Belos Serial Dense Matrix Abstraction

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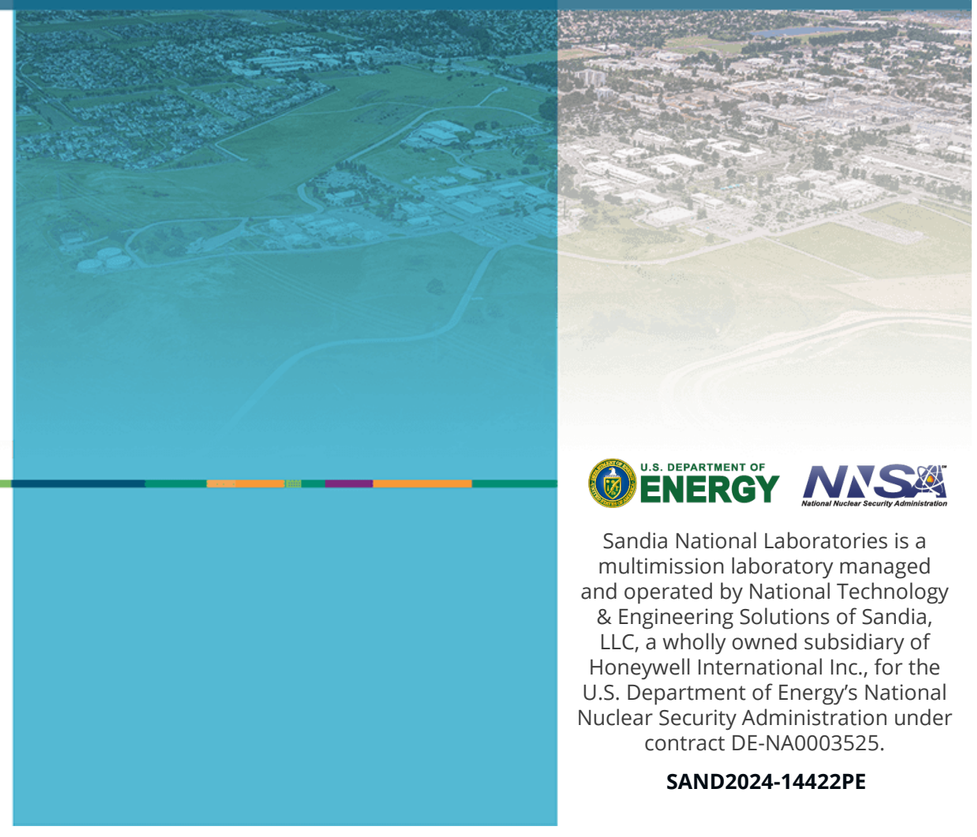

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Belos Templated Linear Solvers

- Next generation linear solver libraries, written in templated C++
  - Iterative methods for solving sparse, matrix-free systems
- Provide a generic interface to a collection of algorithms for solving linear problems
- Algorithms developed with generic programming techniques
  - Algorithmic components:
    - Ease the implementation of complex algorithms
  - Operator/MultiVector interface *(and Teuchos::ScalarTraits)*:
    - Allow the user to leverage their existing software investment
    - Multi-precision solver capability
  - Dense matrix abstract interface (coming soon!)
    - Allows the user to improve performance in advanced architectures
  - Design offers: Interoperability, extensibility, and reusability
- Includes block linear solvers

Belos Solver Categories

Belos provides solvers for:

- Single RHS: $Ax = b$
- Multiple RHS (available simultaneously): $AX = B$
- Multiple RHS (available sequentially): $Ax_i = b_i$, $i=1,\ldots,k$
- Sequential Linear systems: $A_i x_i = b_i$, $i=1,\ldots,k$
- Linear Least Squares: $\min \| Ax - b \|_2$

Leverage research advances of solver community:

- Block methods: block GMRES [Vital], block CG/BICG [O'Leary]
- "Seed" solvers: hybrid GMRES [Nachtigal, et al.]
- "Recycling" solvers for sequences of linear systems: RCG, GCRO-DR [Parks, et al.]
- Restarting, orthogonalization techniques
- Multi-precision methods, communication-avoiding methods

Belos Solvers

Hermitian Systems ($A = A^H$)

- CG / Block CG
- Pseudo-Block CG (Perform single-vector algorithm simultaneously)
- RCG (Recycling Conjugate Gradients)
- PCPG (Projected CG)
- MINRES

Non-Hermitian System ($A \neq A^H$)

- Block GMRES
- Pseudo-Block GMRES (Perform single-vector algorithm simultaneously)
- Block FGMRES (Variable preconditioner)
- Hybrid GMRES
- TFQMR
- GCRO-DR / Block GCRO-DR (Recycling GMRES)
- RCG (Recycling CG)

Linear Least Squares

- LSQR

Belos
(Framework Overview)

$x^{(0)}$ is an initial guess
for $j = 1, 2, ...$
  Solve r from $Mr = b - Ax^{(0)}$
  $v^{(1)} = r/\|r\|_2$
  $s := \|r\|_2 e_1$
  for $i = 1, 2, ..., m$
    Solve w from $Mw = Av^{(i)}$
    for $k = 1, ..., i$
      $h_{k,i} = (w, v^{(k)})$
      $w = w - h_{k,i} v^{(k)}$
    end
    $h_{i+1,i} = \|w\|_2$
    $v^{(i+1)} = w/h_{i+1,i}$
    apply $J_1, ..., J_{i-1}$ on $(h_{1,i}, ..., h_{i+1,i})$
    construct J_i, acting on ith and $(i+1)$st component
    of $h_{.,i}$, such that $(i+1)$st component of $J_i h_{.,i}$ is 0
    $s := J_i s$
    if $s(i+1)$ is small enough then (UPDATE$(\tilde{x}, i)$ and quit)
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GMRES Example

Belos
(Framework Overview)

Multivector Traits

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GMRES Example

Belos
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Problem Classes / Operator Traits

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GMRES Example

[Mat]OrthoManager Class
(ICGS, IMGS, DGKS, SVQB, TSQR)

Belos
(Framework Overview)

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[Mat]OrthoManager Class (ICGS, IMGS, DGKS, SVQB, TSQR)

StatusTest Class

GMRES Example

Belos
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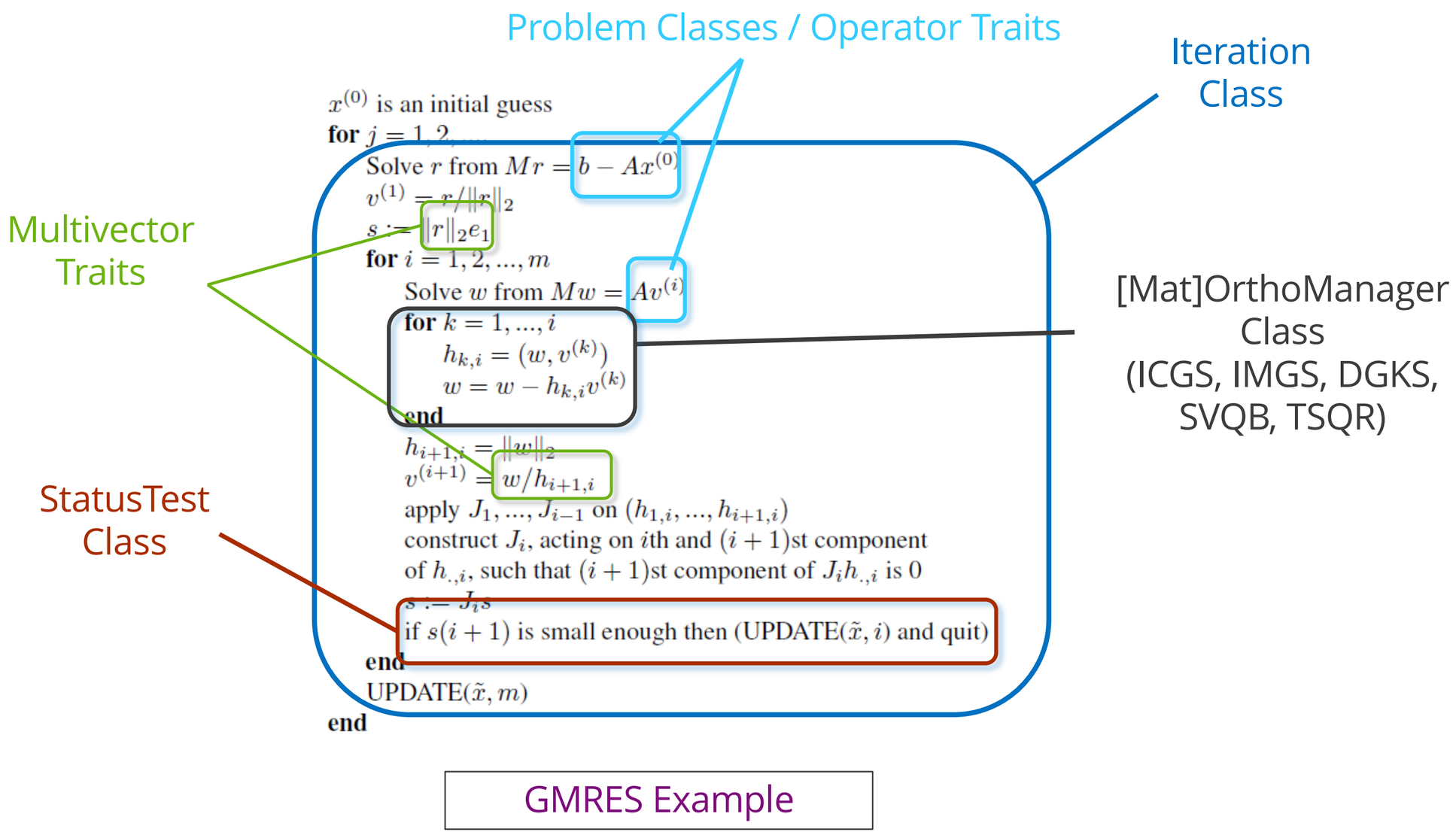

GMRES Example

Belos
(Framework Overview)

SolverManager Class

Problem Classes / Operator Traits

Iteration Class

Multivector Traits

[Mat]OrthoManager Class (ICGS, IMGS, DGKS, SVQB, TSQR)

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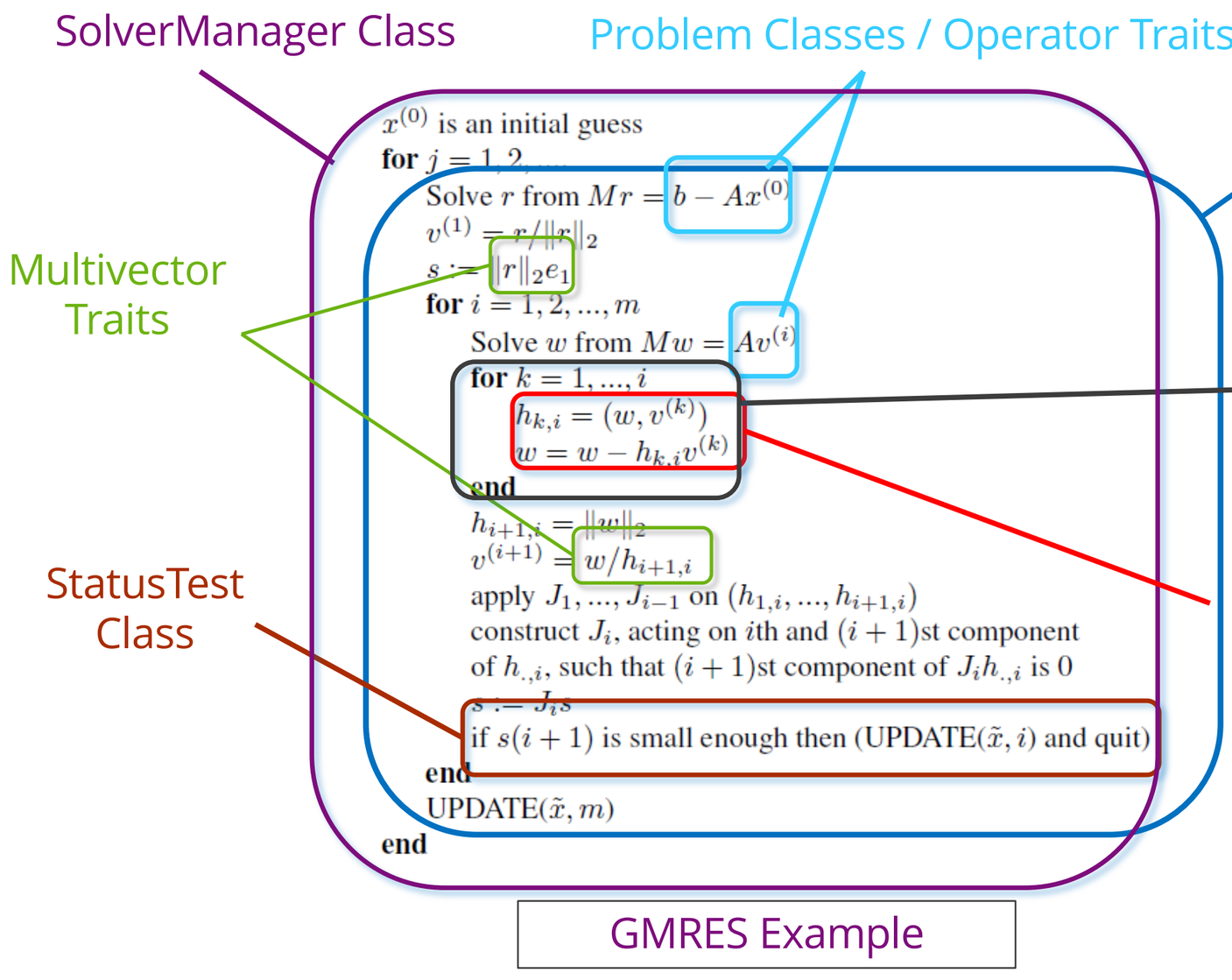


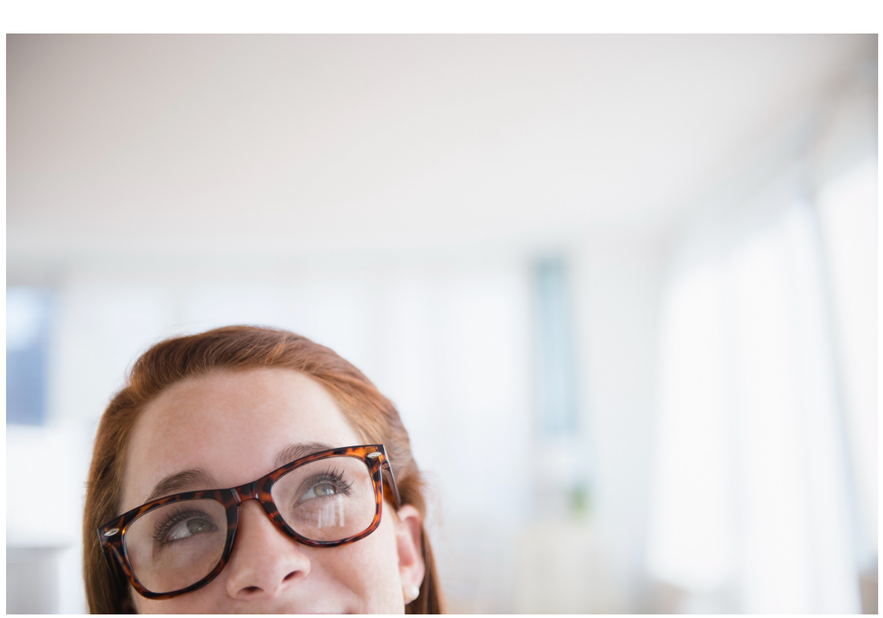
GMRES Example

What is the Dense Matrix Traits interface?

An abstraction of the dense matrix object intended to improve iterative solver performance in advanced architectures

- Default: Teuchos::SerialDenseMatrix<>
- Optionally: Kokkos::DualView<>

So, what is the minimal interface for Belos linear solvers?



What is the Dense Matrix Traits interface?

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static ScalarType & Value( DM& dm, const int i, const int j )
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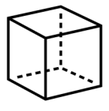

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static int GetNumRows( const DM& dm )
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static int GetStride( const DM& dm )
static void Add( DM& thisDM, const DM& sourceDM)
static void PutScalar( DM& dm, ScalarType value = Teuchos::ScalarTraits<ScalarType>::zero())
static void Scale( DM& dm, ScalarType value)
static void Randomize( DM& dm)
static void Assign( DM& thisDM, const DM& sourceDM)
static typename Teuchos::ScalarTraits<ScalarType>::magnitudeType NormFrobenius( DM& dm)
static typename Teuchos::ScalarTraits<ScalarType>::magnitudeType NormOne( DM& dm)
```

What are the impacts of this change internal to Belos?

Synchronizations are explicitly integrated into Belos solvers and support classes

- Mostly to perform some computation on the dense matrix object
- Sometimes to provide debug information (optional)

* Uses MvDot

Class	# SyncDeviceToHost	Reason
ICGS / IMGS / DGKS	1*	Debugging
BiCGStab / TFQMR	0*	
Block CG	2	Cholesky solve (POTRF/POTRS)
CG / PseudoBlock CG / PseudoBlock Stochastic CG	2*	Extract scalar coefficients
PCPG	6	Extract scalar coefficients (GESVD)
RCG	48*	Recycling subspace (GEMM/GESV/GETRS/SYGV)
Minres	3	Extract scalar coefficients
Block (F)GMRES / PseudoBlock GMRES	3	Update / solve LSQR (ROT/TRSM)
GCRODR	21	Recycling subspace, update / solve LSQR (ROT/TRSM/ GEMM/GETRF/GETRI/GEQRF/UNGQR/GEEV/GESV/GGEVX)
LSQR	2	Debugging

What are the impacts of this change to Belos MV Traits?

The MultiVectorTraits interface has methods with dense matrix/vector object arguments:

```
static void MvTimesMatAddMv( const ScalarType alpha, const MV& A,
                             const DM& B,
                             const ScalarType beta, MV& mv )

static void MvTransMv( const ScalarType alpha, const MV& A, const MV& mv, DM& B)
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```
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```

What about this one?

```
static void MvDot ( const MV& mv, const MV& A, std::vector<ScalarType> &b)
```

Will a synchronization be hidden within this call?

```
Teuchos::ArrayView<ScalarType> av (b);
mv.dot (A, av (0, numVecs));
```

What are the impacts of this change external to Belos?

All of the classes that directly or indirectly use a dense matrix object will have an additional template argument

```
template<class ScalarType, class MV, class OP, class DM = Teuchos::SerialDenseMatrix<int,ScalarType>>
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Direct use of Belos package appears easiest way to employ this new capability

- Thyra interfaces used by Stratimikos may not be compatible with Kokkos::DualView?

What is next for the Dense Matrix Abstraction?

Development and integration of this change has been completed on a fork of Trilinos

- Detailed testing of abstract interface and implementations ☑
- Stokhos, MueLu ☑

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Finalizing the refactor

- Fix remaining testing issues
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Comments / Questions ?