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Outline

1 Why bother?

- 2 Decomposition-aware modelling systems
- SMS++: design goals
- SMS++: basic components
- 5 SMS++: existing Block and Solver
- 6 SMS++: (some of) the missing pieces

Conclusions

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- Programming is hard, good programming is harder, optimization is hard, good programming for optimization is extremely hard
- Typically done early on in the career (you)
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- Selfish version of the altruistic reason: if all this work was readily available decomposition would make a lot more sense, and my own work would be more useful

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Decomposition-aware modelling systems

- Decomposition is complex, but so is any Branch-and-X
- Need general-purpose efficient decomposition software:
 - Cplex does Benders', structure automatic or user hints
 - SCIP^[1] does B&C&P (one-level D-W), pricing & reformulation up to the user (plugins)
 - GCG^[1] extends SCIP with automatic and user-defined (one-level) D-W and recently also a generic (one-level) Benders' approach^[2]
 - D-W approaches for two-stage stochastic programs are implemented in DDSIP^[3] and PIPS^[4], the latter interfaced with StructJuMP^[5]
 - The BaPCoD B&C&P code has been used to develop Coluna.jl^[6], doing one-level D-W and (alpha) Benders', multi-level planned
- No multi-level C++, so we started one

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^[1] https://scipopt.org, https://gcg.or.rwth-aachen.de

^[2] Maher "Implementing the Branch-and-Cut approach for a general purpose Benders' decomposition framework" EJOR, 2021

^[3] https://github.com/RalfGollmer/ddsip

^[4] https://github.com/Argonne-National-Laboratory/PIPS

^[5] https://github.com/StructJuMP/StructJuMP.jl

^[6] https://github.com/atoptima/Coluna.jl

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https://gitlab.com/smspp/smspp-project

Open source (LGPL3)

Public as of February 8, but some 8+ years in the making

What SMS++ is

- A core set of C++-17 classes implementing a modelling system that:
 - explicitly supports the notion of $\texttt{Block} \equiv \texttt{nested structure}$
 - separately provides "semantic" information from "syntactic" details (list of constraints/variables ≡ one specific formulation among many)
 - allows exploiting specialised Solver on Block with specific structure
 - manages any dynamic change in the Block beyond "just" generation of constraints/variables
 - supports reformulation/restriction/relaxation of Block
 - has built-in parallel processing capabilities
 - should be able to deal with almost anything (bilevel, PDE, ...)
- An hopefully growing set of specialized Block and Solver
- In perspective an ecosystem fostering collaboration and code sharing

- An algebraic modelling language: Block / Solver are C++ code (although it provides some modelling-language-like functionalities)
- For the faint of heart: primarily written for algorithmic experts (although users may benefit from having many pre-defined Block)
- Stable: only version 0.4, lots of further development ahead, significant changes in interfaces not ruled out, actually expected (although current Block / Solver very thoroughly tested)
- Interfaced with many solvers: only Cplex, SCIP, MCFClass, StOpt (although the list should hopefully grow)

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A Crude Schematic



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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)
- Possibly alternative abstract representation(s) of a Block:
 - one Objective (but possibly vector-valued)
 - any # of groups of (static) Variable
 - any # of groups of std::list of (dynamic) Variable
 - any # of groups of (static) Constraint
 - any # of groups of std::list of (dynamic) Constraint
 groups of Variable/Constraint can be single (std::list) or
 std::vector (...) or boost::multi_array
- Any # of sub-Blocks (recursively), possibly of specific type (e.g., Block::MMCFBlock has k Block::MCFBlock inside)

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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 => copying a Variable makes a different Variable => 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 ⇒ copying a Constraint makes a different Constraint ⇒ dynamic Constraints 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)



- Real-valued Function
- 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^[56] (since :ThinComputeInterface, and that does)
- FunctionModification[Variables] for "easy" changes reoptimization (shift, adding/removing "quasi separable" Variable)

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CO5Function 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)
- CO5FunctionModification[Variables/LinearizationShift] for "easy" changes ⇒ reoptimization (linearizations shift, some linearizations entries changing in simple ways)
- C15Function supports (partial) Hessians
- Arbitrary hierarchy of :Function possible/envisioned, any one that makes sense for application and/or solution method

Closer to the ground

- ColVariable: Variable: "value = one single real" (possibly $\in \mathbb{Z}$)
- RowConstraint: Constraint: "I ≤ a real ≤ u" ⇒ has dual variable (single real) attached to it
- OneVarConstraint:RowConstraint: "a real" = a single ColVariable = bound constraints
- FRowConstraint:RowConstraint: "a real" given by a Function
- FRealObjective:RealObjective: "value" given by a Function
- LinearFunction:Function: a linear form in ColVariable
- DQuadFunction: Function: a separable quadratic form
- Many things missing (AlgebraicFunction, DenseLinearFunction, Matrix/VectorVariable, ...)

Block and Solver

- Any # of Solver attached to a Block to solve it
- Solver for a specific :Block can use the physical representation — no need for explicit Constraint
 - \Longrightarrow abstract representation of Block only constructed on demand
- However, Variable are always present to interface with Solver (this may change thanks to methods factory)
- 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

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Solver

- Solver = interface between a Block and algorithms solving it
- 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)
 - $\bullet\,$ any # of multiple solutions produced on demand
 - lazily reacts to changes in the data of the Block via Modification
- Slanted towards RealObjective (\approx optimality = up/low bounds)
- CDASolver:Solver is "Convex Duality Aware": bounds are associated to dual solutions (possibly, multiple)
- Provides general events mechanism (ThinComputeInterface does)

Block and Modification

- Most Block components can change, but not all:
 - set of sub-Block
 - $\# \ {\tt and} \ {\tt shape} \ {\tt of} \ {\tt groups} \ {\tt of} \ {\tt Variable}/{\tt Constraint}$
- 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 <code>Modification</code>
 - \implies concerns_Block() mechanism to avoid this to repeat
 - \implies parameter in changing methods to avoid useless <code>Modification</code>
- 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

Support to (coarse-grained) Parallel Computation

- Block can be (r/w) lock()-ed and read_lock()-ed
- Iock()-ing a Block automatically lock()s all inner Block
- lock() (but not read_lock()) sets an owner and records its std::thread::id; other lock() from the same thread fail (std::mutex would not work there)
- Similar mechanism for read_lock(), any # of concurrent reads
- Write starvation not handled yet
- A Solver can be "lent an ID" (solving an inner Block)
- The list of Modification of Solver is under an "active guard" (std::atomic)
- Distributed computation under development, can exploit general serialize/deserialize Block capabilities, Cray/HPE "Fugu" framework

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 \implies "less general" Solution may (automatically) convert in "more general" ones
- Like Block, Solution are tree-structured complex objects
- 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
- RowConstraintSolution:Solution same for dual information (RowConstraint), ColRowSolution for both

Configuration

• 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<>, ...)
- [C/O/R]BlockConfiguration:Configuration set [recursively]:
 - which dynamic Variable/Constraint are generated, how (Solver, time limit, parameters ...)
 - which Solution is produced (what is saved)
 - the ComputeConfiguration:Configuration of any Constraint/Objective that needs one
 - a bunch of other Block parameters
- [R]BlockSolverConfiguration:Configuration set [recursively] which Solver are attached to the Block and their ComputeConfiguration:Configuration
- Can be clear()-ed for cleanup

R³Block

- Often reformulation crucial, but also relaxation or restriction: get_R3_Block() produces one, possibly using sub-Blocks'
- Obvious special case: copy (clone) should always work
- \bullet Available $\mathsf{R}^3\mathsf{Blocks}$:Block-specific, a :Configuration needed
- R³Block completely independent (new Variable/Constraint), useful for algorithmic purposes (branch, fix, solve, ...)
- Solution of R³Block useful to Solver for original Block: map_back_solution() (best effort in case of dynamic Variable)
- Sometimes keeping R³Block 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 R³Block
- :Block is in charge of all this, thus decides what it supports

A lot of other support stuff

- All tree-structured complex objects (Block, Configuration, ...) and Solver have an (almost) automatic factory
- All tree-structured complex objects (...) have methods to serialize/deserialize themselves to netCDF files
- A methods factory for changing the physical representation without knowing of which :Block it exactly is (standardised interface)
- AbstractBlock for constructing a model a-la algebraic language, can be derived for "general Block + specific part"
- PolyhedralFunction[Block], very useful for decomposition
- AbstractPath for indexing any Constranit/Variable in a Block
- FakeSolver:Solver stashes away all Modification, UpdateSolver:Solver immediately forwards/R³Bs them

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Main Existing :Block

- MCFBlock/MMCFBlock: single/multicommodity flow (p.o.c.)
- UCBlock for UC, abstract UnitBlock with several concrete (ThermalUnitBlock, HydroUnitBlock, ...), abstract NetworkBlock with a few concrete (DCNetworkBlock)
- LagBFunction: {CO5Function,Block} transforms any Block (with appropriate Objective) into its dual function
- BendersBFunction: {CO5Function,Block} transforms any Block (with appropriate Constraint) into its value function
- StochasticBlock implements realizations of scenarios into any Block (using methods factory)
- SDDPBlock represents multi-stage stochastic programs suitable for Stochastic Dual Dynamic Programming

Main "Basic" :Solver

- MCFSolver: templated p.o.c. wrapper to MCFClass^[7] for MCFBlock
- DPSolver for ThermalUnitBlock (still needs serious work)
- MILPSolver: constructs matrix-based representation of any "LP" Block: ColVariable, FRowConstraint, FRealObjective with LinearFunction or DQuadFunction
- CPXMILPSolver:MILPSolver and SCIPMILPSolver:MILPSolver wrappers for Cplex and SCIP (to be improved)
- BundleSolver:CDASolver: SMS++-native version of^[8] (still shares some code, dependency to be removed), optimizes any (sum of) C05Function, several (but not all) state-of-the-art tricks
- SDDPSolver: wrapper for SDDP solver StOpt^[9] using StochasticBlock, BendersBFunction and PolyhedralFunction
- SDDPGreedySolver: greedy forward simulator for SDDPBlock

[9] https://gitlab.com/stochastic-control/StOpt

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^[7] https://github.com/frangio68/Min-Cost-Flow-Class

^[8] https://gitlab.com/frangio68/ndosolver_fioracle_project

Our Masterpiece: LagrangianDualSolver

- Works for any Block with natural block-diagonal structure: no Objective or Variable, all Constraint linking the inner Block
- Using LagBFunction stealthily constructs the Lagrangian Dual w.r.t. linking Constraint, R³B-ing or "stealing" the inner Block
- Solves the Lagrangian Dual with appropriate CDASolver (e.g., but not necessarily, BundleSolver), provides dual and "convexified" solution in original Block
- Can attach LagrangianDualSolver and (say) :MILPSolver to same Block, solve in parallel!
- Weeks of work in days/hours (if Block of the right form already)
- Hopefully soon BendersDecompositionSolver (crucial component BendersBFunction existing and tested)
- Multilevel nested parallel heterogeneous decomposition by design (but I'll believe it when I'll see it running)

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The many things that we do not have (yet)

- A relaxation-agnostic Branch-and-X Solver (could recycle OOBB?)
- Many other forms of (among many other things):
 - Variable (Vector/MatrixVariable, FunctionVariable, ...)
 - Constraint (SOCConstraint, SDPConstraint, PDEConstraint, BilevelConstraint, EquilibriumConstraint, ...)
 - Objective (RealVectorObjective, ...)
 - Function (AlgebraicFunction, ...)
- Better handling of many things (groups of stuff, Modification, ...)
- Interfaces with many other general-purpose solvers (GuRoBi, OSISolverInterface, Couenne, OR-tools CP-SAT Solver, ...)
- Many many many more :Block and their specialised :Solver
- Translation layers from real modelling languages (AMPL, JuMP, ...)
- In a word: users/mindshare chicken-and-egg problem

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 - a much-needed step towards higher uptake of parallel methods
 - the missing marketplace for specialised solution methods
 - a step towards a reformulation-aware modelling system^[10]

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• Lots of fun to be had, all contributions welcome

[10] F., Perez Sanchez "Transforming Mathematical Models Using Declarative Reformulation Rules" LNCS, 2011

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