobID (str) -
```

Returns job working directory

Return type str

getNSName()

getPyroFile (jobID, filename, buffSize=1024)

Returns the (remote) PyroFile representation of given file. To create local copy of file represented by PyroFile, use PyroUtil.downloadPyroFile, see PyroUtil.downloadPyroFile()

Parameters

- jobID (str) job identifier (jobID)
- **filename** (str) source file name (on remote server). The filename should contain only base filename, not a path, which is determined by jobManager based on jobID.
- buffSize (int) -

Returns PyroFile representation of given file

Return type PyroFile

getStatus()

registerPyro (daemon, ns, uri, appName, externalDaemon)

Possibility to register the Pyro daemon and nameserver.

Parameters

- daemon (Pyro4. Daemon) Optional pyro daemon
- ns (Pyro4.naming.Nameserver) Optional nameserver
- uri (string) Optional URI of receiver
- appName (string) -
- externalDaemon (bool) Optional parameter when damon was allocated externally.

terminate()

Terminates job manager itself.

terminateJob(jobID)

Terminates the given job, frees the associated recources.

```
Parameters jobID (str) - jobID
```

Returns JOBMAN_OK indicates successfull termination, JOBMAN_ERR means internal error

Return type str

uploadFile (jobID, filename, pyroFile, hkey)

Uploads the given file to application server, files are uploaded to dedicated jobID directory :param str jobID: jobID :param str filename: target file name :param PyroFile pyroFile: source pyroFile :param str hkey: A password string

class mupif.JobManager.RemoteJobManager(decoratee, sshTunnel=None)

Bases: object

Remote jobManager instances are normally represented by auto generated pyro proxy. However, when ssh tunneled connection is established to connect to remote job manager, its instance must be properly terminated. This class is a decorator around pyro proxy object represeting jobManager storing the reference to the ssh tunnel established. Note in case of VPN or direct (plain) connection, the plain Pyro proxy should be used.

The attribute could not be injected into remote instance (using proxy) as the termination has to be done from local computer, where the ssh tunnel has been created. Also different connections (proxies) to the same jobManager can exist.

terminate()

Terminates the application. Terminates the allocated job at jobManager

2.13 mupif.Localizer module

```
class mupif.Localizer.Localizer
     Bases: object
     A Localizer is an abstract class representing an algorithm used to partition space and quicly localize the con-
     tained objects.
     delete(item)
           Deletes the given object from Localizer data structure.
               Parameters item (object) - Object to be removed
     evaluate (functor)
           Returns the list of all objects for which the functor is satisfied.
               Parameters functor (object) – The functor is a class which defines two methods: giveB-
                   Box() which returns an initial functor bbox and evaluate(obj) which should return True if the
                   functor is satisfied for a given object.
               Returns List of all objects
               Return type tuple
     giveItemsInBBox(bbox)
               Parameters bbox (BBox) – Bounding box
               Returns List of all objects which bbox contains and intersects
               Return type tuple
     insert (item)
```

Inserts given object to Localizer. Object is assume to provide giveBBox() method returning bounding

Parameters item (object) - Inserted object

2.14 mupif.MDict module

volume if itself.

```
class mupif.MDict.MValType(type, compulsory)
    Bases: object
    compare(MDTemplate1, MD1)
    flattenDict(init, lkey=")
    validate()
```

2.15 mupif.Mesh module

```
class mupif.Mesh.Mesh
     Bases: object
```

Abstract representation of a computational domain. Mesh contains computational cells and vertices. Derived classes represent structured, unstructured FE grids, FV grids, etc.

Mesh is assumed to provide a suitable instance of cell and vertex localizers.

```
___init___()
```

asHdf5Object (parentgroup, newgroup)

Return the instance as HDF5 object. Complementary to makeFromHdf5Object which will restore the instance from that data.

asVtkUnstructuredGrid()

Return object as a vtk.vtkUnstructuredMesh instance.

Note: This method uses the compiled vtk module (which is a wrapper atop the c++ VTK library) – in contrast to *UnstructuredMesh.getVTKRepresentation*, which uses the pyvtk module (pythononly implementation of VTK i/o supporting only VTK File Format version 2).

cellLabel2Number (label)

Returns local cell number corresponding to given label. If no label found, throws an exception.

Parameters label (str) - Cell label

Returns Cell number

Return type int

Except Label not found

cells()

Iterator over cells.

Returns Iterator over cells

Return type *MeshIterator*

copy()

Returns a copy of the receiver.

Returns A copy of the receiver

Return type Copy of the receiver, e.g. Mesh

Note: DeepCopy will not work, as individual cells contain mesh link attributes, leading to underlying mesh duplication in every cell!

dumpToLocalFile (fileName, protocol=4)

Dump Mesh to a file using a Pickle serialization module.

Parameters

- **fileName** (str) File name
- protocol (int) Used protocol 0=ASCII, 1=old binary, 2=new binary

getCell(i)

Returns i-th cell.

Parameters i (int) - i-th cell

Returns cell

Return type Cell

getCells()

Return all cells as 2x numpy.array; each i-th row contains vertex indices for i-th cell. Does in 2 passes, first to determine maximum number of vertices per cell (to shape the field accordingly). For cells with less vertices than the maximum, excess ones are assigned the invalid value of -1.

```
Returns (cell_types,cell_vertices)
```

Return type (numpy.array,numpy.array)

Note: This method has not been tested yet.

getMapping()

Get mesh mapping.

Returns The mapping associated to a mesh

Return type defined by API

getNumberOfCells()

Return number of cells (finite elements).

Returns The number of Cells

Return type int

qetNumberOfVertices()

Get number of vertices (nodes).

Returns Number of Vertices

Return type int

getVertex(i)

Returns i-th vertex.

Parameters i (int) – i-th vertex

Returns vertex

Return type Vertex

getVertices()

Return all vertex coordinates as 2D (Nx3) numpy.array; each i-th row contains 3d coordinates of the i-th vertex.

Returns vertices

Return type numpy.array

Note: This method has not been tested yet.

internalArraysDigest()

Internal function returning hash digest of all internal data, for the purposes of identity test.

classmethod loadFromLocalFile (fileName)

Alternative constructor which loads an instance from a Pickle module.

Parameters fileName (str) – File name

Returns Returns Mesh instance

Return type Mesh

static makeFromHdf5Object(h5obj)

Create new Mesh instance from given hdf5 object. Complementary to asHdf50bject.

Returns new instance

```
Return type Mesh or its subclass
     vertexLabel2Number (label)
          Returns local vertex number corresponding to given label. If no label found, throws an exception.
               Parameters label (str) – Vertex label
               Returns Vertex number
               Return type int
               Except Label not found
     vertices()
          Iterator over vertices.
               Returns Iterator over vertices
               Return type MeshIterator
class mupif.Mesh.MeshIterator(mesh, type)
     Bases: object
     Class implementing iterator on Mesh components (vertices, cells).
     ___init___(mesh, type)
          Constructor.
               Parameters
                   • mesh (Mesh) - Given mesh
                   • type (str) - Type of mesh, e.g. VERTICES or CELLS
     __iter__()
               Returns Itself
               Return type MeshIterator
     __next__()
               Returns Returns next Mesh components.
               Return type MeshIterator
class mupif.Mesh.UnstructuredMesh
     Bases: mupif.Mesh.Mesh
     Represents unstructured mesh. Maintains the list of vertices and cells.
     The class contains:
        • vertexList: list of vertices
        • cellList: list of interpolation cells
        • vertexOctree: vertex spatial localizer
        • cellOctree: cell spatial localizer

    vertexDict: vertex dictionary

        • cellDict: cell dictionary
       _init___()
          Constructor.
```

```
buildVertexLabelMap ()
    Create a custom dictionary between vertex's label and Vertex instance.
__buildCellLabelMap__()
    Create a custom dictionary between cell's label and Cell instance.
cellLabel2Number (label)
    See Mesh.cellLabel2Number()
copy()
    See Mesh.copy()
getCell(i)
    See Mesh.getCell()
getNumberOfCells()
    See Mesh.getNumberOfCells()
getNumberOfVertices()
    See Mesh.getNumberOfVertices()
getVTKRepresentation()
    Get VTK representatnion of the mesh.
    return: VTK representation of the receiver. Requires pyvtk module. :rtype: pyvtk.UnstructuredGrid
getVertex(i)
    See Mesh.getVertex()
giveCellLocalizer()
    Get the cell localizer.
        Returns Returns the cell localizer.
        Return type Octree
giveVertexLocalizer()
        Returns Returns the vertex localizer.
        Return type Octree
static makeFromPvvtkUnstructuredGrid(ugr)
    Create a new instance of UnstructuredMesh based on pyvtk.UnstructuredGrid object. Cell types are
    mapped between pyvtk and mupif (supported: triangle, tetra, quad, hexahedron).
        Parameters ugr – instance of pyvtk.UnstructuredGrid
        Returns new instance of UnstructuredMesh
static makeFromVtkUnstructuredGrid(ugrid)
    Create a new instance of UnstructuredMesh based on VTK's unstructured grid object. Cell types
    are mapped between VTK and mupif (supported: vtkTriangle, vtkQuadraticTriangle, vtkQuad, vtkTetra,
    vtkHexahedron).
```

Parameters ugrid - instance of vtk.vtkUnstructuredGrid

Returns new instance of UnstructuredMesh

merge (mesh)

Merges receiver with a given mesh. This is based on merging mesh entities (vertices, cells) based on their labels, as they refer to global IDs of each entity, that should be unique.

The procedure used here is based on creating a dictionary for every component from both meshes, where the key is component label so that the entities with the same ID could be easily identified.

```
Parameters mesh (Mesh) - Source mesh for merging
```

```
setup (vertexList, cellList)
```

Initializes the receicer according to given vertex and cell lists.

Parameters

- **vertexList** (tuple) A tuple of vertices
- cellList (tuple) A tuple of cells

```
vertexLabel2Number (label)
```

See Mesh.vertexLabel2Number()

2.16 mupif.MetadataKeys module

Definition of common metadata keys

2.17 mupif.Model module

```
class mupif.Model.Model(metaData={})
    Bases: mupif.MupifObject.MupifObject
```

An abstract class representing an application and its interface (API).

The purpose of this class is to define abstract services for data exchange and steering. This interface has to be implemented/provided by any application. The data exchange is performed by the means of new data types introduced in the framework, namely properties and fields. New abstract data types (properties, fields) allow to hide all implementation details related to discretization and data storage.

```
___init___(metaData={})
```

Constructor. Initializes the application.

Parameters metaData (dict) – Optionally pass metadata.

finishStep(tstep)

Called after a global convergence within a time step is achieved.

```
Parameters tstep (TimeStep. TimeStep) - Solution step
```

```
get (objectTypeID, time=None, objectID=0)
```

Returns the requested object at given time. Object is identified by id.

Parameters

- or FieldID or FunctionID objectTypeID (PropertyID) Identifier of the object
- time (Physics.PhysicalQuantity) Target time
- objectID (int) Identifies object with objectID (optional, default 0)

Returns Returns requested object.

```
getAPIVersion()
```

Returns Returns the supported API version

Return type str, int

getApplicationSignature()

Get application signature.

Returns Returns the application identification

Return type str

getAssemblyTime (tstep)

Returns the assembly time related to given time step. The registered fields (inputs) should be evaluated in this time.

Parameters tstep (TimeStep. TimeStep) - Solution step

Returns Assembly time

Return type Physics. Physical Quantity, TimeStep. TimeStep

getCriticalTimeStep()

Returns a critical time step for an application.

Returns Returns the actual (related to current state) critical time step increment

Return type Physics.PhysicalQuantity

getField (fieldID, time, objectID=0)

Returns the requested field at given time. Field is identified by fieldID.

Parameters

- fieldID (FieldID) Identifier of the field
- time (Physics.PhysicalQuantity) Target time
- **objectID** (*int*) Identifies field with objectID (optional, default 0)

Returns Returns requested field.

Return type Field

getFieldURI (fieldID, time, objectID=0)

Returns the uri of requested field at given time. Field is identified by fieldID.

Parameters

- fieldID (FieldID) Identifier of the field
- time (Physics.PhysicalQuantity) Target time
- objectID (int) Identifies field with objectID (optional, default 0)

Returns Requested field uri

Return type Pyro4.core.URI

getFunction (funcID, time, objectID=0)

Returns function identified by its ID

Parameters

- funcID (FunctionID) function ID
- time (Physics. Physical Quantity) Time when function should to be evaluated
- **objectID** (*int*) Identifies optional object/submesh on which property is evaluated (optional, default 0)

Returns Returns requested function

Return type Function

getMesh (tstep)

Returns the computational mesh for given solution step.

Parameters tstep (TimeStep. TimeStep) - Solution step

Returns Returns the representation of mesh

Return type Mesh

getProperty (propID, time, objectID=0)

Returns property identified by its ID evaluated at given time.

Parameters

- propID (PropertyID) property ID
- time (Physics. Physical Quantity) Time when property should to be evaluated
- **objectID** (*int*) Identifies object/submesh on which property is evaluated (optional, default 0)

Returns Returns representation of requested property

Return type *Property*

getURI()

Returns Returns the application URI or None if application not registered in Pyro

Return type str

 $\verb|initialize| (file=", workdir=", metaData={}\}, validateMetaData=True, **kwargs)|$

Initializes application, i.e. all functions after constructor and before run.

Parameters

- **file** (str) Name of file
- workdir (str) Optional parameter for working directory
- **metaData** (*dict*) Optional dictionary used to set up metadata (can be also set by setMetadata()).
- validateMetaData (bool) Defines if the metadata validation will be called
- kwargs (named_arguments) Arbitrary further parameters

isSolved()

Check whether solve has completed.

Returns Returns true or false depending whether solve has completed when executed in background.

Return type bool

printMetadata(nonEmpty=False)

Print all metadata :param bool nonEmpty: Optionally print only non-empty values :return: None :rtype: None

 $\verb"registerPyro" (pyroDaemon, pyroNS, pyroURI, appName=None, externalDaemon=False)$

Register the Pyro daemon and nameserver. Required by several services

- pyroDaemon (Pyro4.Daemon) Optional pyro daemon
- pyroNS (Pyro4.naming.Nameserver) Optional nameserver

- pyroURI (string) Optional URI of receiver
- appName (string) Optional application name. Used for removing from pyroNS
- **externalDaemon** (bool) Optional parameter when daemon was allocated externally.

removeApp (nameServer=None, appName=None)

Removes (unregisters) application from the name server.

Parameters

- nameServer (Pyro4.naming.Nameserver) Optional instance of a nameServer
- appName (str) Optional name of the application to be removed

restoreState (tstep)

Restore the saved state of an application. :param TimeStep.TimeStep tstep: Solution step

set (obj, objectID=0)

Registers the given (remote) object in application.

Parameters

- or Field.Field or Function.Function obj (Property.Property) Remote object to be registered by the application
- objectID (int) Identifies object with objectID (optional, default 0)

setField (field, objectID=0)

Registers the given (remote) field in application.

Parameters

- **field** (Field.Field) Remote field to be registered by the application
- **objectID** (*int*) Identifies field with objectID (optional, default 0)

setFunction (func, objectID=0)

Register given function in the application.

Parameters

- func (Function.Function) Function to register
- **objectID** (*int*) Identifies optional object/submesh on which property is evaluated (optional, default 0)

setProperty (property, objectID=0)

Register given property in the application

Parameters

- property (Property. Property) Setting property
- **objectID** (*int*) Identifies object/submesh on which property is evaluated (optional, default 0)

$\verb|solveStep| (\textit{tstep}, \textit{stageID} = 0, \textit{runInBackground} = \textit{False})|$

Solves the problem for given time step.

Proceeds the solution from actual state to given time. The actual state should not be updated at the end, as this method could be called multiple times for the same solution step until the global convergence is reached. When global convergence is reached, finishStep is called and then the actual state has to be updated. Solution can be split into individual stages identified by optional stageID parameter. In between the stages the additional data exchange can be performed. See also wait and isSolved services.

- tstep (TimeStep. TimeStep) Solution step
- **stageID** (*int*) optional argument identifying solution stage (default 0)
- **runInBackground** (bool) optional argument, defualt False. If True, the solution will run in background (in separate thread or remotely).

storeState (tstep)

Store the solution state of an application.

```
Parameters tstep (TimeStep. TimeStep) - Solution step
```

terminate()

Terminates the application. Shutdowns daemons if created internally.

wait()

Wait until solve is completed when executed in background.

```
class mupif.Model.RemoteModel(decoratee, jobMan=None, jobID=None, appTunnel=None)
    Bases: object
```

Remote Application instances are normally represented by auto generated pyro proxy. However, when application is allocated using JobManager or ssh tunnel, the proper termination of the tunnel or job manager task is required.

This class is a decorator around pyro proxy object represeting application storing the reference to job manager and related jobID or/and ssh tunnel.

These external attributes could not be injected into Application instance, as it is remote instance (using proxy) and the termination of job and tunnel has to be done from local computer, which has the neccesary communication link established (ssh tunnel in particular, when port translation takes place)

```
getJobID()
```

terminate()

Terminates the application. Terminates the allocated job at jobManager

2.18 mupif.MupifObject module

```
class mupif.MupifObject.MupifObject(jsonFileName=")
    Bases: object
```

An abstract class representing a base Mupif object.

The purpose of this class is to represent any mupif object; it introduce basic methods for getting and setting object metatdata.

```
__init__(jsonFileName=")
```

Constructor. Initializes the object :param str jsonFileName: Optionally instantiate from JSON file

getAllMetadata()

Return type dict

```
getMetadata(key)
```

Returns metadata associated to given key :param key: unique metadataID :return: metadata associated to key, throws TypeError if key does not exist :raises: TypeError

```
{\tt hasMetadata}\ (\textit{key})
```

Returns true if key defined :param key: unique metadataID :return: true if key defined, false otherwise :rtype: bool

printMetadata (nonEmpty=False)

Print all metadata :param bool nonEmpty: Optionally print only non-empty values :return: None :rtype: None

setMetadata(key, val)

Sets metadata associated to given key :param str key: unique metadataID :param val: any type

toJSON (indent=4)

By default, the JSON encoder only understands native Python data types (str, int, float, bool, list, tuple, and dict). Other classes need JSON serialization method :return: string

toJSONFile (filename, indent=4)

updateMetadata (dictionary)

Updates metadata's dictionary with a given dictionary :param dict dictionary: Dictionary of metadata

validateMetadata(template)

Validates metadata's dictionary with a given dictionary :param dict template: Schema for json template

2.19 mupif.Octree module

```
class mupif.Octree.Octant (octree, parent, origin, size)
    Bases: object
```

Defines Octree Octant: a cell containing either terminal data or its child octants. Octree is used to partition space by recursively subdividing the root cell (square or cube) into octants. Octants can be terminal (containing the data) or can be further subdivided into children octants. Each terminal octant contains the objects with bounding box within the octant.

```
__init__ (octree, parent, origin, size)
```

The contructor. Octant class contains:

- data: Container storing the indexed objects (cells, vertices, etc)
- children: Container storing the children octants (if not terminal).
- octree: Link to octree object
- parent: Link to parent Octant
- origin: Coordinates of Octant lower left corner
- size: Dimension of Octant

Parameters

- octree (Octree) Link to octree object
- parent (Octree) Link to parent Octant
- origin (tuple) coordinates of octant lower left corner
- **size** (*float*) Size (dimension) of receiver

childrenIJK()

Returns iterator over receiver children

Returns iterator over 3-tuples with child indices; functionally equivalent to 3 nested loops, a bit faster and more readable.

```
containsBBox (_bbox)
```

Returns True if BBox contains or intersects the receiver.

delete(item, itemBBox=None)

Deletes/removes the given object from receiver

Parameters

- item (object) object to remove
- itemBBox (BBox.BBox) Optional parameter to specify bounding box of the object to be removed

divide()

Divides the receiver locally, creating child octants.

evaluate (functor)

Evaluate the given functor on all containing objects. The functor should define getBBox() function to return functor bounding box. Only the objects within this bouding box will be processed. Functor should also define evaluate method accepting object as a parameter.

```
Parameters functor (object) - Functor
```

giveDepth()

Returns Returns the depth (the subdivision level) of the receiver (and its children)

qiveItemsInBBox (itemList, bbox)

Returns the list of objects inside the given bounding box. Note: an object can be included several times, as can be assigned to several octants.

Parameters

- itemList (list) list containing the objects matching the criteria
- bbox (BBox.BBox) target bounding box

giveMyBBox()

Returns Receiver's BBox

Return type BBox.BBox

```
insert (item, itemBBox=None)
```

Insert given object into receiver container. Object is inserted only when its bounding box intersects the bounding box of the receiver. If the number of stored objects exceeds the limit, the receiver is adaptively refined and objects distributed to children octants.

Parameters

- item (object) object to insert
- itemBBox (BBox.BBox) Optional parameter determining the BBox of the object

isTerminal()

Returns True if octree is the terminal cell

```
class mupif.Octree.Octree(origin, size, mask)
```

```
Bases: mupif.Localizer.Localizer
```

An octree is used to partition space by recursively subdividing the root cell (square or cube) into octants. Octants can be terminal (containing the data) or can be further subdivided into children octants partitioning the parent. Each terminal octant contains the objects with bounding box within the octant. Octree contains at least one octant, called root octant, with geometry large enough to contain all potential objects. Such a partitiong can significantly speed up spatial serches on objects.

Each object that can be inserted is assumed to provide giveBBox() returning its bounding box.

Octree implementation supports 1D, 2D and 3D setting. This is controlled by Octree mask. Octree mask is a tuple containing 0 or 1 values. If corresponding mask value is nonzero, receiver is subdivided in corresponding coordinate direction.

```
__init__ (origin, size, mask)
The constructor.
```

Parameters

- origin (tuple) coordinates of lower left corner of the root octant.
- **size** (float) dimension (size) of the root octant
- mask (tuple) boolean tuple, where true values determine the coordinate indices in which octree octants are subdivided

```
delete (item)
    Removes the given object from octree. See Octant.delete()

evaluate (functor)
    Evaluate the given functor on all containing objects. See Octant.evaluate()

giveDepth()
    See Octant.giveDepth()

giveItemsInBBox (bbox)
    Returns the list of objects inside the given bounding box. See Octant.giveItemsInBBox()

insert (item)
    Inserts given object into octree. See Octant.insert()
```

2.20 mupif.Property module

```
class mupif.Property.ConstantProperty(value, propID, valueType, units, time=None, objec-
tID=0, metaData={})
Bases: mupif.Property.Property
```

Property is a characteristic value of a problem, that does not depend on spatial variable, e.g. homogenized conductivity over the whole domain. Typically, properties are obtained by postprocessing results from lover scales by means of homogenization and are parameters of models at higher scales.

Property value can be of scalar, vector, or tensorial type. Property keeps its value, objectID, time and type.

```
__init__ (value, propID, valueType, units, time=None, objectID=0, metaData={})
Initializes the property.
```

- value (tuple) A tuple (array) representing property value
- propID (PropertyID) Property ID
- **valueType** (ValueType) Type of a property, i.e. scalar, vector, tensor. Tensor is by default a tuple of 9 values, being compatible with Field's tensor.
- **time** (*Physics.PhysicalQuantity*) Time when property is evaluated. If None (default), no time dependence
- units (Physics. Physical Units or string) Property units or string

• **objectID** (*int*) – Optional ID of problem object/subdomain to which property is related, default = 0

convertToUnit (unit)

Change the unit and adjust the value such that the combination is equivalent to the original one. The new unit must be compatible with the previous unit of the object.

```
Parameters unit (C\{str\}) – a unit
```

Raises TypeError – if the unit string is not a known unit or a unit incompatible with the current one

dumpToLocalFile (fileName, protocol=4)

Dump Property to a file using Pickle module

Parameters

- **fileName** (str) File name
- protocol (int) Used protocol 0=ASCII, 1=old binary, 2=new binary

getTime()

Returns Receiver time

Return type *PhysicalQuantity* or None

```
getValue (time=None, **kwargs)
```

Returns the value of property in a tuple. :param Physics.PhysicalQuantity time: Time of property evaluation :param **kwargs: None.

Returns Property value as an array

Return type tuple

inUnitsOf (*units)

Express the quantity in different units. If one unit is specified, a new PhysicalQuantity object is returned that expresses the quantity in that unit. If several units are specified, the return value is a tuple of PhysicalObject instances with with one element per unit such that the sum of all quantities in the tuple equals the original quantity and all the values except for the last one are integers. This is used to convert to irregular unit systems like hour/minute/second.

```
Parameters units (C\{str\}) – one units
```

Returns one physical quantity

Return type L{PhysicalQuantity} or C{tuple} of L{PhysicalQuantity}

Raises TypeError – if any of the specified units are not compatible with the original unit

classmethod loadFromLocalFile(fileName)

Alternative constructor from a Pickle module

```
Parameters fileName (str) - File name
```

Returns Property instance

Return type *Property*

```
class mupif.Property.Property (propID, valueType, units, objectID=0, metaData={})
```

```
\textbf{Bases:} \qquad \textit{mupif.MupifObject.MupifObject,} \qquad \textit{mupif.Physics.PhysicalQuantities.} \\ \textit{PhysicalQuantity} \\
```

Property is a characteristic value of a problem, that does not depend on spatial variable, e.g. homogenized conductivity over the whole domain. Typically, properties are obtained by postprocessing results from lover scales by means of homogenization and are parameters of models at higher scales.

Property value can be of scalar, vector, or tensorial type. Property keeps its value, objectID, time and type.

```
__init__(propID, valueType, units, objectID=0, metaData={})
Initializes the property.
```

Parameters

- propID (PropertyID) Property ID
- **valueType** (ValueType) Type of a property, i.e. scalar, vector, tensor. Tensor is by default a tuple of 9 values, being compatible with Field's tensor.
- units (Physics.PhysicalUnits or string) Property units or string
- objectID (int) Optional ID of problem object/subdomain to which property is related, default = 0

getObjectID()

Returns property objectID.

Returns Object's ID

Return type int

getPropertyID()

Returns type of property.

Returns Receiver's property ID

Return type PropertyID

getUnits()

Returns representation of property units.

Returns Returns receiver's units (Units)

Return type PhysicalQuantity

```
getValue (time=None, **kwargs)
```

Returns the value of property in a tuple. :param Physics.PhysicalQuantity time: Time of property evaluation :param **kwargs: Arbitrary keyword arguments, see documentation of derived classes.

Returns Property value as an array

Return type tuple

getValueType()

Returns the value type of property.

Returns Property value type

Return type *mupif.PropertyID*

2.21 mupif.PyroFile module

```
class mupif.PyroFile.PyroFile (filename, mode, buffsize=1024, compressFlag=False)
    Bases: object
```

Helper Pyro class providing an access to local file. It allows to receive/send the file content from/to remote site (using Pyro) in chunks of configured size.

```
close()
```

Closes the associated file handle.

getChunk()

Reads and returns next buffsize bytes from open (should be opened in read mode). The returned chunk may contain less bytes if not enough data can be read, or can be empty if end-of-file is reached. :return: Returns next chunk of data read from the file :rtype: str

getTerminalChunk()

Reads and returns the terminal bytes from source. In case of of source without compression, an empty string should be returned, in case of compressed stream the termination sequence is returned (see zlib flush(Z_FINAL)) :rtype: str

setBuffSize (buffSize)

Allows to set the receiver buffer size. :param int buffSize: new buffer size

setChunk (buffer)

Writes the given chunk of data into the file, which should be opened in write mode.

Parameters buffer (str) – data chunk to append

setCompressionFlag()

Sets the compressionFlag to True

2.22 mupif.PyroUtil module

```
class mupif.PyroUtil.SSHContext(userName=", sshClient='manual', options=", sshHost=")
Bases: object
```

Helper class to store ssh tunnel connection details. It is parameter to different methods (connectJobManager, allocateApplicationWithJobManager, etc.). When provided, the corresponding ssh tunnel connection is established and associated to proxy using decorator class to make sure it can be terminated properly.

mupif.PyroUtil.allocateApplicationWithJobManager(ns, jobMan, natPort, hkey, sshContext=None)

Request new application instance to be spawned by given jobManager.

Parameters

- ns (Pyro4.naming.Nameserver) running name server
- **jobMan** (*jobManager*) **jobmanager** to use
- natPort (int) nat port on a local computer for ssh tunnel for the application
- hkey (str) A password string
- sshContext (sshContext) describing optional ssh tunnel connection detail

Returns Application instance

Return type Model.RemoteModel

Raises Exception – if allocation of job fails

mupif.PyroUtil.allocateNextApplication (ns, jobMan, natPort, sshContext=None)
Request new application instance to be spawned by given jobManager

- ns (Pyro4.naming.Nameserver) running name server
- jobMan jobmanager to use
- natPort (int) nat port on a local computer for ssh tunnel for the application

:param sshContext describing optional ssh tunnel connection detail

Returns Application instance

Return type Model.RemoteModel

Raises Exception – if allocation of job fails

mupif.PyroUtil.connectApp (ns, name, hkey, sshContext=None)

Connects to a remote application, creates the ssh tunnel if necessary

Parameters

- ns (Pyro4.naming.Nameserver) Instance of a nameServer
- name (str) Name of the application to be connected to
- hkey (str) A password string

Returns Application Decorator (docorating pyro proxy with ssh tunnel instance)

Return type Instance of an application decorator

Raises Exception - When cannot find registered server or Cannot connect to application

mupif.PyroUtil.connectApplicationsViaClient(fromContext, fromApplication, toApplication)

Create a reverse ssh tunnel so one server application can connect to another one.

Typically, steering_computer creates connection to server1 and server2. However, there is no direct link server1-server2 which is needed for Field operations (getField, setField). Assume a working connection server1-steering_computer on NAT port 6000. This function creates a tunnel steering_computer:6000 and server2:7000 so server2 has direct access to server1's data.

steering_computer / from server1:6000 to server2:7000

Parameters

- fromContext (SSHContext) Remote application
- **fromApplication** (Model.Model) Application object from which we want to create a tunnel
- toApplication (Model.Model) Application object to which we want to create a tunnel

Returns Instance of sshTunnel class

Return type sshTunnel

mupif.PyroUtil.connectJobManager (ns, jobManName, hkey, sshContext=None)

Connect to jobManager described by given jobManRec and create an optional ssh tunnel

:param jobManName name under which jobmanager is registered on NS :param str hkey: A password string :param sshContext describing optional ssh tunnel connection detail

Returns (JobManager proxy, jobManager Tunnel)

Return type JobManager.RemoteJobManager

Raises Exception – if creation of a tunnel failed

mupif.PyroUtil.connectNameServer(nshost, nsport, hkey, timeOut=3.0)

Connects to a NameServer.

- nshost (str) IP address of nameServer
- **nsport** (*int*) Nameserver port.
- hkey (str) A password string
- timeOut (float) Waiting time for response in seconds

Returns NameServer

Return type Pyro4.naming.Nameserver

Raises Exception – When can not connect to a LISTENING port of nameserver

mupif.PyroUtil.downloadPyroFile (newLocalFileName, pyroFile, compressFlag=False) Allows to download remote file (pyro ile handle) to a local file.

Parameters

- newLocalFileName (str) path to a new local file on a client.
- pyroFile (PyroFile.PyroFile) representation of existing remote server's file
- **compressFlag** (bool) will activate compression during data transfer (zlib)

mupif.PyroUtil.downloadPyroFileFromServer(newLocalFileName, pyroFile, compress-Flag=False)

See :func:'downloadPyroFileFromServer'

mupif.PyroUtil.getIPfromUri(uri)

Returns IP address of the server hosting given URI, e.g. return 127.0.0.1 from string PYRO:obj_b178eed8e1994135adf9864725f1d50f@127.0.0.1:5555 :param str uri: URI from an object

Returns IP address

Return type string

mupif.PyroUtil.getNATfromUri(uri)

Return NAT port from URI, e.g. return 5555 from string PYRO:obj_b178eed8e1994135adf9864725f1d50f@127.0.0.1:5555

Parameters uri (str) - URI from an object

Returns NAT port number

Return type int

mupif.PyroUtil.getNSAppName (jobname, appname)

Get application name.

Parameters

- jobname (str) Arbitrary string concatenated in the outut
- appname (str) Arbitrary string concatenated in the outut

Returns String of concatenated arguments

Return type str

mupif.PyroUtil.getNSConnectionInfo(ns, name)

Returns component connection information stored in name server :return (host, port, nathost, natport) tuple :rtype: tuple

mupif.PyroUtil.getNSmetadata(ns, name)

Returns name server metadata for given entry identified by name :return entry metadata :rtype: list of strings

mupif.PyroUtil.getObjectFromURI(uri, hkey)

Returns object from given URI, e.g. returns a field :param str uri: URI from an object :param str hkey: A password string

Returns Field, Property etc.

Return type object including hkey

mupif.PyroUtil.getUserInfo()

Returns tuple containing (username, hostname)

Return type tuple of strings

Runs a simple application server

Parameters

- **server** (str) Host name of the server (internal host name)
- port (int) Port number on the server where daemon will listen (internal port number)
- **nathost** (str) Hostname of the server as reported by nameserver, for secure ssh tunnel it should be set to 'localhost' (external host name)
- natport (int) Server NAT port as reported by nameserver (external port)
- **nshost** (str) Hostname of the computer running nameserver
- nsport (int) Nameserver port
- appName (str) Name of registered application
- app (instance) Application instance
- hkey (str) A password string
- daemon Reference to already running daemon, if available. Optional parameter.

Raises Exception – if can not run Pyro4 daemon

mupif.PyroUtil.runDaemon (host, port, hkey, nathost=None, natport=None)

Runs a daemon without registering to a name server :param str(int) host: Host name where daemon runs. This is typically a localhost :param int or tuple port: Port number where daemon will listen (internal port number) or tuple of possible ports :param str hkey: A password string :param str(int) nathost: Hostname of the server as reported by nameserver, for secure ssh tunnel it should be set to 'localhost' (external host name) :param int natport: Server NAT port, optional (external port)

:return Instance of the running daemon, None if a problem :rtype Pyro4.Daemon

Registers and runs given jobManager server

- **server** (*str*) Host name of the server (internal host name)
- port (int) Port number on the server where daemon will listen (internal port number)
- **nathost** (str) Hostname of the server as reported by nameserver, for secure ssh tunnel it should be set to 'localhost' (external host name)
- natport (int) Server NAT port as reported by nameserver (external port)
- **nshost** (str) Hostname of the computer running nameserver

- **nsport** (*int*) Nameserver port
- appName (str) Name of job manager to be registered at nameserver
- hkey (str) A password string
- jobman Jobmanager
- daemon Reference to already running daemon, if available. Optional parameter.

mupif.PyroUtil.runServer (server, port, nathost, natport, nshost, nsport, appName, hkey, app, daemon=None, metadata=None)

Runs a simple application server

Parameters

- **server** (*str*) Host name of the server (internal host name)
- port (int) Port number on the server where daemon will listen (internal port number)
- **nathost** (str) Hostname of the server as reported by nameserver, for secure ssh tunnel it should be set to 'localhost' (external host name)
- natport (int) Server NAT port as reported by nameserver (external port)
- **nshost** (str) Hostname of the computer running nameserver
- nsport (int) Nameserver port
- appName (str) Name of registered application
- app (instance) Application instance
- hkey (str) A password string
- daemon Reference to already running daemon, if available. Optional parameter.
- metadata set of strings that will be the metadata tags associated with the object registration. See PyroUtil.py for valid tags. The metadata string "connection:server:port:nathost:natport" will be automatically generated.

Raises Exception – if can not run Pyro4 daemon

Bases: object

Helper class to represent established ssh tunnel. It defines terminate and __del__ method to ensure correct tunnel termination.

terminate()

Terminate the connection.

mupif.PyroUtil.uploadPyroFile (clientFileName, pyroFile, hkey, size=1024, compressFlag=False) Allows to upload given local file to a remote location (represented by Pyro file hanfdle).

- clientFileName (str) path to existing local file on a client where we are
- pyroFile (PyroFile.PyroFile) representaion of remote file, this file will be created
- hkey (str) A password string
- size (int) optional chunk size. The data are read and written in byte chunks of this size
- compressFlag (bool) will activate compression during data transfer (zlib)

mupif.PyroUtil.uploadPyroFileOnServer (clientFileName, pyroFile, hkey, size=1024, compress-Flag=False)

See :func:'downloadPyroFile'

2.23 mupif.RemoteAppRecord module

class mupif.RemoteAppRecord.RemoteAppRecord(app, appTunnel, jobMan, jobManTunnel, jobID)

Bases: object

Class keeping internal data on remote application. The data contain: * appTunnel: reference to application ssh tunnel * jobMan: reference to jobManager * jobManTunnel: reference to jobManager tunnel representation * jobID: jobID of application .. automethod:: __init__

appendNextApplication (app, appTunnel, jobID)

Append next application on existing instance :param Application app: application instance :param subprocess.Popen appTunnel: ssh tunnel subprocess representing ssh tunnel to application process :param string jobID: application jobID

getApplication (num=0)

Returns application instance :param int num: number of application, default 0 :return: Instance of Application

getApplicationUri(num=0)

Returns application uri :param int num: number of application, default 0 :return: uri

getJobID (num=0)

getJobManager()

terminateAll()

Terminates all remote applications in app[] including their ssh tunnels. Terminates also jobManager and the associated ssh tunnel.

terminateApp(num)

Terminates app[num] and its ssh tunnel. Job manager and its tunnel remains untouched. :param int num: number of application

2.24 mupif.SimpleJobManager module

Bases: mupif.JobManager.JobManager

Simple job manager using Pyro thread pool based server. Requires Pyro servertype=thread pool based (SERVERTYPE config item). This is the default value. For the thread pool server the amount of worker threads to be spawned is configured using THREADPOOL_SIZE config item (default value set to 16).

However, dee to GIL (Global Interpreter Lock of python the actual level of achievable concurrency is low. The threads created from a single python context are executed sequentially. This implementation is suitable only for servers with a low workload.

__init__(daemon, ns, appAPIClass, appName, jobManWorkDir, maxJobs=1)
Constructor.

Parameters

• daemon (Pyro4. Daemon) - running daemon for SimpleJobManager

```
• ns (Pyro4.naming.Nameserver) - running name server
                 • appAPIClass (Application) - application class
                 • appName (str) – application name
                 • jobManWorkDir(str) - see JobManager.__init__()
                 • maxJobs (int) - see JobManager. init ()
     allocateJob (user, natPort)
          Allocates a new job.
          See JobManager.allocateJob()
             Except unable to start a thread, no more resources
     getApplicationSignature()
             Returns application name
             Return type str
     getStatus()
          Returns a list of tuples for all running jobIDs :return: a list of tuples (jobID, running time, user) :rtype: a
          list of (str, float, str)
     terminateJob(jobID)
          Terminates the given job, frees the associated recources.
          See JobMSimpleJobManageranager.terminateJob()
class mupif.SimpleJobManager.SimpleJobManager2 (daemon, ns, appAPIClass, appName,
                                                           portRange, jobManWorkDir, serverCon-
                                                           figPath, serverConfigFile, serverConfig-
                                                           Mode, jobMan2CmdPath, maxJobs=1,
                                                           jobMancmdCommPort=10000)
     Bases: mupif.JobManager.JobManager
     Simple job manager 2. This implementation avoids the problem of GIL lock by running application server under
     new process with its own daemon.
     allocateJob (user, natPort)
          Allocates a new job.
          See JobManager.allocateJob() :except: unable to start a thread, no more resources
     getApplicationSignature()
          See SimpleJobManager.getApplicationSignature()
     getPyroFile (jobID, filename, mode='r', buffSize=1024)
          See JobManager.getPyroFile()
     getStatus()
          See JobManager.getStatus()
     terminate()
          Terminates job manager itself.
     terminateAllJobs()
          Terminates all registered jobs, frees the associated recources.
     terminateJob(jobID)
          Terminates the given job, frees the associated recources.
          See JobManager.terminateJob()
```

```
uploadFile (jobID, filename, pyroFile, hkey)
See JobManager.uploadFile()
```

2.25 mupif.TimeStep module

```
class mupif. TimeStep. TimeStep (t, dt, targetTime, units=None, n=1)
Bases: object
```

Class representing a time step. The following attributes are used to characterize a time step:

```
||- - - ||(time-dt)- - - i-th time step(dt) - - - ||(time)- - - - ||- - - - ||(targetTime)
```

Note: Individual models (applications) assemble their governing equations at specific time, called asssembly-Time, this time is reported by individual models. For explicit model, asssembly time is equal to timeStep.timetimestep.dt, for fully implicit model, assembly time is equal to timeStep.time

```
\_init\_(t, dt, targetTime, units=None, n=1)
Initializes time step.
```

Parameters

- t (PQ.PhysicalQuantity) Time(time at the end of time step)
- dt (PQ.PhysicalQuantity) Step length (time increment), type depends on 'units'
- targetTime (PQ.PhysicalQuantity. targetTime is not related to particular time step rather to the material model (load duration, relaxation spectra etc.)) target simulation time (time at the end of simulation, not of a single TimeStep)
- or str units (PQ.PhysicalUnit) optional units for t, dt, targetTime if given as float values
- **n** (*int*) Optional, solution time step number, default = 1

```
getNumber()
```

Returns Receiver's solution step number

Return type int

getTargetTime()

Returns Target time

Return type PQ.PhysicalQuantity

getTime()

Returns Time

Return type PQ.PhysicalQuantity

getTimeIncrement()

Returns Time increment

Return type PQ.PhysicalQuantity

2.26 mupif.Timer module

```
class mupif.Timer.Timer
Bases: object

Class for measuring time.

__enter__()
    Remembers time at calling this function.

__exit__(*args)
    Remembers time at calling this function and calculates the difference to __enter_().
```

2.27 mupif.Util module

mupif.Util.NoneOrInt(arg)

Check if None or Int types. :param str,int arg: Parameter

Returns argument (converted to int)

Return type None of int

mupif.Util.changeRootLogger(newLoggerName)

Change root logger by giving a new file name. Useful in parallel processes on a single machine.

Returns Nothing

mupif.Util.getParentParser()

Parent parser for controlling running mode. Used in MuPIF's examples. Mode 0-local (default), 1-ssh, 2-VPN with option -m.

Returns parent parser object

Return type argparse object

```
mupif.Util.quadratic_real(a, b, c)
```

Finds real roots of quadratic equation: $ax^2 + bx + c = 0$. By substituting x = y-t and t = a/2, the equation reduces to $y^2 + (b-t^2) = 0$ which has easy solution $y = +/-sqrt(t^2-b)$

Parameters

- a (float) Parameter from quadratic equation
- **b** (float) Parameter from quadratic equation
- c (float) Parameter from quadratic equation

Returns Two real roots if they exist

Return type tuple

```
mupif.Util.setupLogger(fileName, level=10)
```

Set up a logger which prints messages on the screen and simultaneously saves them to a file. The file has the suffix '.log' after a loggerName.

Parameters

- **fileName** (str) file name, the suffix '.log' is appended.
- level (object) logging level. Allowed values are CRITICAL, ERROR, WARNING, INFO, DEBUG, NOTSET

Return type logger instance

2.28 mupif. Vertex module

class mupif.Vertex.Vertex(number, label, coords=None)

```
Bases: object
Represent a vertex. Vertices define the geometry of interpolation cells. Vertex is characterized by its position,
number and label. Vertex number is locally assigned number, while label is a unique number referring to source
application.
  _init___(number, label, coords=None)
     Initializes the vertex.
         Parameters
             • number (int) - Local vertex number
             • label (int) - Vertex label
             • coords (tuple) – 3D position vector of a vertex
__repr__()
         Returns Receiver's number, label, coordinates
         Return type string
getBBox()
         Returns Receiver's bounding-box (containing only one point)
         Return type mupif.BBox.BBox
getCoordinates()
         Returns Receiver's coordinates
         Return type tuple
getNumber()
         Returns Number of the instance
         Return type int
```

2.29 mupif.VtkReader2 module

• **fieldID** (FieldID) – Field type (displacement, strain, temperature ...)

- units (PhysicalUnit) field units
- time (Physical Quantity) time
- name (str) name of the field to visualize
- filename (str) -
- type (int) type of value of the field (1:Scalar, 3:Vector, 6:Tensor)

Returns Field of unknowns

Return type Field

 $\verb|mupif.VtkReader2.readMesh| (\textit{numNodes}, \textit{nx}, \textit{ny}, \textit{nz}, \textit{coords})|$

Reads structured 3D mesh

Parameters

- numNodes (int) Number of nodes
- nx (int) Number of elements in x direction
- ny (int) Number of elements in y direction
- nz (int) Number of elements in z direction
- coords (tuple) Coordinates for each nodes

Returns Mesh

Return type Mesh

2.30 mupif.Workflow module

```
class mupif.Workflow.Workflow(metaData={})
    Bases: mupif.Model.Model
```

An abstract class representing a workflow and its interface (API).

The purpose of this class is to represent a workflow, its abstract services for data exchange and steering. This interface has to be implemented/provided by any workflow. The Workflow class inherits from Application allowing to treat any workflow as model(application) in high-level workflow.

```
___init___(metaData={})
```

Constructor. Initializes the workflow

Parameters metaData (dict) – Optionally pass metadata.

getAPIVersion()

Returns Returns the supported API version

Return type str, int

getApplicationSignature()

Get application signature.

Returns Returns the application identification

Return type str

initialize (file=", workdir=", targetTime=PhysicalQuantity(0.0, 's'), metaData={}, validateMeta-Data=True, **kwargs)

Initializes application, i.e. all functions after constructor and before run.

Parameters

- file (str) Name of file
- workdir (str) Optional parameter for working directory
- targetTime (PhysicalQuantity) target simulation time
- **metaData** (*dict*) Optional dictionary used to set up metadata (can be also set by setMetadata())
- validateMetaData (bool) Defines if the metadata validation will be called
- **kwargs** (named_arguments) Arbitrary further parameters

solve (runInBackground=False)

Solves the workflow.

The default implementation solves the problem in series of time steps using solveStep method (inheritted) until the final time is reached.

Parameters runInBackground (bool) – optional argument, default False. If True, the solution will run in background (in separate thread or remotely).

```
updateStatus (status, progress=0)
```

Updates the workflow status. The status is submitted to workflow monitor. The self.workflowMonitor should be (proxy) to workflowManager :param str status: string describing the workflow status (initialized, running, failed, finished) :param int progress: integer number indicating execution progress (in percent)

2.31 mupif.WorkflowMonitor module

class mupif.WorkflowMonitor.WorkflowMonitor

Bases: mupif.MupifObject.MupifObject

An class implementing workflow monitor; a server keeping track of individual workflow executions and their status. It internally maintains workflows dict, where keys are workflow execution IDs, and values are dicts containing metadata.

```
init ()
```

Constructor. Initializes the monitor server

getAllMetadata()

Returns all metadata :return dict: all metadata

```
updateMetadata (key, valueDict)
```

Updates the entry. :param str key: unique execution ID of workflow, application, etc. :param dict value-Dict: metadata

2.32 mupif.dataID module

Module defining PropertyID and FieldID as enumeration, e.g. concentration, velocity. class Enum allows accessing members by .name and .value FunctionID is deprecated and will be removed

```
class mupif.dataID.FieldID
    Bases: enum.IntEnum
```

This class represents the supported values of field IDs, e.g. displacement, strain, temperature. Immutable class Enum allows accessing members by .name and .value methods

```
FID_BucklingShape = 10
    FID Concentration = 6
    FID_Displacement = 1
    FID DomainNumber = 12
    FID ESI VPS Displacement = 10001
    FID FibreOrientation = 11
    FID_Humidity = 5
    FID_Material_number = 9
    FID Strain = 2
    FID Stress = 3
    FID_Temperature = 4
    FID_Thermal_absorption_surface = 8
    FID_Thermal_absorption_volume = 7
class mupif.dataID.FunctionID
    Bases: enum.IntEnum
    This classenumeration represent the supported values of FunctionID, e.g. FuncID_ProbabilityDistribution
    FuncID_ProbabilityDistribution = 1
class mupif.dataID.PropertyID
    Bases: enum.IntEnum
    Enumeration class defining Property IDs. These are used to uniquely determine the canonical keywords identi-
    fiing individual properties.
    PID_Acceleration = 1018
    PID_Amphiphilicity = 1035
    PID_Angular_acceleration = 1024
    PID Angular velocity = 1023
    PID AsorptionSpectrum = 26
    PID_Bond_label = 1015
    PID_Bond_type = 1016
    PID CROSSLINKER TYPE = 92003
    PID CROSSLINKONG DENSITY = 92007
    PID_Charge = 1083
    PID_Charge_density = 1084
    PID_Chemical_specie = 1004
    PID_ChipSpectrum = 17
    PID_Cohesion_energy_density = 1078
    PID_Cohesive_group = 1118
    PID_Collision_operator = 1103
```

```
PID CompositeAxialYoung = 9000
PID_CompositeInPlanePoisson = 9004
PID_CompositeInPlaneShear = 9002
PID_CompositeInPlaneYoung = 9001
PID CompositeTransversePoisson = 9005
PID CompositeTransverseShear = 9003
PID_Concentration = 1
PID_Contact_angle = 1034
PID_Coupling_time = 1065
PID CriticalLoadLevel = 48
PID_Crystal_storage = 1010
PID_CumulativeConcentration = 2
PID_Current = 1054
PID_Cutoff_distance = 1066
PID DENSITY = 92100
PID DENSITY OF FUNCTIONALIZATION = 92009
PID Debye length = 1040
PID_Deflection = 36
PID_Delta_displacement = 1056
PID Demo Integral = 9992
PID_Demo_Max = 9991
PID_Demo_Min = 9990
PID_Demo_Value = 9994
PID Demo Volume = 9993
PID_Density = 1047
PID_Description = 1085
PID_Dielectric_constant = 1069
PID Diffusion coefficient = 1029
PID Diffusion velocity = 1075
PID_Direction = 1001
PID_Distribution = 1051
PID_Dynamic_pressure = 1070
PID_Dynamic_viscosity = 1027
PID_EModulus = 37
PID_ESI_VPS_BUCKL_LOAD = 91007
PID ESI VPS CRIMP STIFFNESS = 91003
```

PID ESI VPS FIRST FAILURE ELE = 91004 PID ESI VPS FIRST FAILURE MOM = 91001 PID_ESI_VPS_FIRST_FAILURE_PLY = 91005 PID ESI VPS FIRST FAILURE ROT = 91002 PID ESI VPS FIRST FAILURE VAL = 91000 PID ESI VPS MOMENT = 90019 PID_ESI_VPS_MOMENT_CURVE = 91008 $PID_ESI_VPS_PLY1_E0c1 = 90011$ PID ESI VPS PLY1 E0t1 = 90002 PID ESI VPS PLY1 E0t2 = 90003 PID_ESI_VPS_PLY1_E0t3 = 90004 PID_ESI_VPS_PLY1_G012 = 90005 PID ESI VPS PLY1 G013 = 90007 PID ESI VPS PLY1 G023 = 90006 PID ESI VPS PLY1 NU12 = 90008 PID ESI VPS PLY1 NU13 = 90010 PID ESI VPS PLY1 NU23 = 90009 PID ESI VPS PLY1 RHO = 90012 PID_ESI_VPS_PLY1_S12 = 90018 PID ESI VPS PLY1 XC = 90015 PID ESI VPS PLY1 XT = 90014 PID_ESI_VPS_PLY1_YC = 90017 PID_ESI_VPS_PLY1_YT = 90016 PID ESI VPS ROTATION = 90020 PID ESI VPS ROTATION CURVE = 91009 PID_ESI_VPS_SECFO_1 = 90023 PID_ESI_VPS_SECFO_2 = 90024 PID ESI VPS TEND = 90001 PID ESI VPS THNOD 1 = 90021PID_ESI_VPS_THNOD_2 = 90022 PID_ESI_VPS_TOTAL_MODEL_MASS = 91006 PID_ESI_VPS_hPLY = 90013 PID Electric field = 1086 PID Electron mass = 1087 PID Electrostatic field = 1088

PID_EmissionSpectrum = 24

```
PID_Energy = 1089
PID_Energy_well_depth = 1067
PID_Equation_of_state_coefficient = 1033
PID_Euler_angles = 1058
PID ExcitationSpectrum = 25
PID ExtensionalInPlaneStiffness = 49
PID_ExtensionalOutOfPlaneStiffness = 50
PID_External_applied_force = 1057
PID_External_forcing = 1105
PID_FILLER_CONCENTRATION = 92008
PID_FILLER_DESIGNATION = 92004
PID_Final = 1055
PID_Flow_type = 1106
PID Flux = 1071
PID Force = 1045
PID Friction coefficient = 1031
PID Full = 1082
PID_Hamaker_constant = 1037
PID_Heat_conductivity = 1090
PID_Height = 34
PID_Homogenized_stress_tensor = 1072
PID_InclusionAspectRatio = 8005
PID_InclusionPoisson = 8003
PID InclusionVolumeFraction = 8004
PID_InclusionYoung = 8002
PID_Index = 1108
PID_Initial_viscosity = 1091
PID InverseCumulativeDist = 28
PID_Ion_valence_effect = 1039
PID_KPI01 = 9996
PID_Kinematic_viscosity = 1028
PID_LEDCCT = 20
PID_LEDColor_x = 18
PID_LEDColor_y = 19
PID LEDRadiantPower = 21
PID_LEDSpectrum = 16
```

PID Label = 1003 PID_Lattice_parameter = 1112 PID_Lattice_spacing = 1042 PID_Lattice_vectors = 1012 PID Length = 33 PID Linear constant = 1092 PID_LocalBendingStiffness = 53 PID_MOLECULAR_WEIGHT = 92001 PID_Magnitude = 1116 $PID_Major = 1079$ $PID_Mass = 1021$ PID_Material_type = 1005 PID MatrixPoisson = 8001 PID_MatrixYoung = 8000 PID_Maximum_Courant_number = 1114 PID Maximum viscosity = 1093 PID_Minimum_viscosity = 1094 PID_Minor = 1080 PID_Moment_inertia = 1096 PID Momentum = 1095 PID_Name_UC = 1011 PID_None = 1111 PID_NumberOfFluorescentParticles = 29 PID NumberOfRays = 15 PID_Number_of_cores = 1115 PID_Number_of_physics_states = 1117 PID_Number_of_time_steps = 1044 PID_Occupancy = 1014 PID_Order_parameter = 1052 PID_Original_position = 1053 PID_POLYDISPERSITY_INDEX = 92002 PID_PRESSURE = 92011 PID_ParticleMu = 30 PID_ParticleNumberDensity = 22 PID ParticleRefractiveIndex = 23 PID_ParticleSigma = 31

```
PID Patch = 1081
PID_Phase_interaction_strength = 1036
PID_PhosphorEfficiency = 32
PID_PoissonRatio = 38
PID PoissonRatio12 = 44
PID PoissonRatio13 = 43
PID_PoissonRatio23 = 42
PID_Poisson_ratio = 1061
PID Position = 1000
PID_Potential_energy = 1097
PID_Power_law_index = 1098
PID_Pressure = 1049
PID_Probability_coefficient = 1030
PID Radius = 1019
PID_Reference_density = 1104
PID RefractiveIndex = 14
PID_Relative_velocity = 1074
PID_Relaxation_time = 1099
PID_Restitution_coefficient = 1062
PID Rolling friction = 1063
PID_SMILE_FILLER_MOLECULAR_STRUCTURE = 92006
PID_SMILE_MODIFIER_MOLECULAR_STRUCTURE = 92005
PID_SMILE_MOLECULAR_STRUCTURE = 92000
PID Scaling coefficient = 1032
PID ScatteringCrossSections = 27
PID_Shape_center = 1006
PID_Shape_length = 1007
PID Shape radius = 1008
PID Shape side = 1009
PID_ShearInPlaneStiffness = 51
PID_ShearModulus12 = 47
PID_ShearModulus13 = 46
PID_ShearModulus23 = 45
PID ShearOutOfPlaneStiffness = 52
PID_Simulation_domain_dimensions = 1025
PID_Simulation_domain_origin = 1026
```

```
PID Size = 1020
PID_Smoothing_length = 1041
PID_Sphericity = 1059
PID_Status = 1002
PID Steady state = 1113
PID Strain tensor = 1073
PID_Stress_tensor = 1076
PID_Surface_tension = 1100
PID_Symmetry_lattice_vectors = 1013
PID_TEMPERATURE = 92010
PID_TRANSITION_TEMPERATURE = 92101
PID_Temperature = 1050
PID_Thermodynamic_ensemble = 1109
PID Thickness = 35
PID_Time = 1101
PID Time step = 1043
PID Torque = 1046
PID_UserTimeStep = 9995
PID_Van_der_Waals_radius = 1068
PID Variable = 1110
PID_Vector = 1107
PID_Velocity = 3
PID_Viscosity = 1102
PID Volume = 1022
PID Volume fraction = 1064
PID_Volume_fraction_gradient = 1077
PID_YoungModulus1 = 39
PID YoungModulus2 = 40
PID YoungModulus3 = 41
PID_Young_modulus = 1060
PID_Zeta_potential = 1038
PID_conductivity_green_phosphor = 9
PID_conductivity_red_phosphor = 8
PID_effective_conductivity = 5
PID_mean_radius_green_phosphor = 11
PID_mean_radius_red_phosphor = 10
```

```
PID_standard_deviation_green_phosphor = 13
PID_standard_deviation_red_phosphor = 12
PID_transient_simulation_time = 4
PID_volume_fraction_green_phosphor = 7
PID volume fraction red phosphor = 6
```

2.33 mupif.operatorUtil module

Bases: mupif.operatorUtil.OperatorInteraction
Derived class implementing different communication channels.

```
checkOperatorResponse(workflowID, jobID)
```

Check IMAP server if there is operator's response. :param: str workflowID: unique workflow ID :param: str jobID: unique jobID :return: tuple of bool confirming existence of the message and body of the message :rtype: bool, str

```
contactOperator (workflowID, jobID, msgBody)
```

Sends an email to the operator. :param: str workflowID: unique workflow ID :param: str jobID: unique jobID :param: str msgBody: message from operator. The message should contain an empty dictionary entry which should be filled

```
class mupif.operatorUtil.OperatorInteraction
    Bases: object
```

Generic class to represent interaction with an operator. Derived classes implement different communication channels.

```
checkOperatorResponse(workflowID, jobID)
```

Check operator response and return received data :param: str workflowID: unique workflow ID :param: str jobID: unique jobID :return: tuple (ret, Data), where ret is False if response not received, True otherwise and Data contains the operator response. :rtype: (bool, str)

```
contactOperator (workflowID, jobID, msgBody)
```

Contact operator. :param: str workflowID: unique workflow ID :param: str jobID: unique jobID :param: str msgBody: message to operator. Recomended to store all paramaters into dictionary and convert dictionary into json string representation.

2.34 mupif.valueType module

Enumeration defining supported types of field and property values, e.g. scalar, vector, tensor

```
class mupif.valueType.ValueType
    Bases: enum.IntEnum
    An enumeration.
Scalar = 1
```

```
Tensor = 3
Vector = 2
static fromNumberOfComponents(i)
    Parameters i(int) - number of components
    Returns value type corresponding to the number of components
RuntimeError is raised if i does not match any value known.
```

This is a MuPIF module (Multi-Physics Integration Framework)

```
class mupif.FieldID
    Bases: enum.IntEnum
```

This class represents the supported values of field IDs, e.g. displacement, strain, temperature. Immutable class Enum allows accessing members by .name and .value methods

```
Enum allows accessing members by .name and .value methods
    FID_BucklingShape = 10
    FID Concentration = 6
    FID_Displacement = 1
    FID_DomainNumber = 12
    FID_ESI_VPS_Displacement = 10001
    FID FibreOrientation = 11
    FID_Humidity = 5
    FID_Material_number = 9
    FID_Strain = 2
    FID Stress = 3
    FID Temperature = 4
    FID_Thermal_absorption_surface = 8
    FID_Thermal_absorption_volume = 7
class mupif.FunctionID
    Bases: enum. IntEnum
    This classenumeration represent the supported values of FunctionID, e.g. FuncID_ProbabilityDistribution
    FuncID_ProbabilityDistribution = 1
class mupif.PropertyID
    Bases: enum. IntEnum
    Enumeration class defining Property IDs. These are used to uniquely determine the canonical keywords identi-
    fiing individual properties.
    PID Acceleration = 1018
    PID_Amphiphilicity = 1035
    PID_Angular_acceleration = 1024
```

```
PID_Angular_velocity = 1023
PID_AsorptionSpectrum = 26
PID_Bond_label = 1015
PID_Bond_type = 1016
PID CROSSLINKER TYPE = 92003
PID CROSSLINKONG DENSITY = 92007
PID_Charge = 1083
PID_Charge_density = 1084
PID_Chemical_specie = 1004
PID_ChipSpectrum = 17
PID_Cohesion_energy_density = 1078
PID_Cohesive_group = 1118
PID_Collision_operator = 1103
PID_CompositeAxialYoung = 9000
PID_CompositeInPlanePoisson = 9004
PID CompositeInPlaneShear = 9002
PID_CompositeInPlaneYoung = 9001
PID_CompositeTransversePoisson = 9005
PID_CompositeTransverseShear = 9003
PID Concentration = 1
PID_Contact_angle = 1034
PID_Coupling_time = 1065
PID_CriticalLoadLevel = 48
PID Crystal storage = 1010
PID CumulativeConcentration = 2
PID_Current = 1054
PID_Cutoff_distance = 1066
PID DENSITY = 92100
PID DENSITY OF FUNCTIONALIZATION = 92009
PID_Debye_length = 1040
PID_Deflection = 36
PID_Delta_displacement = 1056
PID_Demo_Integral = 9992
PID_Demo_Max = 9991
PID Demo Min = 9990
PID_Demo_Value = 9994
```

```
PID Demo Volume = 9993
PID_Density = 1047
PID_Description = 1085
PID Dielectric constant = 1069
PID Diffusion coefficient = 1029
PID Diffusion velocity = 1075
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PID_Distribution = 1051
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PID_Dynamic_viscosity = 1027
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PID ESI VPS FIRST FAILURE PLY = 91005
PID ESI VPS FIRST FAILURE ROT = 91002
PID ESI VPS FIRST FAILURE VAL = 91000
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PID ESI VPS PLY1 YT = 90016
```

```
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```

```
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```

```
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```

```
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PID_Viscosity = 1102
```

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    PID_Volume_fraction = 1064
    PID_Volume_fraction_gradient = 1077
    PID_YoungModulus1 = 39
    PID YoungModulus2 = 40
    PID YoungModulus3 = 41
    PID_Young_modulus = 1060
    PID_Zeta_potential = 1038
    PID_conductivity_green_phosphor = 9
    PID_conductivity_red_phosphor = 8
    PID_effective_conductivity = 5
    PID_mean_radius_green_phosphor = 11
    PID_mean_radius_red_phosphor = 10
    PID_standard_deviation_green_phosphor = 13
    PID_standard_deviation_red_phosphor = 12
    PID transient simulation time = 4
    PID_volume_fraction_green_phosphor = 7
    PID_volume_fraction_red_phosphor = 6
class mupif.ValueType
    Bases: enum.IntEnum
    An enumeration.
    Scalar = 1
    Tensor = 3
    Vector = 2
    {\tt static} from Number Of Components (i)
           Parameters i(int) – number of components
           Returns value type corresponding to the number of components
        RuntimeError is raised if i does not match any value known.
```

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Acknowledgement

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