

Debugging Scientific Software

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Inria, DiverSE

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Scientific software: what is it and why is it important?

Scientific computing

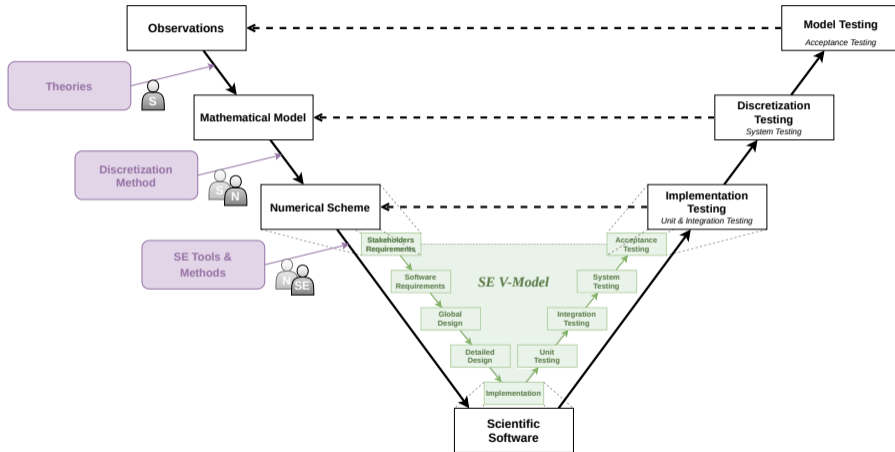
Use of advanced computing capabilities to solve complex problems, aiming to predict the behavior or outcome of a system, man-made or otherwise.

Why is it important?

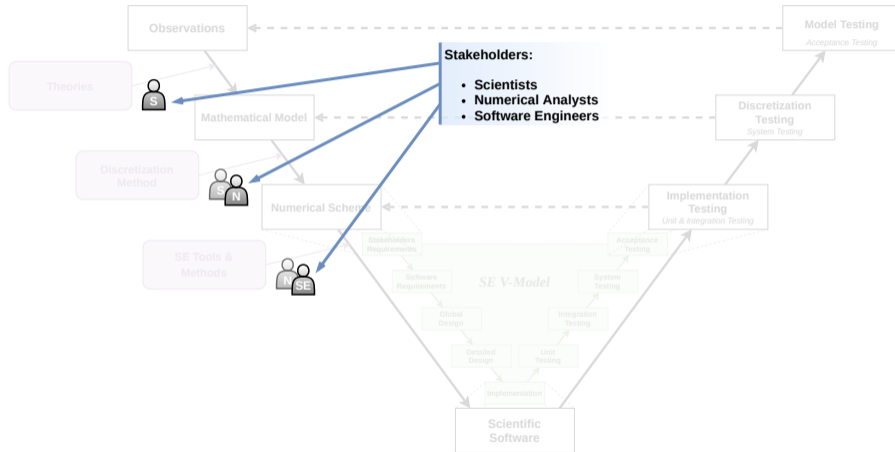
Aerospace engineering, mechanical engineering, material science, chemistry, medicine and many more disciplines, but also...

Basis of scientific findings shaping **policy regarding wicked problems** such as COVID-19 or climate change.

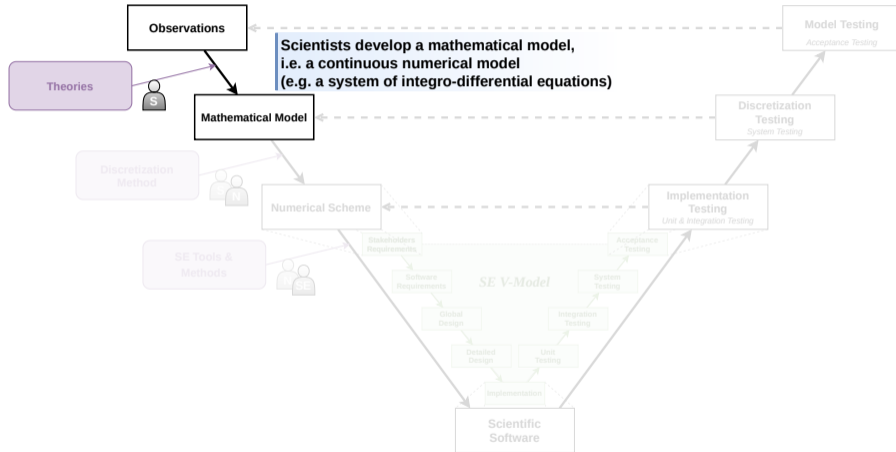
The engineering of scientific software



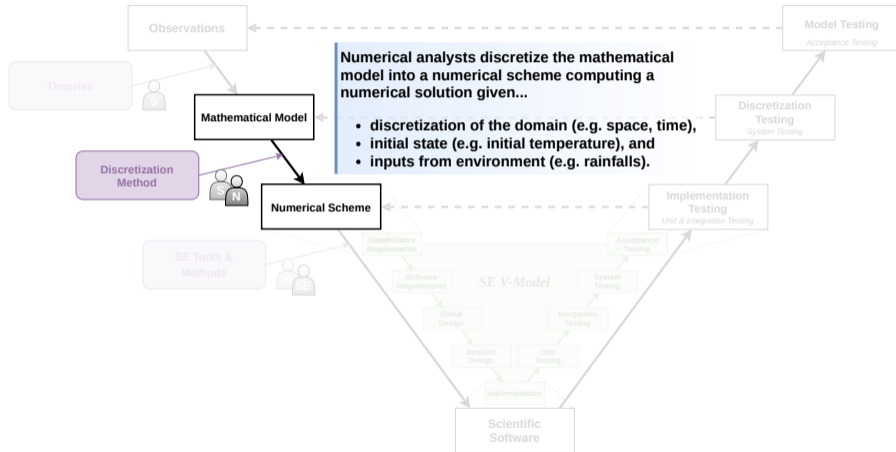
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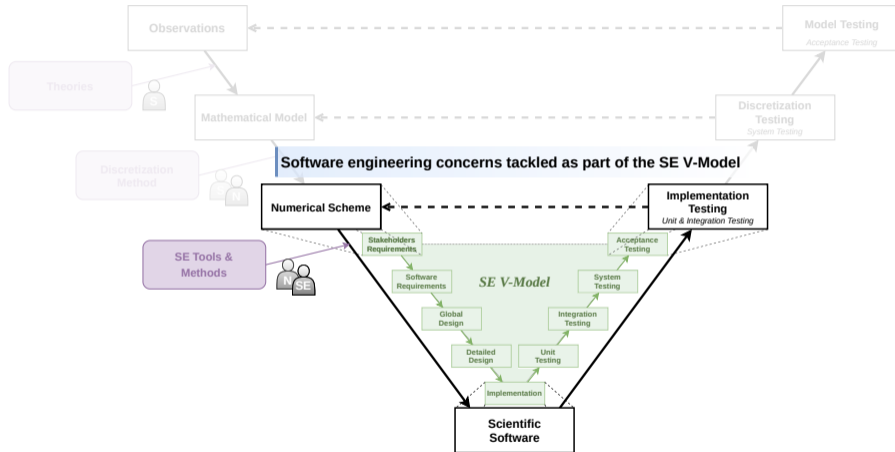
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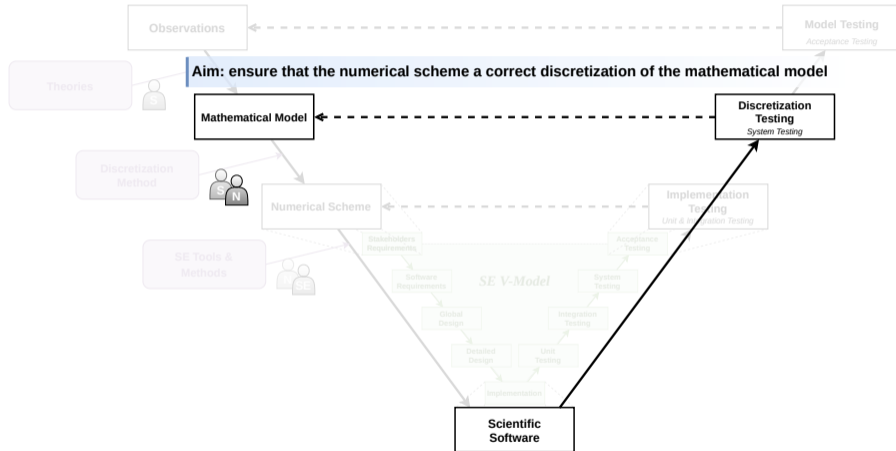
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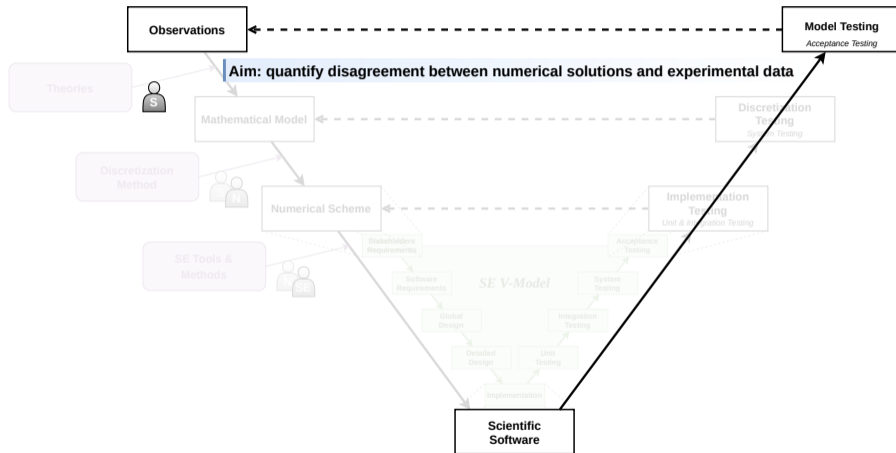
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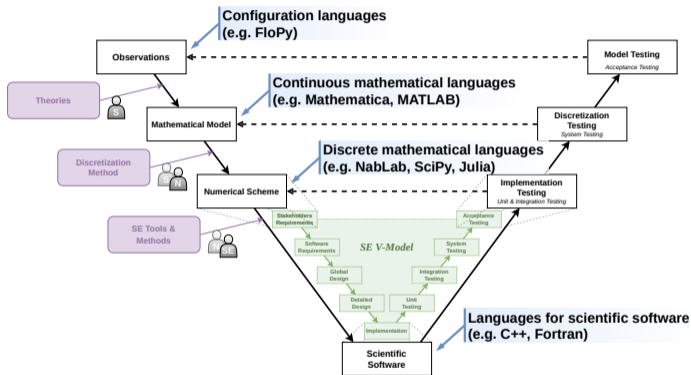
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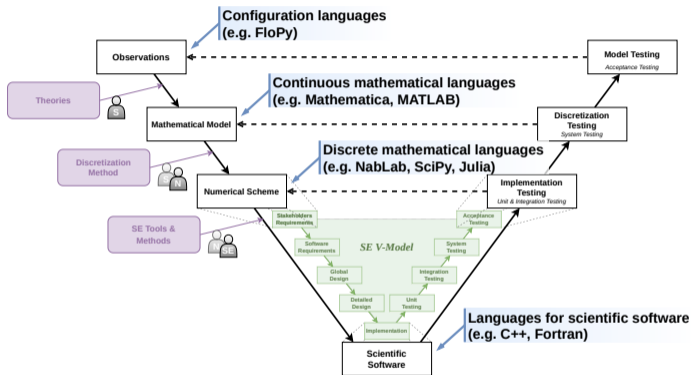


Language matters! Power comes with responsibility!



We investigated the impact of language choice through the **balance of responsibilities** between language users and language designers.

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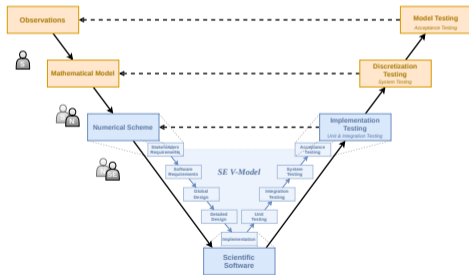
We investigated the impact of language choice through the **balance of responsibilities** between language users and language designers.

Balance of responsibilities: languages for mathematical models

Example languages

Mathematica, MATLAB

Balance of responsibilities



Language users

- Model testing to assess mathematical model fidelity
- Discretization testing on the derived scientific software

Language designers

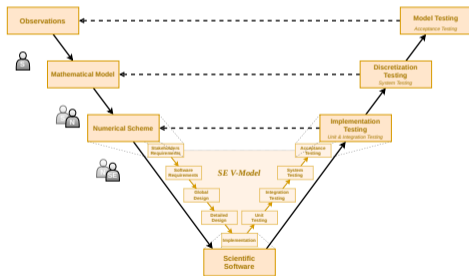
- Discretization testing of the provided continuous mathematical constructs
- Software engineering V&V concerns
- Providing tools for discretization testing

Balance of responsibilities: languages for scientific software

Example languages

C++, Fortran

Balance of responsibilities



Language users

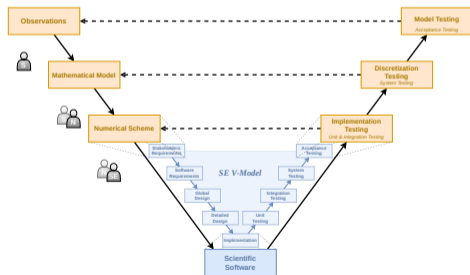
- Software engineering V&V concerns
- Implementation testing
- Discretization testing
- Model testing

Balance of responsibilities: languages for numerical schemes

Example languages

NabLab, Julia, SciPy, GNU Octave

Balance of responsibilities



Language users

- Implementation testing
- Discretization testing
- Model testing

Language designers

- Software engineering V&V concerns
- Implementation testing of the provided discrete mathematical constructs
- **Providing tools for implementation testing**

NabLab: Executable DSL (xDSL) for **numerical analysis**.

Abstract syntax: Metamodel reifying **domain concepts**, e.g.,

- Matrices, vectors, scalars
- Algebraic expressions over those
- Mathematical functions
- Iterative control structures

Operational semantics:

- Metamodel defining **model state** during the execution
- Set of execution rules \Rightarrow **Interpreter**

Example NABLAB model: IterativeHeatEquation

Example NabLab model: Solving the heat equation with iterative numerical method.

```
iterate n while (t^{n+1} < stopTime && n+1 < maxIterations),  
    k while (residual > ε && check(k+1 < maxIterationsK));  
  
UpdateU: VcEcells(), u^{n+1, k+1}{c} = u^{n}{c} + α{c, c} * u^{n+1, k}{c} +  
    Σ{d∈neighbourCells(c)} (α{c, d} * u^{n+1, k}{d});  
ComputeResidual: residual = Max{j ∈ cells()}(abs(u^{n+1, k+1}{j} - u^{n+1, k}{j}));  
ComputeTn: t^{n+1} = t^{n} + δt;
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Example invariant to check: $\text{residual}_{n,k} > \text{residual}_{n,k+1}$

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ComputeTn:  $t^{n+1} = t^n + \delta t;$ 
```

Example invariant to check: $\text{residual}_{n,k} > \text{residual}_{n,k+1}$

Available facilities:

- Output capabilities \Rightarrow designed for **production use**, not debugging.

```
VtkOutput
{
  periodReferenceVariable = iterativeHeatEquation.n;
  outputVariables = iterativeHeatEquation.u as "Temperature";
}
```

- Interactive debugging \Rightarrow **impractical** for such highly iterative software.

```
UpdateU: VcEcells(), u^{n+1, k+1}{c} =
  u^{n}{c} +  $\alpha$ {c, c} * u^{n+1, k}{c} +
   $\sum_{d \in \text{neighbourCells}(c)}$  ( $\alpha$ {c, d} * u^{n+1, k}{d});
```

Preferred approach:

- ▶ **Logging and monitoring** of domain-specific properties (e.g., physics conservation laws, numerical invariants).

General obstacles to **domain-level** logging and monitoring facilities for xDSLs:

- Restricted DSL expressivity:
 - Introducing language constructs **goes against SoC** (e.g., printf, if)
 - **Different expressivity** than offered by the DSL might be required
- Domain-specificness:
 - Cannot reuse libraries through **domain concepts** (e.g., Apache log4x)
 - Additional development costs **for each DSL** to support

Logging and monitoring are often **dependent on one another**:

- Monitoring can **operate on derived data** obtained through logging mechanisms
- Logging can be **triggered or altered** upon (in)validation of monitored properties

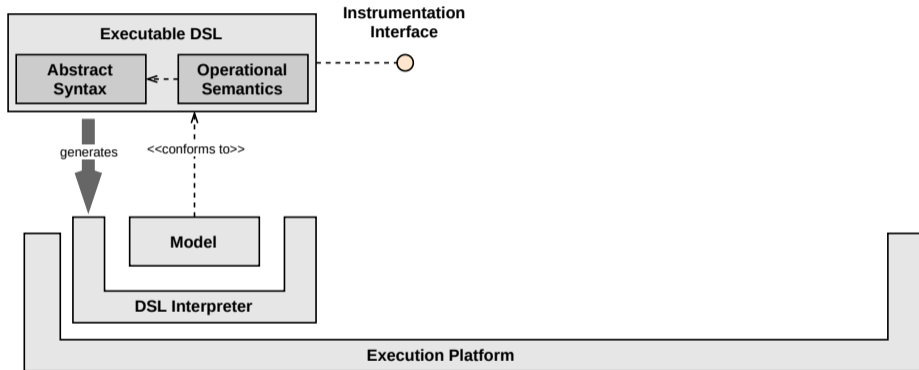
Yet, obstacles prevent **domain experts** from leveraging these complementarities:

- Requires **DSL support** for logging and monitoring frameworks
- Requires **domain-level interoperability** between frameworks

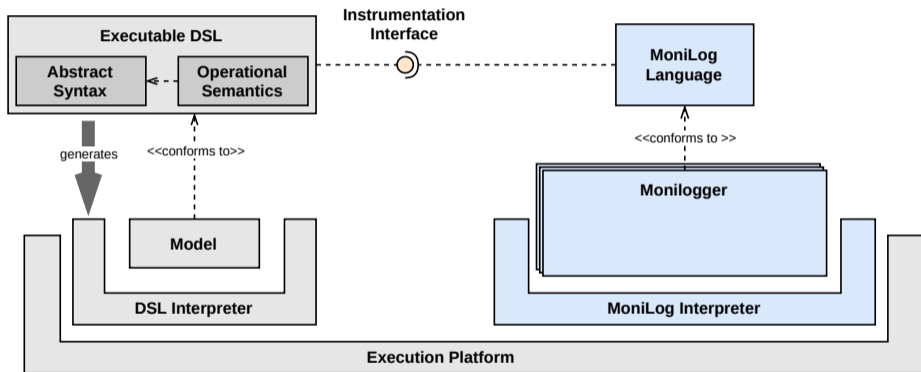
Proposed solution: `MONILOG`

- ▶ **Language-agnostic, unifying framework** for runtime monitoring and logging allowing to define loggers, runtime monitors and combinations of the two, a.k.a. *moniloggers*.

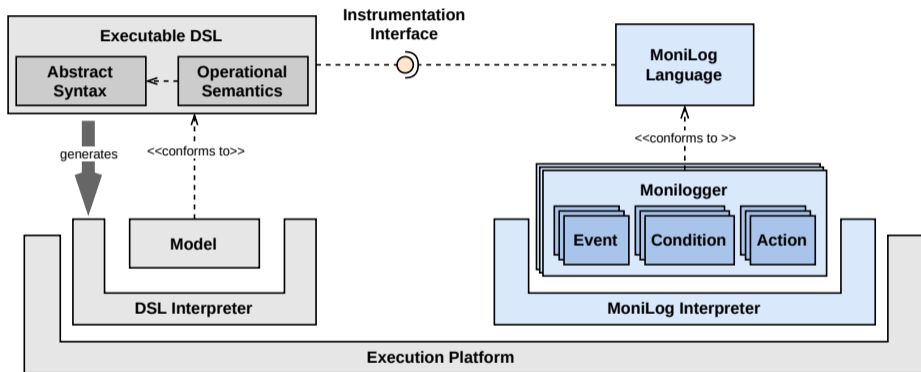
Overview of the approach



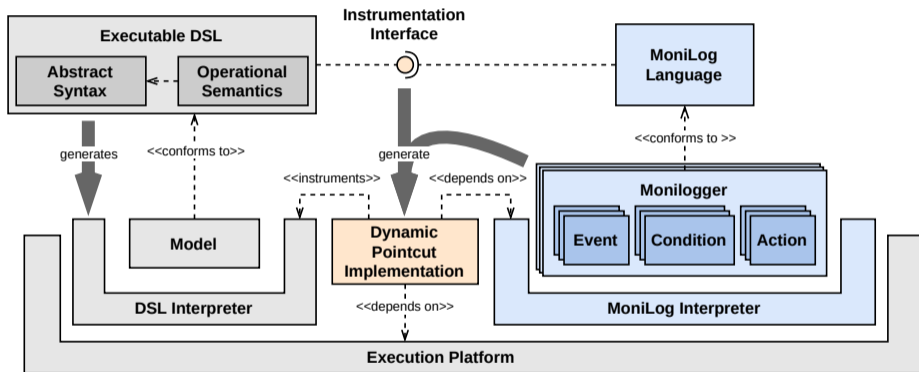
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Overview of the approach



A MONILOG specification allows to

- define instrumentation-specific variables,
- declare the execution events of interest,
- register moniloggers to these events, which can
 - update instrumentation variables,
 - access the execution state of the running model,
 - evaluate expressions with languages available on the execution platform,
 - call various appenders (e.g., file, message queue, console),
 - start/stop moniloggers

Example use on NABLAB

```
IterativeHeatEquation-MonitorResidual.mnlg
package iterativeheatequation

import org.gemoc.monilog.stl.*
import fr.cea.nabla.monilog.nablablib.*
import IterativeHeatEquation.*

@setup {
  prevResidual = 1.0;
}

@event ComputeTnReturned {
  after call ComputeTn
}

@event ResidualUpdated {
  after call ComputeResidual
}

@monilogger correctResidual {
  when ResidualUpdated
  if (context(residual) > prevResidual)
  then {
    NabLabConsoleAppender.call(
      StringLayout.call("[n={0,number,000}, k={1,number,00}] " +
        "Incorrect residual! " +
        "current residual: {2,number,0.0E0}, " +
        "previous residual: {3,number,0.0E0}",
        context(n), context(k), context(residual), prevResidual));
    correctResidual.stop();
    resetResidual.stop();
  } else {
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    prevResidual = context(residual);
  }
}

@monilogger resetResidual {
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  }
}

IterativeHeatEquation.n
InitD: VcCells(), D{c} = 1.0;

ComputeDeltaTn:  $\delta t = \text{Min}(c\text{Cells}()) \{V\{c\}/D\{c\}\} * 0.1;$ 
ComputeV: V{cCells()}, V{ij} = 0.5 *  $\sum\{p\text{NodesOfCell}()\}\{\text{det}(X\{p\}, X\{p+1\})\};$ 
ComputeFaceLength: VfFaces(), faceLength{f} = 0.5 *  $\sum\{p\text{NodesOfFace}()\}\{\text{norm}(X\{p\}, X\{p+1\})\};$ 
ComputeFaceConductivity: VfFaces(), faceConductivity{f} = 2.0 *  $\|f\{c\}c\text{CellsOfFace}()\};$ 

// Assembling of the diffusion matrix
@ComputeAlphaCoeff: VcCells(), {
  let R aDiag = 0.0;
  @ VdNeighbourCells(c), VfCommonFace(c,d), {
    let R aExtraDiag =  $\delta t / V\{c\} * \{faceLength\{f\} * faceConductivity\{f\} / n\{a\{c, d\}\} = a\text{ExtraDiag};$ 
    aDiag = aDiag + aExtraDiag;
  }
  a{c, c} = -aDiag;
}

UpdateU: VcCells(),  $u^{n+1, k+1}\{c\} = u^n\{n\}\{c\} + a\{c, c\} * u^{n+1, k}\{c\} + \sum\{d\text{EdgesOfCell}()\}\{d\text{NodesOfFace}()\}\{u^{n+1, k}\{j\} - u^{n+1, k}\{i\}\};$ 
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Console
NabLab Console
[n=018, k=09] current residual: 1.1E-6, previous residual: 1.8E-6
[n=018, k=10] current residual: 7.0E-7, previous residual: 1.1E-6
[n=018, k=11] current residual: 4.4E-7, previous residual: 7.0E-7
[n=018, k=12] current residual: 2.8E-7, previous residual: 4.4E-7
[n=018, k=13] current residual: 1.8E-7, previous residual: 2.8E-7
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[n=018, k=17] current residual: 3.6E-8, previous residual: 5.3E-8
[n=018, k=18] current residual: 2.5E-8, previous residual: 3.6E-8
[n=018, k=19] current residual: 1.7E-8, previous residual: 2.5E-8
[n=018, k=20] current residual: 1.2E-8, previous residual: 1.7E-8
[n=018, k=21] current residual: 8.5E-9, previous residual: 1.2E-8
[n=019, k=01] current residual: 9.0E-3, previous residual: 1.0E0
[n=019, k=02] current residual: 7.0E-4, previous residual: 9.0E-3
[n=019, k=03] current residual: 1.0E-4, previous residual: 7.0E-4
[n=019, k=04] current residual: 2.4E-5, previous residual: 1.0E-4
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[n=019, k=06] current residual: 3.9E-6, previous residual: 8.4E-6
[n=019, k=07] current residual: 1.9E-6, previous residual: 3.9E-6
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residual decreases while iterating over k

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ComputeDeltaTn:  $\delta t = \text{Min}(c\text{Cells}())\{V\{c\}/D\{c\} * 0.1;$ 
ComputeV: VjCells(), V{j} = 0.5 *  $\sum\{p\text{NodesOfCell}()\}\{\text{det}(X\{p\}, X\{p+1\});$ 
ComputeFaceLength: VfFaces(), faceLength{f} = 0.5 *  $\sum\{p\text{NodesOfFace}()\}\{\text{norm}(X\{p\}, X\{p+1\});$ 
ComputeFaceConductivity: VfFaces(), faceConductivity{f} = 2.0 *  $\|(\text{cCellsOfFace}()$ 

// Assembling of the diffusion matrix
@ComputeAlphaCoeff: VcCells(), {
  R aDiag = 0.0;
  neighbourCells(c), VfCommonFace(c,d), {
    let R aExtraDiag =  $\delta t / V\{c\} * (\text{faceLength}\{f\} * \text{faceConductivity}\{f\} / n$ 
    a{c, d} = aExtraDiag;
    aDiag = aDiag + aExtraDiag;
  }
  a{c, c} = -aDiag;
}

UpdateU: VcCells(),  $u^{n+1, k+1}\{c\} = u^n\{c\} + a\{c, c\} * u^{n+1, k}\{c\} + \sum\{d\text{En}$ 
ComputeResidual: residual =  $\text{Max}\{j \in \text{cells}()\}\{\text{abs}(u^{n+1, k+1}\{j\} - u^{n+1, k}\{j}\);$ 
ComputeTn:  $t^{n+1} = t^n + \delta t;$ 

Console
NabLab Console
[n=018, k=09] current residual: 1.1E-6, previous residual: 1.8E-6
[n=018, k=10] current residual: 7.0E-7, previous residual: 1.1E-6
[n=018, k=11] current residual: 4.4E-7, previous residual: 7.0E-7
[n=018, k=12] current residual: 2.8E-7, previous residual: 4.4E-7
[n=018, k=13] current residual: 1.8E-7, previous residual: 2.8E-7
[n=018, k=14] current residual: 1.2E-7, previous residual: 1.8E-7
[n=018, k=15] current residual: 8.0E-8, previous residual: 1.2E-7
[n=018, k=16] current residual: 5.3E-8, previous residual: 8.0E-8
[n=018, k=17] current residual: 3.6E-8, previous residual: 5.3E-8
[n=018, k=18] current residual: 2.5E-8, previous residual: 3.6E-8
[n=018, k=19] current residual: 1.7E-8, previous residual: 2.5E-8
[n=018, k=20] current residual: 1.2E-8, previous residual: 1.7E-8
[n=018, k=21] current residual: 8.5E-9, previous residual: 1.2E-8
[n=019, k=01] current residual: 9.0E-3, previous residual: 1.0E0
[n=019, k=02] current residual: 7.0E-4, previous residual: 9.0E-3
[n=019, k=03] current residual: 1.0E-4, previous residual: 7.0E-4
[n=019, k=04] current residual: 2.4E-5, previous residual: 1.0E-4
[n=019, k=05] current residual: 8.4E-6, previous residual: 2.4E-5
[n=019, k=06] current residual: 3.9E-6, previous residual: 8.4E-6
[n=019, k=07] current residual: 1.9E-6, previous residual: 3.9E-6
[n=019, k=08] current residual: 1.1E-6, previous residual: 1.9E-6
```

Example use on NABLAB

The image shows a screenshot of the NABLAB environment with two code windows and a console window. The left window, `IterativeHeatEquation-MonitorResidual.mnlg`, contains monitoring and logging code. The right window, `IterativeHeatEquation.n`, contains the main simulation code. The console window at the bottom shows the output of the simulation.

Code in `IterativeHeatEquation-MonitorResidual.mnlg`:

```
package iterativeheatequation
import org.gemoc.monitors.stl.*
import fr.cea.nablab.*
import IterativeHeatEquation

@setup {
  prevResidual = 1.0;
}

@event ComputeTnReturned {
  after call ComputeTn
}

@event ResidualUpdated {
  after call ComputeResidual
}

@monilogger correctResidual {
  when ResidualUpdated
  if (context(residual) > prevResidual)
  then {
    NabLabConsoleAppender.call(
      StringLayout.call("[n={0,number,000}, k={1,number,00}] " +
        "Incorrect residual! " +
        "current residual: {2,number,0.0E0}, " +
        "previous residual: {3,number,0.0E0}",
        context(n), context(k), context(residual), prevResidual));
    correctResidual.stop();
    resetResidual.stop();
  } else {
    NabLabConsoleAppender.call(
      StringLayout.call("[n={0,number,000}, k={1,number,00}] " +
        "current residual: {2,number,0.0E0}, " +
        "previous residual: {3,number,0.0E0}",
        context(n), context(k), context(residual), prevResidual));
    prevResidual = context(residual);
  }
}

@monilogger resetResidual {
  when ComputeTnReturned
  {
    prevResidual = 1.0;
  }
}
```

Code in `IterativeHeatEquation.n`:

```
InitD: VcCells(), D{c} = 1.0;

ComputeDeltaTn:  $\delta t = \text{Min}(c\text{Cells}())\{V\{c\}/D\{c\} * 0.1;$ 
ComputeV: VjCells(), V{j} = 0.5 *  $\sum\{p\text{NodesOfCell}()\}\{\text{det}(X\{p\}, X\{p+1\});$ 
ComputeFaceLength: VfFaces(), faceLength{f} = 0.5 *  $\sum\{p\text{NodesOfFace}()\}\{\text{norm}(X\{p\}, X\{p+1\});$ 
ComputeFaceConductivity: VfFaces(), faceConductivity{f} = 2.0 *  $\prod\{c\text{CellsOfFace}()\}\{D\{c\};$ 

// Assembling of the diffusion matrix
@ComputeAlphaCoeff: VcCells(), {
  R aDiag = 0.0;
  neighbourCells(c), VfCommonFace(c,d), {
    let R aExtraDiag =  $\delta t / V\{c\} * \{faceLength\{f\} * faceConductivity\{f\} / n$ 
    a{c, d} = aExtraDiag;
    aDiag = aDiag + aExtraDiag;
  }
  a{c, c} = -aDiag;
}

UpdateU: VcCells(),  $u^{n+1, k+1}\{c\} = u^n\{c\} + a\{c, c\} * u^{n+1, k}\{c\} + \sum\{d\text{EdgesOfCell}()\}\{D\{d\} * u^{n+1, k}\{d\} - u^{n+1, k}\{c\}\};$ 
ComputeResidual: residual =  $\text{Max}\{j \in \text{cells}()\}\{\text{abs}(u^{n+1, k+1}\{j\} - u^{n+1, k}\{j\});$ 
ComputeTn:  $t^{n+1} = t^n + \delta t;$ 
```

Console Output:

```
NabLab Console
[n=018, k=09] current residual: 1.1E-6, previous residual: 1.8E-6
[n=018, k=10] current residual: 7.0E-7, previous residual: 1.1E-6
[n=018, k=11] current residual: 4.4E-7, previous residual: 7.0E-7
[n=018, k=12] current residual: 2.8E-7, previous residual: 4.4E-7
[n=018, k=13] current residual: 1.8E-7, previous residual: 2.8E-7
[n=018, k=14] current residual: 1.2E-7, previous residual: 1.8E-7
[n=018, k=15] current residual: 8.0E-8, previous residual: 1.2E-7
[n=018, k=16] current residual: 5.3E-8, previous residual: 8.0E-8
[n=018, k=17] current residual: 3.6E-8, previous residual: 5.3E-8
[n=018, k=18] current residual: 2.5E-8, previous residual: 3.6E-8
[n=018, k=19] current residual: 1.7E-8, previous residual: 2.5E-8
[n=018, k=20] current residual: 1.2E-8, previous residual: 1.7E-8
[n=018, k=21] current residual: 8.5E-9, previous residual: 1.2E-8
[n=019, k=01] current residual: 9.0E-3, previous residual: 1.0E0
[n=019, k=02] current residual: 7.0E-4, previous residual: 9.0E-3
[n=019, k=03] current residual: 1.0E-4, previous residual: 7.0E-4
[n=019, k=04] current residual: 2.4E-5, previous residual: 1.0E-4
[n=019, k=05] current residual: 8.4E-6, previous residual: 2.4E-5
[n=019, k=06] current residual: 3.9E-6, previous residual: 8.4E-6
[n=019, k=07] current residual: 1.9E-6, previous residual: 3.9E-6
[n=019, k=08] current residual: 1.1E-6, previous residual: 1.9E-6
```

Annotations:

- Initializing variable storing value of previous residual:** Points to `prevResidual = 1.0;` in the `setup` block.
- Declaring events of interest:** Points to `ComputeTnReturned` and `ResidualUpdated` event declarations.
- residual decreases while iterating over k:** Points to the `correctResidual` monilogger logic.

Example use on NABLAB

The image displays a NABLAB code editor with two files open: `IterativeHeatEquation-MonitorResidual.mnlg` and `IterativeHeatEquation.n`. The left pane shows the monitor code, and the right pane shows the simulation code. A console window at the bottom shows the output of the simulation.

Annotations:

- Initializing variable storing value of previous residual:** Points to `prevResidual = 1.0;` in the `setup` block.
- Declaring events of interest:** Points to `event ComputeTnReturned` and `event ResidualUpdated`.
- Checking the invariant:** Points to the `correctResidual` block.
- residual decreases while iterating over k:** Points to the `ComputeResidual` line in the `UpdateU` block.

Code Snippets:

```
package iterativeheatequation
import org.gemoc.monitors.stl.*
import fr.cea.nabl.*
import IterativeHeatEquation

@setup {
  prevResidual = 1.0;
}

@event ComputeTnReturned {
  after call ComputeTn
}

@event ResidualUpdated {
  after call ComputeResidual
}

@monilogger correctResidual {
  when ResidualUpdated
  if (context(residual) > prevResidual)
  then {
    NabLabConsoleAppender.call(
      StringLayout.call("[n={0,number,000}, k={1,number,00}] " +
        "Incorrect residual! " +
        "current residual: {2,number,0.0E0}, " +
        "previous residual: {3,number,0.0E0}",
        context(n), context(k), context(residual), prevResidual));
    correctResidual.stop();
    resetResidual.stop();
  }
  else {
    NabLabConsoleAppender.call(
      StringLayout.call("[n={0,number,000}, k={1,number,00}] " +
        "current residual: {2,number,0.0E0}, " +
        "previous residual: {3,number,0.0E0}",
        context(n), context(k), context(residual), prevResidual));
    prevResidual = context(residual);
  }
}

@monilogger resetResidual {
  when ComputeTnReturned
  {
    prevResidual = 1.0;
  }
}
```

```
InitID: VcCells(), D{c} = 1.0;

ComputeDeltaTn:  $\delta t = \text{Min}(c\text{Cells}()) \{V\{c\}/D\{c\} * 0.1;$ 
ComputeV: V{cCells()}, V{j} = 0.5 *  $\sum\{p\text{NodesOfCell}()\}\{\text{det}(X\{p\}, X\{p+1\});$ 
ComputeFaceLength: V{Faces()}, faceLength{f} = 0.5 *  $\sum\{p\text{NodesOfFace}()\}\{\text{norm}(X\{p\}, X\{p+1\});$ 
ComputeFaceConductivity: V{Faces()}, faceConductivity{f} = 2.0 *  $\|f\{c\}\{c\text{CellsOfFace}()\};$ 

// Assembling of the diffusion matrix
@ComputeAlphaCoeff: VcCells(), {
  R aDiag = 0.0;
  neighbourCells(c), V{CommonFace(c,d), {
    let R aExtraDiag =  $\delta t / V\{c\} * \{faceLength\{f\} * faceConductivity\{f\} / n$ 
    a{c, d} = aExtraDiag;
    aDiag = aDiag + aExtraDiag;
  }
  a{c, c} = -aDiag;
}

UpdateU: VcCells(),  $u^{n+1, k+1}\{c\} = u^n\{c\} + \alpha\{c, c\} * u^{n+1, k}\{c\} + \sum\{d\text{En}$ 
ComputeResidual: residual =  $\text{Max}\{j \in \text{cells}()\}\{\text{abs}(u^{n+1, k+1}\{j\} - u^{n+1, k}\{j\});$ 
ComputeTn:  $t^{n+1} = t^n + \delta t;$ 
```

Console Output:

```
NabLab Console
[n=018, k=09] current residual: 1.1E-6, previous residual: 1.8E-6
[n=018, k=10] current residual: 7.0E-7, previous residual: 1.1E-6
[n=018, k=11] current residual: 4.4E-7, previous residual: 7.0E-7
[n=018, k=12] current residual: 2.8E-7, previous residual: 4.4E-7
[n=018, k=13] current residual: 1.8E-7, previous residual: 2.8E-7
[n=018, k=14] current residual: 1.2E-7, previous residual: 1.8E-7
[n=018, k=15] current residual: 8.0E-8, previous residual: 1.2E-7
[n=018, k=16] current residual: 5.3E-8, previous residual: 8.0E-8
[n=018, k=17] current residual: 3.6E-8, previous residual: 5.3E-8
[n=018, k=18] current residual: 2.5E-8, previous residual: 3.6E-8
[n=018, k=19] current residual: 1.7E-8, previous residual: 2.5E-8
[n=018, k=20] current residual: 1.2E-8, previous residual: 1.7E-8
[n=018, k=21] current residual: 8.5E-9, previous residual: 1.2E-8
[n=019, k=01] current residual: 9.0E-3, previous residual: 1.0E0
[n=019, k=02] current residual: 7.0E-4, previous residual: 9.0E-3
[n=019, k=03] current residual: 1.0E-4, previous residual: 7.0E-4
[n=019, k=04] current residual: 2.4E-5, previous residual: 1.0E-4
[n=019, k=05] current residual: 8.4E-6, previous residual: 2.4E-5
[n=019, k=06] current residual: 3.9E-6, previous residual: 8.4E-6
[n=019, k=07] current residual: 1.9E-6, previous residual: 3.9E-6
[n=019, k=08] current residual: 1.1E-6, previous residual: 1.9E-6
```

Example use on NABLAB

The image displays a screenshot of the NABLAB code editor with two files open: `IterativeHeatEquation-MonitorResidual.mnlg` and `IterativeHeatEquation.n`. The left pane shows the monitoring code, and the right pane shows the simulation code. A console window at the bottom shows the output of the simulation.

Annotations:

- Initializing variable storing value of previous residual:** Points to `prevResidual = 1.0;` in the `setup` block.
- Declaring events of interest:** Points to `event ComputeTnReturned` and `event ResidualUpdated`.
- Checking the invariant:** Points to the `if (context(residual) > prevResidual)` condition in the `correctResidual` block.
- Logging the values of interest and storing residual for next iteration:** Points to the `correctResidual.call` and `resetResidual.call` blocks.
- residual decreases while iterating over k:** Points to the `correctResidual` block.

Code Snippets:

```
package iterativeheatequation
import org.gemc.monitors.*
import fr.cea.nablab.*
import IterativeHeatEquation

@setup {
  prevResidual = 1.0;
}

@event ComputeTnReturned {
  after call ComputeTn
}

@event ResidualUpdated {
  after call ComputeResidual
}

@monilogger correctResidual {
  when ResidualUpdated
  if (context(residual) > prevResidual)
  then {
    NabLabConsoleAppender.call(
      StringLayout.call(["n={0,number,000}, k={1,number,00} " +
        "Incorrect residual! " +
        "current residual: {2,number,0.0E0}, " +
        "previous residual: {3,number,0.0E0}",
        context(n), context(k), context(residual), prevResidual));
    correctResidual.stop();
    resetResidual.stop();
  } else {
    NabLabConsoleAppender.call(
      StringLayout.call(["n={0,number,000}, k={1,number,00} " +
        "current residual: {2,number,0.0E0}, " +
        "previous residual: {3,number,0.0E0}",
        context(n), context(k), context(residual), prevResidual));
    prevResidual = context(residual);
  }
}

@monilogger resetResidual {
  when ComputeTnReturned
  {
    prevResidual = 1.0;
  }
}
```

```
IterativeHeatEquation.n
InitD: VcCells(), D{c} = 1.0;

ComputeDeltaTn:  $\delta t = \text{Min}(c\text{Cells}()) \{V\{c\}/D\{c\} * 0.1;$ 
ComputeV: VfCells(), V{j} = 0.5 *  $\sum\{p\text{NodesOfCell}(j)\}(\text{det}(X\{p\}, X\{p+1\}));$ 
ComputeFaceLength: VfFaces(), faceLength{f} = 0.5 *  $\sum\{p\text{NodesOfFace}(f)\}(\text{norm}(X\{p\}, X\{p+1\}));$ 
ComputeFaceConductivity: VfFaces(), faceConductivity{f} = 2.0 *  $\|f\{c\}E\{c\}\text{OfFace}(f);$ 

// Assembling of the diffusion matrix
@ComputeAlphaCoeff: VcCells(), {
  R aDiag = 0.0;
  neighbourCells(c), VfCommonFace(c,d), {
    let R aExtraDiag =  $\delta t / V\{c\} * (\text{faceLength}\{f\} * \text{faceConductivity}\{f\}) / n;$ 
    a{c, d} = aExtraDiag;
    aDiag = aDiag + aExtraDiag;
  }
  a{c, c} = -aDiag;
}

UpdateU: VcCells(),  $u^{n+1, k+1}\{c\} = u^n\{c\} + a\{c, c\} * u^{n+1, k}\{c\} + \sum\{d\text{EdgesOfCell}(c)\}(\text{norm}(u^{n+1, k}\{d\} - u^{n+1, k}\{c\}));$ 
ComputeResidual: residual =  $\text{Max}\{j \in \text{cells}()\}(\text{abs}(u^{n+1, k+1}\{j\} - u^{n+1, k}\{j}\));$ 
ComputeTn:  $t^{n+1} = t^n + \delta t;$ 
```

Console Output:

```
NabLab Console
[n=018, k=09] current residual: 1.1E-6, previous residual: 1.8E-6
[n=018, k=10] current residual: 7.0E-7, previous residual: 1.1E-6
[n=018, k=11] current residual: 4.4E-7, previous residual: 7.0E-7
[n=018, k=12] current residual: 2.8E-7, previous residual: 4.4E-7
[n=018, k=13] current residual: 1.8E-7, previous residual: 2.8E-7
[n=018, k=14] current residual: 1.2E-7, previous residual: 1.8E-7
[n=018, k=15] current residual: 8.0E-8, previous residual: 1.2E-7
[n=018, k=16] current residual: 5.3E-8, previous residual: 8.0E-8
[n=018, k=17] current residual: 3.6E-8, previous residual: 5.3E-8
[n=018, k=18] current residual: 2.5E-8, previous residual: 3.6E-8
[n=018, k=19] current residual: 1.7E-8, previous residual: 2.5E-8
[n=018, k=20] current residual: 1.2E-8, previous residual: 1.7E-8
[n=018, k=21] current residual: 8.5E-9, previous residual: 1.2E-8
[n=019, k=01] current residual: 9.0E-3, previous residual: 1.0E0
[n=019, k=02] current residual: 7.0E-4, previous residual: 9.0E-3
[n=019, k=03] current residual: 1.0E-4, previous residual: 7.0E-4
[n=019, k=04] current residual: 2.4E-5, previous residual: 1.0E-4
[n=019, k=05] current residual: 8.4E-6, previous residual: 2.4E-5
[n=019, k=06] current residual: 3.9E-6, previous residual: 8.4E-6
[n=019, k=07] current residual: 1.9E-6, previous residual: 3.9E-6
[n=019, k=08] current residual: 1.1E-6, previous residual: 1.9E-6
```

Example use on NABLAB

The image displays a screenshot of the NABLAB environment with two code editors and a console window. The left editor shows the main simulation logic, and the right editor shows the underlying mathematical model. A console window at the bottom shows the output of the simulation.

Left Editor: IterativeHeatEquation-MonitorResidual.mnlg

```
package iterativeheatequation
import org.gemc.monitors.*
import fr.cea.nabl.*
import IterativeHeatEquation.*

@setup {
  prevResidual = 1.0;
}

@event ComputeTnReturned {
  after call ComputeTn
}

@event ResidualUpdated {
  after call ComputeResidual
}

@monilogger correctResidual {
  when ResidualUpdated
  if (context(residual) > prevResidual)
  then {
    NabLabConsoleAppender.call(
      StringLayout.call(["n={0,number,000}, k={1,number,00}" +
        "Incorrect residual!" +
        "current residual: {2,number,0.0E0}, " +
        "previous residual: {3,number,0.0E0}",
        context(n), context(k), context(residual), prevResidual));
    correctResidual.stop();
    resetResidual.stop();
  } else {
    NabLabConsoleAppender.call(
      StringLayout.call(["n={0,number,000}, k={1,number,00}" +
        "current residual: {2,number,0.0E0}, " +
        "previous residual: {3,number,0.0E0}",
        context(n), context(k), context(residual), prevResidual));
    prevResidual = context(residual);
  }
}

@monilogger resetResidual {
  when ComputeTnReturned
  {
    prevResidual = 1.0;
  }
}
```

Right Editor: IterativeHeatEquation.n

```
InitD: VcCells(), D{c} = 1.0;

ComputeDeltaTn:  $\delta t = \text{Min}(c\text{Cells}())\{V\{c\}/D\{c\} * 0.1;$ 
ComputeV: VjCells(), V{j} = 0.5 *  $\sum\{p\text{NodesOfCell}()\}\{\text{det}(X\{p\}, X\{p+1\});$ 
ComputeFaceLength: VfFaces(), faceLength{f} = 0.5 *  $\sum\{p\text{NodesOfFace}()\}\{\text{norm}(X\{p\}, X\{p+1\});$ 
ComputeFaceConductivity: VfFaces(), faceConductivity{f} = 2.0 *  $\|{c1\text{CellsOfFace}()\}\{V\{c1\}/D\{c1\};$ 

// Assembling of the diffusion matrix
@ComputeAlphaCoeff: VcCells(), {
  R aDiag = 0.0;
  neighbourCells(c), VfCommonFace(c,d), {
    let R aExtraDiag =  $\delta t / V\{c\} * \{faceLength\{f\} * faceConductivity\{f\} / n$ 
    a{c, d} = aExtraDiag;
    aDiag = aDiag + aExtraDiag;
  }
  a{c, c} = -aDiag;
}

UpdateU: VcCells(),  $u^{n+1, k+1}\{c\} = u^n\{c\} + \alpha\{c, c\} * u^{n+1, k}\{c\} + \sum\{d\text{EdgesOfCell}()\}\{d\text{NodesOfCell}()\}\{u^{n+1, k}\{d\} - u^{n+1, k}\{c\}\};$ 
ComputeResidual: residual =  $\text{Max}\{j \in \text{cells}()\}\{\text{abs}(u^{n+1, k+1}\{j\} - u^{n+1, k}\{j\});$ 
ComputeTn:  $t^{n+1} = t^n + \delta t;$ 
```

Console Output:

```
NabLab Console
[n=018, k=09] current residual: 1.1E-6, previous residual: 1.8E-6
[n=018, k=10] current residual: 7.0E-7, previous residual: 1.1E-6
[n=018, k=11] current residual: 4.4E-7, previous residual: 7.0E-7
[n=018, k=12] current residual: 2.8E-7, previous residual: 4.4E-7
[n=018, k=13] current residual: 1.8E-7, previous residual: 2.8E-7
[n=018, k=14] current residual: 1.2E-7, previous residual: 1.8E-7
[n=018, k=15] current residual: 8.0E-8, previous residual: 1.2E-7
[n=018, k=16] current residual: 5.3E-8, previous residual: 8.0E-8
[n=018, k=17] current residual: 3.6E-8, previous residual: 5.3E-8
[n=018, k=18] current residual: 2.5E-8, previous residual: 3.6E-8
[n=018, k=19] current residual: 1.7E-8, previous residual: 2.5E-8
[n=018, k=20] current residual: 1.2E-8, previous residual: 1.7E-8
[n=018, k=21] current residual: 8.5E-9, previous residual: 1.2E-8
[n=019, k=01] current residual: 9.0E-3, previous residual: 1.0E0
[n=019, k=02] current residual: 7.0E-4, previous residual: 9.0E-3
[n=019, k=03] current residual: 1.0E-4, previous residual: 7.0E-4
[n=019, k=04] current residual: 2.4E-5, previous residual: 1.0E-4
[n=019, k=05] current residual: 8.4E-6, previous residual: 2.4E-5
[n=019, k=06] current residual: 3.9E-6, previous residual: 8.4E-6
[n=019, k=07] current residual: 1.9E-6, previous residual: 3.9E-6
[n=019, k=08] current residual: 1.1E-6, previous residual: 1.9E-6
```

Annotations:

- Initializing variable storing value of previous residual
- Declaring events of interest
- Checking the invariant
- residual decreases while iterating over k
- Logging the values of interest and storing residual for next iteration
- Resetting stored residual to 1.0 after each iteration over n

- Applicable to **Java-based** interpreters
- **Non-intrusive** w.r.t. language definition
- Instrumentation interface = aspects **weaved into the interpreter:**

```
pointcut interpretJob(Job job, Context context) :
call(public static void fr.cea.nabla.ir.interpreter.JobInterpreter.interprete(Job, Context)) &&
args(job, context);

after(Job job, Context context) : interpretJob(job, context) {
    notifyAfter(job.getName(), null, context);
}

before(Job job, Context context) : interpretJob(job, context) {
    notifyBefore(job.getName(), context);
}
```

Implementation – Truffle language implementation framework

- Applicable to languages with a **Truffle-based** interpreter (e.g., Python, R)
- Can evaluate expressions in **any language** installed on the GraalVM
- Instrumentation interface **part of language definition**:

```
public abstract class NablaWriteVariableNode
    extends NablaInstructionNode
    implements InstrumentableNode, TruffleObject {
    @Override
    public boolean hasTag(Class<? extends Tag> tag) {
        return tag.equals(StandardTags.WriteVariableTag.class) || super.hasTag(tag);
    }
}
```

Research questions:

- RQ#1** How does the proposed approach allow to combine runtime monitoring and logging to extract relevant data from running models?
- ▶ Answered through demonstration cases similar to the provided example.
- RQ#2** How is the overhead induced by the approach affected by different scenarios?
- ▶ Answered through quantitative evaluation

RQ#1: Demonstration case (Coarsen Interval)

```
IterativeHeatEquation-CoarsenInterval.mnlg
package heatequation

import org.gemoc.monilog.stl.*
import fr.cea.nabla.monilog.nablalib.*
import IterativeHeatEquation.*

import "/home/vagrant/workspace/NabLabExamples/Utils.js" as jsutils

setup {
  currentTime = 0.0;
  outputInterval = 0.0001;
  stdev = 1.0;
  dateString = js(jsutils.getDate);
  filePath = "/home/vagrant/workspace/NabLabExamples/dumps/";
}

event ComputeTnReturned {
  after call ComputeTn
}

monillogger LogTemperature {
  when ComputeTnReturned
  if (currentTime + outputInterval <= context(t_n))
  then {
    stdev = js(jsutils.stdev(context(u_n)));
    FileAppender.call(
      StringLayout.call(
        "{0,number,0.0000}, {1,number,0.000E0}",
        context(t_n),
        stdev),
      StringLayout.call("{0}iterativeheatequation-{1}.csv", filePath, dateString));
    currentTime = currentTime + outputInterval;
  }
}

monillogger CoarsenInterval {
  when ComputeTnReturned
  if (stdev <= 0.20)
  then {
    outputInterval = 0.01;
    CoarsenInterval.stop;
  }
}
```

- Log standard deviation of u_n to file at interval of 0.0001
- When standard deviation less than 0.2, increase interval to 0.01
- ▶ Derived data leveraged by monitor
- ▶ Monitor affects logger behavior

RQ#2: Quantitative evaluation

Setup:

CPU: Intel® Core™ i7-9850H CPU @ 2.60GHz × 12

OS: Ubuntu 20.04.2, VM: GraalVM 21.1.0

Overhead induced by 3 MONILOG specifications over simulation times from 0.2 to 1.0

AspectJ:

baseline: from $\approx 42.6\text{s}$ to $\approx 134.89\text{s}$

absolute: from $\approx 8.75\text{s}$ to $\approx 18.27\text{s}$

relative: from $\approx 26\%$ to $\approx 16\%$

Truffle:

baseline: from $\approx 10.21\text{s}$ to $\approx 29.76\text{s}$

absolute: from $\approx 2.75\text{s}$ to $\approx 4.85\text{s}$

relative: from $\approx 36.5\%$ to $\approx 19.5\%$

- ▶ Suitable for **debugging** as absolute overhead reasonably low on shorter execution times, and relative overhead decreases by 40 to 50% on longer execution times.

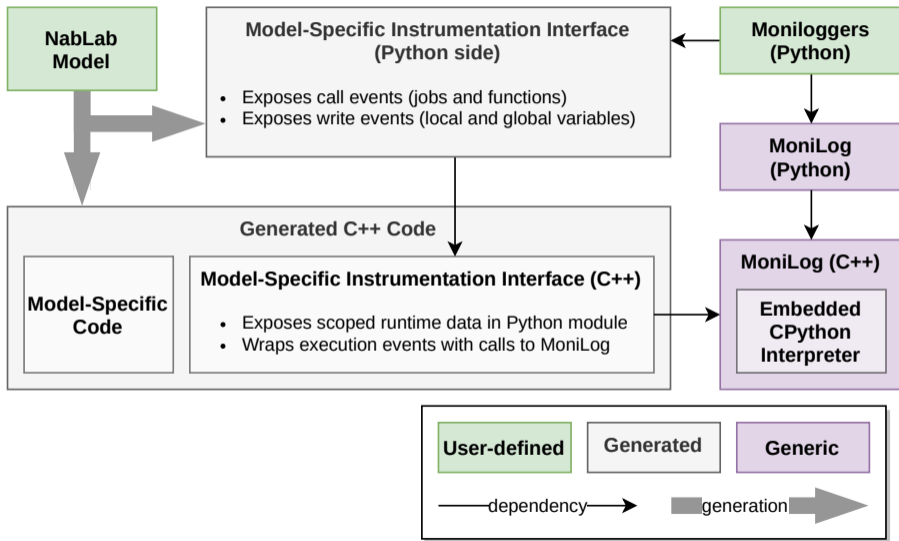
Prerequisites:

- MONILOG host language interpreter embeddable in target language
- Extend code generators to generate model-specific instrumentation interface

The generated model-specific instrumentation interface is split between:

- the target language of the DSL's code generator, to expose runtime data and events of the model, and
- the host language of MONILOG, to execution events of the model from moniloggers.

MONILOG for compiled DSLs (ongoing work)



Example use of Python-based MONILOG

```
src > iterativeheatequation > logStdev.py > ...
1  import iterativeheatequation as ihe
2  from monilog import *
3  import statistics
4
5  currentTime = 0
6  outputInterval = 0.0001
7  stdev = 1.0
8
9  @after(ihe.ComputeTn)
10 def logTemperature(context):
11     global currentTime
12     global outputInterval
13     global stdev
14     currentTime += outputInterval
15     if (currentTime <= context.t_n):
16         stdev = statistics.stdev(context.u_n)
17         print("[ " + str(context.t_n) + " ] stdev=" + str(stdev))
18
19 @after(ihe.ComputeTn)
20 def coarsenInterval(context):
21     global stdev
22     global outputInterval
23     if (stdev <= 0.20):
24         outputInterval = 0.01
25         coarsenInterval.stop()
```

- High-level languages allow scientists and numerical analysts to focus on their area of expertise and **associated V&V concerns**.
- Designers of high-level languages must **guarantee correctness and performance** of derived scientific software.
- Designers must furthermore **give tools to address the V&V concerns** corresponding to the level of abstraction of the language.
- In the context of **languages for numerical schemes** such as NABLAB, MONILOG is particularly suited to this thanks to:
 - its combination of **logging and monitoring**,
 - its ability to use the **best suited languages** for the task (e.g., Python for data analysis)

Thank you for your attention!

When Scientific Software Meets Software Engineering

Leroy, Dorian, Sallou, June, Bourcier, Johan, Combemale, Benoit Computer 2021

Monilogging for executable domain-specific languages

Leroy, Dorian, Lelandais, Benoît, Oudot, Marie-Pierre, Combemale, Benoit In Proceedings of the 14th ACM SIGPLAN International Conference on Software Language Engineering 2021