SMS++: a Structured Modelling System with Applications to Energy Optimization

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Outline

PGMO

- Project "Consistent Dual Signals and Optimal Primal Solutions" (2012–2018): initial implementation of SMS++ (Ph.D. Thesis[5])
- Project "Advanced Modeling Tools for Decomposition Methods to Energy Optimization Problems" (2016):
  develop general Benders' decomposition code
- Superseded by Project "Multilevel Heterogeneous Distributed Decomposition for Energy Planning with SMS++" (to start RSN):
  generic multi-level decomposition (arbitrary combination of Benders', Lagrange and whatever)

The plan4res H2020 project

- The plan4res project (www.plan4res.eu):

  > "An end-to-end planning and operation tool, composed of a set of optimization models based on an integrated modelling of the pan-European Energy System"

- Plus IT infrastructure, plus lots of data, plus 3 case studies

- An accurate depiction of long-term effects of strategic choices on the pan-European Energy System ≡

  modelling the next 30 years with 1h timescale

  and huge amounts of uncertainty over everything

- An unfeasibly large optimization problem

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- An unfeasibly large optimization problem with lots of structure

- Schedule a set of generating units to satisfy the demand at each node of the transmission network at each time instant of the horizon
- Two versions: simulation (only costs) and operation (also schedules)
- Three natural sources of structure: unit, time, and network
- Relaxing demand constraints decomposes by unit and network: one problem per unit across all horizon, a network problem per instant
- Indeed, Lagrangian Relaxation historically[1] the go-to approach for both simulation and operations[2,3]

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[1] van Ackooij, Danti Lopez, F., Lacalandra, Tahanan "Large-scale Unit Commitment Under Uncertainty [...]" *AOR*, 2018

[2] Borghetti, F., Lacalandra, Nucci "Lagrangian Heuristics Based on Disaggregated Bundle Methods for Hydrothermal Unit Commitment", *IEEE Transactions on Power Systems*, 2003

[3] Dubost, Gonzalez, Lemaréchal "A primal-proximal heuristic applied to french unit-commitment problem" *Math. Prog.* 2005

UC Lagrangian approaches

- A lot of network structure:
  - Dynamic Programming[4] for simple single thermal units, but not for complex ones[5]
  - Min-Cost Flows[6] for simple hydro valleys, but not for complex ones[7]
  - Laplacian of graph[8] for simple network constraints, but not for complex ones[9]
  - other stuff (ROR hydro, solar/wind, small-scale storage, demand response, smart grids, ...) usually "easy"
- Efficient algorithms for simple cases
- At least some hope for complex cases (real-world operations)

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4 F., Gentile "Solving Nonlinear Single-Unit Commitment Problems with Ramping Constraints" *Op. Res.* 2006

5 Tavlaridis-Gyparakis "Decomposition Techniques for Large-Scale Energy Optimization Problems" *Ph.D. Thesis*, 2018

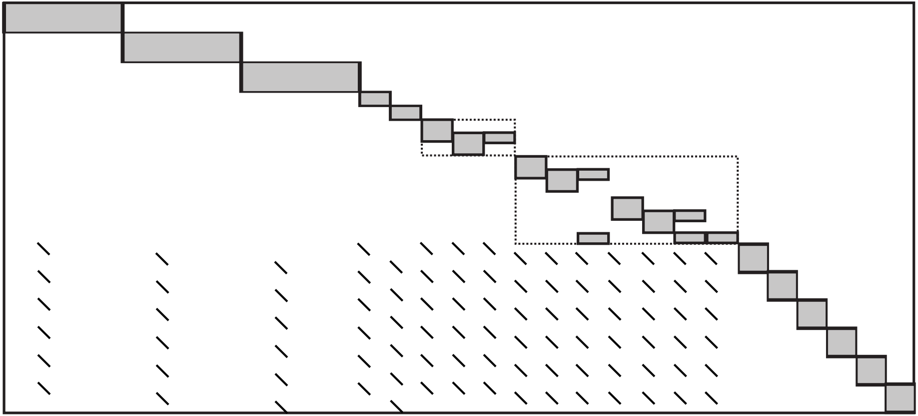
6 F., Manca "A Computational Study of Cost Reoptimization for Min Cost Flow Problems" *INFORMS JOC*, 2006

7 Sahraoui, Bendotti, D'Ambrosio "Real-world hydro-power unit-commitment [...]" *Energy*, 2017

8 F., Serra Capizzano "Spectral Analysis of (Sequences of) Graph Matrices" *SIMAX*, 2001

9 Bienstock, Chertkov, Harnett "Chance-constrained optimal power flow [...]" *SIAM Review* 2014

- A lot of network structure spread around (≈ multicommodity flow)



- Nontrivial linking constraints

Can We Deal With Such a Structure?

- Of course we can, in fact with several different approaches:
  - Lagrangian decomposition[10] and related methods[11], even in parallel[12]
  - Structured Interior-Point methods[13]
  - Structured active-set (simplex) methods[14]
  - Structured Dantzig-Wolfe decomposition[15,16]
  - ...
- Unclear which is better for the application at hand, since have to be solved many times with changing data ≡ reoptimization

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10 F., Gallo "A Bundle type dual-ascent approach to linear multicommodity min cost flow problems" *INFORMS JOC*, 1999

11 Grigoriadis, Khachiyan "An exponential function reduction method for block angular convex programs" *Networks*, 1995

12 Cappanera, F. "Symmetric and asymmetric parallelization of a cost-decomposition algorithm [...]" *INFORMS JOC*, 2003

13 Castro "Solving difficult multicommodity problems through a specialized interior-point algorithm" *Ann. OR*, 2003

14 McBride "Progress made in solving the multicommodity flow problem" *SIOPT*, 1998

15 F., Gendron "A stabilized structured Dantzig-Wolfe decomposition method" *Math. Prog.*, 2013

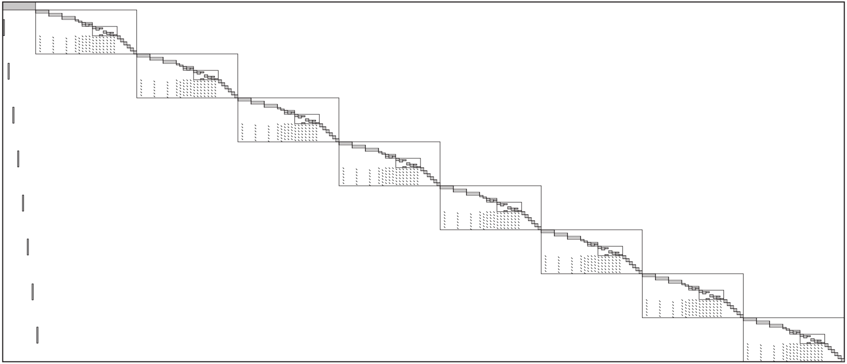
16 Mamer, McBride "A decomposition-based pricing procedure for large-scale linear programs [...]" *Man. Sci.*, 2000

Mid Level: Seasonal storage valuation

- Unit-Commitment is a short-term problem, lacks long-term strategies
- Issue: cost of water (none) / minimum reservoir volume (very low)
  $\Longrightarrow$ lot of water used early on $\Longrightarrow$ no water most of the year
- Hydro production most useful for peak shaving every day
- Computing value of water left in the reservoirs at horizon end
  $\equiv$ the value function of UC w.r.t. max water constraints
  (naturally convex if Lagrangian relaxation = convexification[17] used)
- A mid-term (1y) stochastic program: uncertain inflows, demands, ...
- Stochastic dual dynamic programming[18,19]
  with multiple EUC inside (in principle $\approx$ 365)

[17] Lemaréchal, Renaud "A geometric study of duality gaps, with applications" *Math. Prog.* 2001
[18] Pereira, Pinto "Multi-stage stochastic optimization applied to energy planning" *Math. Prog.*, 1991
[19] van-Ackooij, Warin "On conditional cuts for Stochastic Dual Dynamic Programming" arXiv:1704.06205, 2017

A Picture is Worth 1000 words



- Standard structure for (DP +) Benders' decomposition
- Whenever you do Benders' you can do Lagrange[20] and vice-versa[21]
- Very many different variants, which is best/feasible??

[20] Guignard, Kim "Lagrangean decomposition: a model yielding stronger lagrangean bounds" *Math. Prog.* 1987

[21] Kennington, Shalaby "An Effective Subgradient Procedure for Minimal Cost Multicommodity Flow Problems" *Man. Sci.* 1977

- The energy system changes all the time, but modifications slow, extremely costly, with huge inertia
- Demand and production subject to very significant uncertainties: climate = RES production + demand, shifts in consumption patterns (EV, cryptocurrencies, . . .), new technologies (shale, LED, . . .), geo-political factors (energy security), economical factors (boost or boom), regulatory factors (EU energy market, . . .), political factors (CO_2 emission treaties, nuclear power, . . .), . . .
- Planning long-term evolution very hard, yet necessary
- 20/30 years, 2/5 years steps (multi-level recourse), many scenarios

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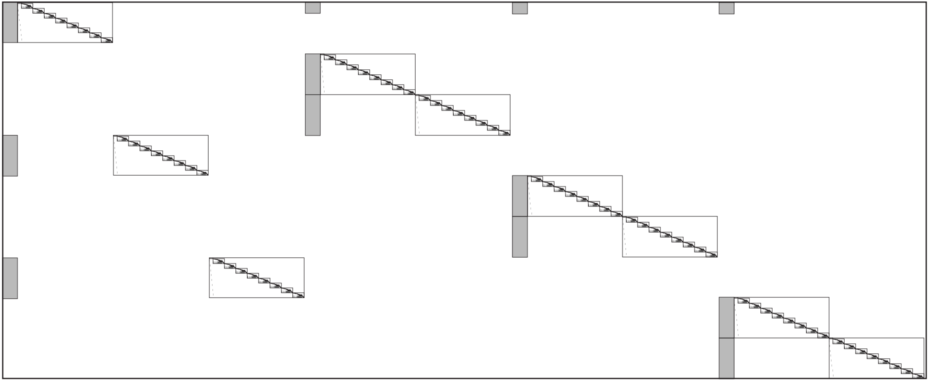


- Huge size, multiple nested structure
- Still OK for either Benders or Lagrange
- Benders + DP + Benders + Lagrange + Graph or . . . ???

How Do you Solve Such a Thing?

- Modeling system: easily construct a huge, flat = unstructured matrix to be passed to a general-purpose, flat solver
- Some solvers offer one-level decomposition (Benders, CG = DW)
- Attempts at automatically recovering structure from a matrix[22], but only one level and anyway conceptually awkward
- Only one tool (that I know of) for multiple nested structure[23,24], but only solves continuous problems by Interior Point methods
- Nothing for multilevel, heterogeneous approaches (such as, but not only, decomposition), e.g., allowing specialized solvers for each block
- So far

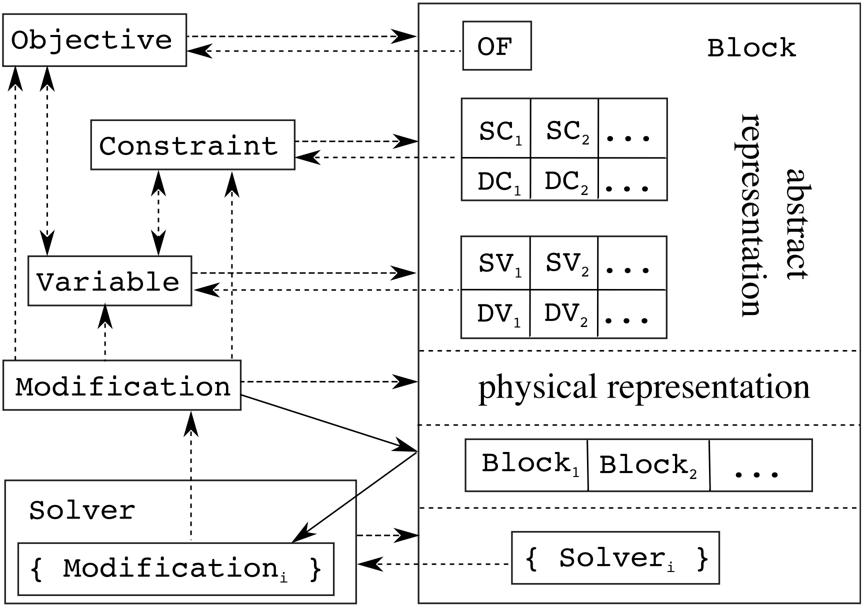
[22] Furini, Lübbecke, Traversi et. al. "Automatic Dantzig–Wolfe reformulation of mixed integer programs" *Math. Prog.* 2015
[23] Gondzio, Grothey "Exploiting Structure in Parallel Implementation of Interior Point Methods [. . .]" *Comput. Man. Sci.*, 2009
[24] Colombo et al. "A Structure-Conveying Modelling Language for Mathematical [. . .] Programming" *Mathe. Prog. Comp.*, 2009

Outline

What We Want

- A modelling language/system which:
  - explicitly supports the notion of block ≡ nested structure
  - separately provides "semantic" information from "syntactic" details (list of constraints/variables ≡ one specific formulation among many)
  - allows exploiting specialised solvers on blocks with specific structure
  - caters all needs of complex methods: dynamic generation of constraints/variables, modifications in the data, reoptimization, ...
- C++ library: set of "core" classes, easily extendable
- Why C++? A number of reasons:
  - all serious solvers are written in C/C++
  - we all love it (especially `C++11/14/17/20`)
  - tried with Julia/JuMP, but could not handle well C++ interface

The Core SMS++


Objective
OF
Block
Constraint
SC1 SC2 ...
DC1 DC2 ...
abstract representation
Variable
SV1 SV2 ...
DV1 DV2 ...
Modification
physical representation
Block1 Block2 ...
Solver
{ Modificationi }
{ Solveri }

Block

- Block = abstract class representing the general concept of "a part of a mathematical model with a well-understood identity"
- Each :Block a model with specific structure (e.g., MCFBlock:Block = a Min-Cost Flow problem)
- Physical representation of a Block: whatever data structure is required to describe the instance (e.g., G, b, c, u)
- Abstract representation of a Block:
  - one Objective (but possibly vector-valued)
  - any # of groups of (pointers) to (static) Variable
  - any # of groups of std::list of (pointers) to (dynamic) Variable
  - any # of groups of (pointers) to (static) Constraint
  - any # of groups of std::list of (pointers) to (dynamic) Constraint

  groups of Variable/Constraint can be single (std::list) or std::vector (. . .) or boost::multi_array thanks to boost::any
- Any # of sub-Blocks (recursively), possibly of specific type (e.g., Block::MMCFBlock can have k Block::MCFBlock inside)

Variable

- Abstract concept, thought to be extended (a matrix, a function, ...)
- Does not even have a value
- Knows which `Block` it belongs to
- Can be fixed and unfixed to/from its current value (whatever that is)
- Influences a set of `Constraint`/`Objective`/`Function` (actually, a set of `ThinVarDepInterface`)
- Fundamental design decision: "name" of a `Variable` = its memory address $\Longrightarrow$ copying a `Variable` makes a different `Variable` $\Longrightarrow$ dynamic `Variables` always live in `std::lists`
- `VariableModification:Modification` (fix/unfix)

Constraint

- Abstract concept, thought to be extended (any algebraic constraint, a matrix constraint, a PDE constraint, bilevel program, . . .)
- Depends from a set of `Variable` (`:ThinVarDepInterface`)
- Either satisfied or not by the current value of the `Variable`, checking it possibly costly (`:ThinComputeInterface`)
- Knows which `Block` it belongs to
- Can be relaxed and enforced
- Fundamental design decision: "name" of a `Constraint` = its memory address $\Longrightarrow$ copying a `Constraint` makes a different `Constraint` $\Longrightarrow$ dynamic `Constraint`s always live in `std::lists`
- `ConstraintModification:Modification` (relax/enforce)

Objective

- Abstract concept, does not specify its return value (vector, set, . . .)
- Either minimized or maximized
- Depends from a set of `Variable` (`:ThinVarDepInterface`)
- Must be evaluated w.r.t. the current value of the `Variable`, possibly a costly operation (`:ThinComputeInterface`)
- `RealObjective:Objective` implements "value is an extended real"
- Knows which `Block` it belongs to
- Same fundamental design decision . . .
  (but there is no such thing as a dynamic `Objective`)
- `ObjectiveModification:Modification` (change verse)

Function

- `Function` only deals with (real) values
- Depends from a set of `Variable` (`:ThinVarDepInterface`)
- Must be evaluated w.r.t. the current value of the `Variable`, possibly a costly operation (`:ThinComputeInterface`)
- Approximate computation supported in a quite general way[25] (since `:ThinComputeInterface`, and that does)
- Asynchronous evaluation still not defined
- `FunctionModification[Variables]` for "easy" changes $\Longrightarrow$ reoptimization (shift, adding/removing "quasi separable" `Variable`)

[25] van Ackooij, F. "Incremental bundle methods using upper models" *SIOPT*, 2018

C05Function and C15Function

- C05Function/C15Function deal with 1st/2nd order information (not necessarily continuous)
- General concept of "linearization" (gradient, convex/concave subgradient, Clarke subgradient, ...)
- Multiple linearizations produced at each evaluation (local pool)
- Global pool of linearizations for reoptimization:
  - convex combination of linearizations
  - "important linearization" (at optimality)
- C05FunctionModification[Variables/LinearizationShift] for "easy" changes $\Longrightarrow$ reoptimization (linearizations shift, some linearizations entries changing in simple ways)
- C15Function supports Hessians, unclear how much reoptimization possible/useful

- Generic concept of "something depending on a set of `Variable`"
- Specific implementation demanded to derived classes for efficiency
- "Abstract" STL-like iterator and const-iterator for access
- Other specific methods to describe/search the set
- Specific twist: a `:ThinVarDepInterface` is constructed after and destructed before "its" `Variable`, `clear()` method to avoid un-necessary data structure updating during destruction

ThinComputeInterface

- Generic concept of "something that can take time to evaluate"
- Specific provisions for the fact that the computation can:
  - end in several ways (OK, error, stopped, ...) and be resumedx
  - be influenced by `int`/`double`/`std::string` parameters which can be gathered in a `ComputeConfig:Configuration` object (flexible)
- Defaults so that "simple" objects with no parameter do nothing
- Clear rules about effect of changes in the underlying object during and after `compute()` to allow for "reoptimization"
- Changes may be "explicit" (a `Modification` issued) or "implicit" (changing a `Variable` value do not trigger a `Modification`)
- Asynchronous `compute()` not done yet, TBD soon with Cray™ help: changes in this interface will do the trick everywhere

Block and Solver

- Any # of Solver attached to a Block to solve it
- :Solver for a specific :Block can use the physical representation
  $\Longrightarrow$ no need for explicit Constraint
  $\Longrightarrow$ abstract representation of Block only constructed on demand
- However, Variable are always present (interface with Solver)
- A general-purpose Solver uses the abstract representation
- Dynamic Variable/Constraint can be generated on demand (user cuts/lazy constraints/column generation)
- For a Solver attached to a Block:
  - Variable not belonging to the Block are constants
  - Constraint not belonging to the Block are ignored

  (belonging = declared there or in any sub-Block recursively)
- Objective of sub-Blocks summed to that of father Block if has same verse, otherwise min/max

Solver

- Solver = interface between a Block and algorithms solving it
- Solver:ThinComputeInterface, inherits and extends interface
- Each Solver attached to a single Block, from which it picks all the data, but any # of Solver can be attached to the same Block
- Solutions are written directly into the Variable of the Block
- Individual Solver can be attached to sub-Block of a Block
- Tries to cater for all the important needs:
  - optimal and sub-optimal solutions, provably unbounded/unfeasible
  - time/resource limits for solutions, but restarts (reoptimization)
  - any # of multiple solutions produced on demand
  - lazily reacts to changes in the data of the Block via Modification
- Somehow slanted towards RealObjective (optimality guarantees = upper and lower bounds)
- CDASolver:Solver is "Convex Duality Aware": bounds are associated to dual solutions (possibly, multiple)

Block and Modification

- Most Block components can change, but not all:
  - set of sub-Block
  - # and shape of groups of Variable/Constraint
- Any change is communicated to each interested Solver (attached to the Block or any of its ancestor) via a Modification object
- anyone_there() $\equiv \exists$ interested Solver (Modification needed)
- However, two different kinds of Modification (what changes):
  - physical Modification, only specialized Solver concerned
  - abstract Modification, only Solver using it concerned
- Abstract Modification used to keep both representations in sync
  $\Longrightarrow$ a single change may trigger more than one Modification
  $\Longrightarrow$ concerns_Block() mechanism to avoid this to repeat
  $\Longrightarrow$ parameter in changing methods to avoid useless Modification
- Specialized Solver disregard abstract Modification and vice-versa
- A Block may refuse to support some changes (explicitly declaring it)

Modification

- Almost empty base class, then everything has its own derived ones
- Heavy stuff can be attached to a `Modification` (e.g., added/deleted dynamic `Variable`/`Constraint`)
- Each `Solver` has the responsibility of cleaning up its list of `Modification` (smart pointers → memory eventually released)
- `Solver` supposedly reoptimize to improve efficiency, which is easier if you can see all list of changes at once (lazy update)
- `GroupModification` to (recursively) pack many `Modification` together ⟹ different "channels" in `Block`
- `Modification` processed in the arrival order to ensure consistency
- A `Solver` may optimize the changes (`Modifications` may cancel each outer out ...), but its responsibility

Solution

- Block produces Solution object, possibly using its sub-Blocks'
- Solution can read() its own Block and write() itself back
- Solution is Block-specific rather than Solver-specific
- Solution may save dual information
- Solution may save only a specific subset of primal/dual information
- Linear combination of Solution supported $\Longrightarrow$ "less general" Solution may (automatically) convert in "more general" ones
- Like Block, Solution are tree-structured complex objects

- Block a tree-structured complex object $\Longrightarrow$
  Configuration for them a (possibly) tree-structured complex object
- But also SimpleConfiguration<T>:Configuration
  (T an int, a double, a std::pair<>, ...)
- BlockConfiguration:Configuration sets (recursively):
  - which dynamic Variable/Constraint are generated, how (Solver, time limit, parameters ...)
  - which Solution is produced (what is saved)
  - a bunch of other Block parameters
- BlockSolverConfiguration:Configuration sets (recursively) which Solver are attached to the Block and their ComputeConfiguration:Configuration
- Both can be set (recursively) at once

R^3Block

- Often reformulation crucial, but also relaxation or restriction: `get_R3_Block()` produces one, possibly using sub-`Block`s'
- Obvious special case: copy (clone) should always work
- Available R^3Blocks `:Block`-specific, a `:Configuration` needed
- R^3Block completely independent (new `Variable`/`Constraint`), useful for algorithmic purposes (branch, fix, solve, . . .)
- Solution of R^3Block useful to `Solver` for original `Block`: `map_back_solution()` (best effort in case of dynamic `Variable`)
- Sometimes keeping R^3Block in sync with original necessary: `map_forward_Modification()`, task of original `Block`
- `map_forward_solution()` and `map_back_Modification()` useful, e.g., dynamic generation of `Variable`/`Constraint` in the R^3Block
- `:Block` is in charge of all this, thus decides what it supports

Other useful stuff

- un_any_thing() template functions/macros to extract (std::vector or boost::multi_array of) (std::list of) Variable/Constraint out of a boost_any and work on that
- All tree-structured complex objects (Block, Configuration, Solution) have an (almost) completely automatic factory
- All tree-structured complex objects (...) have methods to serialize/deserialize themselves to netCDF files
- All objects have ">>" std::stream operator, some (Block) also have "<<"

Closer to the ground

- `ColVariable:Variable`: "value = one single real" (possibly $\in \mathbb{Z}$)
- `RowConstraint:Constraint`: "$l \leq$ a real $\leq u$" $\Longrightarrow$ has dual variable (single real) attached to it
- `OneVarConstraint:RowConstraint`: "a real" = a single `ColVariable` $\equiv$ bound constraints
- `FRowConstraint:RowConstraint`: "a real" given by a `Function`
- `FRealObjective:RealObjective`: "value" given by a `Function`
- `LinearFunction:Function`: a linear form in `ColVariable`
- `ColVariableSolution:Solution` uses the abstract representation of any `Block` that only have (`std::vector` or `boost::multi_array` of) (`std::list` of) `ColVariables` to read/write the solution
- `FakeSolver:Solver`: just stashes away all `Modification`

Outline

S*MILPBlock and MILPSolver

- SimpleMILPBlock:Block: an un-structured set of FRowConstraint and one FRealObjective with only LinearFunction on an un-structured set of ColVariable, possibly with attached OneVarConstraint but no sub-Block

- StructuredMILPBlock:SimpleMILPBlock: all sub-Block can be SimpleMILPBlock (hence also StructuredMILPBlock), generic linking constraints are defined among the variables of the father Block and of the sub-Block

TBD MILPSolver:Solver: passes to Cplex any Block that only has any # of groups of ColVariable and FRowConstraint, and a FRealObjective, all with LinearFunction only

TBD MILPSolver to be transformed in "generic" MILP solver interface with a sub-class for SCIP

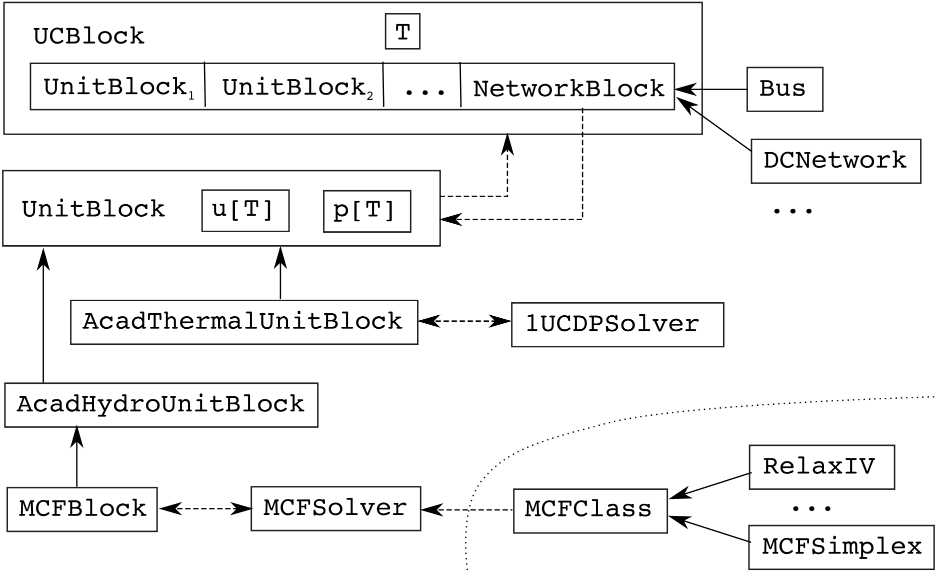
MCFBlock and MCFSolver

- MCFBlock:Block: a Min-Cost Flow Problem
- MCFSolver:Solver: solves a MCFBlock forwarding the MCFClass interface (www.di.unipi.it/optimize/Software/MCF.html) and its existing solvers (<MCFClass>)
- First complete implementation of a Block/Solver pair, with almost all mechanisms (physical/abstract Modification, R^3Block, ...) save for dynamic stuff and sub-Block
- Everything seems to fit, but testing still underway

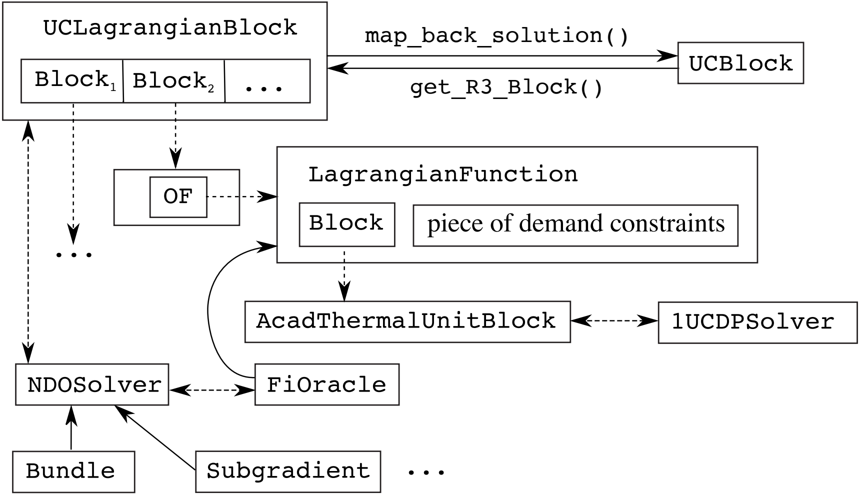
LagrangianFunction [TBD]

- LagrangianFunction:C05Function has one isolated Block + set of (say) LinearFunction to define Lagrangian term
- evaluate() = Block.get_registered_solvers()[i].solve(): asynchronous Solver $\Longrightarrow$ asynchronous Function
- Solution extracted from Block $\equiv$ linearization
- Solver provides local pool
- LagrangianFunction handles global pool
- All changes lead to reoptimization-friendly C05FModification
- BendersFunction should be quite similar

UCBlock and Companion Classes [TBD]



UCLagrangianBlock [TBD]



- Independent from details of units/network
- Multi-level decomposition now (perhaps) possible

Outline

A Lot of Work, Then Maybe Conclusions

- Current pre-beta version sitting tight on GitLab

  `gitlab.com/frangio68/sms_plus_plus_project`

  Private repository, but any interested onlooker/contributor just ask
- Two quite good, (2+1)-years, 2^{15} €/ year, post-doc positions open

  `https://www.unipi.it/ateneo/bandi/assegni/asse2018/inf/28nov2018`

  Deadline 28/11, thanks for helping disseminate
- About time, too, because a lot of work still ahead of us
- True large-scale application still to come, `Solver` to be written
- Asynchronous still to be figured out (but very relevant), good Cray™ folks will lend a helping hand here
- Clearly not for the faint of heart . . .

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  but when it'll work it will be useful in many applications

We are trying. Anyone cares to join?

Acknowledgements

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