

Codee Training: Write Accelerated Code at Expert Level

Codee: Automated Code Inspection for Modernization and Optimization

NERSC Codee Training Series

September 5-6, 2024

Schedule

Day 1 (Thursday 5th, 9:00 - 12:30 PDT)	Day 2 (Friday 6th, 9:00 - 12:30 PDT) Codee: Automated Analysis of Large-Scale Fortran/C/C++ Codes			
Codee: Automated Code Inspection for Modernization and Optimization				
Lecture:	Lecture:			
 Codee's command-line tool Open Catalog of Best Practices for Fortran/C/C++ Modernization and Optimization for CPU and GPU Demo using Fortran: HIMENO modernization 	 Codee's command-line tool using compilation databases Automated testing of large codes using Codee on Perlmutter Use case: Optimizing the Weather Research and Ecrocasting Model with OpenMR Offlord and Codea 			
 HIMENO optimization through GPU parallelism Demo using C/C++: MATMUL optimization through CPU parallelism Hands-on: PI, MATMUL, COULOMB, HIMENO 	 Demo using Fortran: Putting it all together with HYCOM Demo using C/C++: Putting it all together with MBedTLS Hands-on: HYCOM, NUCCOR, ATMUX, LULESHmk, MBedTLS 			

Your Main **Drivers** for Simulation Software?

• Simulation software demands **high-speed computations** and **maintainable code**.

• <u>1. Modernize your code:</u>

- Adopt modern programming practices to increase code quality and facilitate maintenance:
 - Update legacy code; e.g.: F77 → F2018, C++98 → C++20.
 - Ensure portability across compilers; no vendor-specific language extensions.
 - Leverage new language features; e.g.: Fortran modules, C++ smart pointers.
- The modernization process helps **find bugs** and **avoid introducing hidden bugs** during maintenance.
- As a result, the modernization process helps ensure code **correctness**.

<u>2. Optimize performance:</u>

• Overall, enforce modernization before addressing performance optimization.

Fortran/C/C++ on NERSC

- Widely used in:
 - Aerospace
 - Automotive
 - Climate & Weather
 - o Defense
 - Energy & Utilities
 - High Performance Computing
 - Manufacturing
 - Oil and Gas
 - Scientific Research
- Employed by most NERSC users.



Fraction of Users (%)

Source: https://portal.nersc.gov/project/m888/nersc10/workload/N10 Workload Analysis.latest.pdf

Language First appeared in		TIOBE Index 2024		
Fortran	1957	10th		
С	1972	3rd		
C++	1985	2nd		

codee

USE CASE: FORTRAN MODERNIZATION **Thoughts of the Fortran community on modernization**

"Always use IMPLICIT NONE everywhere. It is amazing how many bugs this can find and avoid compared to the default typing rules."

"All subprograms should be CONTAINed. Generally in modules, but also in the main program unit. <...> Again, amazing how many interface bugs show up when this is enforced."

"Many many more could be suggested. Here are a few in no specific order that help compilers find more bugs at compile time, and help programs scale better:

- Always specify intent attributes for dummy arguments.
- Always use assumed shape for array dummy arguments."

"Always use Standard conforming code. **Turn on all warnings** (e.g., -std=f2018 -Wall with gfortran) and fix any issues by using Standard conforming code. There are really very few compiler extensions from the Olden Days that do not have modern, Standard conforming, replacements."

Source:

https://fortran-lang.discourse.group/t/our-initiative-to-publish-the-fortran-lang-top-10-recommendation-for-fortran-modernization-is-it-really-new-or-even-feasible/7774/18

1. Strict compliance with modern Fortran standards

Remove legacy features deleted from recent Fortran standards, as they might not be supported by recent compilers, and avoid compiler-specific extensions, ensuring that the code remains compatible across various development environments.

2. Declare procedures in modules

Declare related procedures within an importable module to enhance code modularity, reusability, and readability. This practice also helps avoid runtime errors related to implicit interfaces. Separate the definition of procedures into modules and their implementation into submodules, leveraging incremental compilation to reduce build times

3. Restrict data visibility with modules

Encapsulate globally accessible data, such as common blocks, within modules. This approach allows for controlled access interfaces, improving code readability and minimizing side effects from global data storage.

4. Improve dummy arguments semantics

Enhance the definitions of dummy arguments to make the behavior of procedures more predictable and transparent, helping avoid common issues related to incorrect assumptions about data type, flow, or structure.

5. Improve data type consistency and management

Ensure the consistency of data types by avoiding implicit typing and standardizing the code on a fixed set of real kinds, improving readability and portability across different development environments. Use derived data types to represent complex multi-field structures. Leverage pointers and allocatable arrays for safer memory handling.

6. Avoid legacy control-flow constructs

Replace outdated and error-prone control-flow constructs with more robust and maintainable language features from recent standards, improving code maintainability and reducing the likelihood of bugs.

7. Enhance source code semantics

Leverage elements from recent Fortran standards to further improve the clarity and intent of code statements beyond previous recommendations.

8. Adherence to code conventions

Establish and adhere to a consistent coding standard, such as variable naming rules of free-form format, to promote readability and ease collaboration among developers.

9. Adopt modern development practices

Integrate modern development practices, such as automated testing, version control, or dependency managers, to enhance the quality, maintainability, collaboration, and distribution of Fortran software.

10. Proper C/C++ interoperability

Ensure seamless interoperability between Fortran and C/C++ to allow Fortran programs to effectively interact with a wide range of systems and libraries written in other languages (e.g., high-performance environments).



USE CASE: FORTRAN MODERNIZATION Top 20 Checks for Fortran Modernization

- [M01] Tune compiler flags to mark non-standard and removed features in modern Fortran standards.
- [M01] Consider using more standard-compliant compilers like gfortran to flag non-standard and removed features.
- [M01] Consider replacing GNU Fortran non-standard constructs to favor portability
- [M02] PWR068: Encapsulate external procedures within modules to avoid the risks of calling implicit interfaces.
- [M03] PWR073: Transform common block into a module for better data encapsulation.
- [M03] PWR069: Use the keyword only to explicitly state what to import from a module.
- [M04] PWR008: Declare the intent for each procedure argument.
- [M04] PWR070: Declare array dummy arguments as assumed-shape arrays.
- [M05] PWR007: Always use implicit none to disable implicit declarations.
- [M05] PWR071: Prefer real(kind=kind_value) for declaring consistent floating types.
- [M06] PWR063: Avoid using legacy and old-style Fortran constructs.
- [M07] PWR003: Explicitly declare pure functions.
- [M07] Add an explicit parameter attribute to constant variables.
- [M07] PWR072: Add an explicit save attribute when initializing variables in their declaration.
- [M10] Consider using Fortran modules instead of C/C++ header files

Open Catalog of Best Practices for Modernization and Optimization

Check		Fortran	С	C++	Autofix
Moderniz	ation				
<u>PWR007</u>	Disable implicit declaration of variables	\checkmark			\checkmark
<u>PWR068</u>	Encapsulate external procedures within modules to avoid the risks of calling implicit interfaces	1			
<u>PWR070</u>	Declare array dummy arguments as assumed-shape arrays	\checkmark			
Many mor	e!				
Optimizat	ion				
<u>PWR050</u>	Consider applying multithreading parallelism to forall loop	1	1	✓	\checkmark
<u>PWR055</u>	Consider applying offloading parallelism to forall loop	\checkmark	1	1	\checkmark
<u>PWD006</u>	Missing deep copy of non-contiguous data to the GPU	\checkmark	1	1	
Many mor	e!				



Codee: Value Proposition

WHAT

HOW

WHERE

Community-guided Top Recommendations Open Catalog on Best Practices



First **Top 10 Recommendations for Fortran Modernization** published on February 2024

Containing **80+ checks** as of August 2024, with curated documentation and examples Automated analysis of Codee 2024.3 reported 64.603 checks in WRF running on Perlmutter

USE CASE: FORTRAN MODERNIZATION Success Stories using Open Source Software

Code	Domain	Metrics with Codee 2024.3.0 (Aug. 2024)
CP2K 1.3M lines of code	Quantum chemistry and solid state physics software package	1344 files, 5431 functions, 9549 loops successfully analyzed and 17 non-analyzed files in 13 m 33 s
OpenRadioss 1.1M lines of code	Finite element solver for dynamic event analysis	3477 files, 6541 functions, 39636 loops successfully analyzed and 0 non-analyzed files in 31 m 6 s
WRF 960K lines of code	Weather Research and Forecasting	508 files, 9722 functions, 26519 loops successfully analyzed (64603 checkers) and 0 non-analyzed files in 1 h 17 m 18 s
ICON 646K lines of code	Weather, climate, and environmental prediction	1143 files, 6959 functions, 7801 loops successfully analyzed (6098 checkers) and 7 non-analyzed files in 9 m 34 s
SIESTA 398K lines of code	First-principles Materials Simulation	967 files, 2956 functions, 2254 loops successfully analyzed (3291 checkers) and 25 non-analyzed files in 2 m 16 s
PHASTA 64K lines of code	Parallel Hierarchic Adaptive Stabilized Transient Analysis of compressible and incompressible Navier Stokes equations	284 files, 608 functions, 1086 loops successfully analyzed (1420 checkers) and 0 non-analyzed files in 6 m 35 s
HYCOM 44K lines of code	HYbrid Coordinate Ocean Model	50 files, 251 functions, 2058 loops successfully analyzed (2965 checkers) and 0 non-analyzed files in 53.85 s
EAP-patterns 4K lines of code	Patterns from an Eulerian cell AMR application	12 files, 88 functions, 164 loops successfully analyzed and 0 non-analyzed files in 1037 ms

Codee: Main Features

O_{\circ}

Static Analysis

Automatically analyze every line of code to find and fix modernization and optimization opportunities.



Code Coverage

Obtain code coverage metrics and discover lines that are not being analyzed.



Reports

Get a deeper understanding of your code's health with analysis reports.



Autofix

Automatically generate fixes for

opportunities, always under the

control of the programmer and

preserving 100% code correctness.

 $\mathcal{O}_{\mathcal{I}}$

CI/CD automation

Integrate with CI/CD systems, automatically testing every code change and pull request.



Self-hosting

Execution on the local system, retraining full control of your code and privacy.

Codee provides a systematic, predictable workflow that is a complement to other software development tools, such as the compiler, profiler, or debugging tools.

Codee: Suggested Basic Workflow



O. Compiler Invocation

```
cat -n matmul.f90
$
    subroutine matmul(n, A, B, C)
1
2
      double precision, dimension(n, n), intent(in) :: A, B
3
      double precision, dimension(n, n), intent(out) :: C
4
5
      ! Initialization
6
      do i = 1, n
7
        do j = 1, n
8
        C(i, j) = 0.0
9
        end do
10
      end do
11
12
     ! Accumulation
13
     do i = 1, n
     do j = 1, n
14
15
       do k = 1, n
16
          C(i, j) = C(i, j) + A(i, k) * B(k, j)
17
          end do
18
     end do
19
    end do
20
    end subroutine matmul
```

\$ gfortran matmul.f90

1. Technical Debt Report



\$ codee technical-debt -- gfortran matmul.f90

TECHNICAL DEBT REPORT

This report quantifies the technical debt associated with the modernization of legacy code by assessing the extent of refactoring required for language constructs. The score is determined based on the number of language constructs necessitating refactoring to bring the source code up to modern standards. Additionally, the metric identifies the impacted source code segments, detailing affected files, functions, and loops.

Score	Affected	d files Affect	ed functi	ons Affecte	d loo	ps	
 10	1	1		 <i>I</i> .		(Score and affected source code
12	T	T		4			
TECHN	ICAL DEB	F BREAKDOWN					
Lines	of code	Analysis time	Checkers	Technical	debt	score	
16		12 ms	12	12			

1 file, 1 function, 5 loops successfully analyzed (12 checkers) and 0 non-analyzed files in 12 ms

2. Screening with Ranking Report



\$ codee screening -- gfortran matmul.f90

SCREENING REPORT

	lines of	F code	Analysis	time <mark># checks</mark> Profiling
				Total checks triggered
	16		13 ms	12 n/a
RANKING OF CHECKERS		EUKERS	Checks ordered by priority	
	Checker	Level	Priority	# Title
	PWR039	L1	P27	I consider loop interchange to improve the locality of reference and enable vectorization
	PWR068	L1	P27	1 Encapsulate external procedures within modules to avoid the risks of calling implicit interfaces
	RMK015	L1	P27	1 Tune compiler optimization flags to increase the speed of the code
	PWR003	L1	P18	1 Explicitly declare pure functions
	PWR008	L1	P18	1 Declare the intent for each procedure parameter
	PWR070	L1	P18	1 Declare array dummy arguments as assumed-shape arrays
	PWR071	L2	P6	2 Prefer real(kind=kind_value) for declaring consistent floating types
	PWR007	L2	P6	1 Disable implicit declaration of variables
	PWR035	L3	P2	1 Avoid non-consecutive arrav access to improve performance
	RMK010	L3	P0	2 The vectorization model states the loop is not a SIMD opportunity due to strided memory

accesses





\$ codee roi -- gfortran matmul.f90

ROI ANALYSIS SUMMARY

This analysis underscores the tangible benefits Codee brings to the development process, not only in terms of savings in development effort, but also in realizing significant cost efficiencies for the organization.

Impact on Development Effort:

This report identifies critical areas within the source code that necessitate attention from the development team, and forecasts a significant reduction in workload by an estimated 223 hours.

Without Codee With Codee	Hours saved	
		Saved hours
235 hours 12 hours	223 hours	

Impact on Cost Savings:

Considering a standard developer's workload of approximately 1800 hours/year, Codee's intervention translates to saving an equivalent to 0.12 (223h / 1800h) developers working full-time. Assuming an average cost of a developer for the company (salary + associated costs) of €100,000, this amounts to cost savings of €12,388 (€100,000 x 0.12).

Developer hours/vear	Number of devs. saved/vear	Developer salarv/vear	Total costs saved/vear	
				Saved cost
1800 hours	0.12	€100,000	€12,388	

ROI CALCULATION BREAKDOWN

<...>

codee

4. Checks Report

\$ codee checks -- gfortran matmul.f90

CHECKS REPORT

matmul.f90:6:3 [PWR039] (level: L1): Consider loop interchange to improve the locality of reference and enable vectorization
matmul.f90:1:1 [PWR068] (level: L1): Encapsulate external procedures within modules to avoid the risks of calling implicit interfaces
matmul.f90 [RMK015] (level: L1): Tune compiler optimization flags to increase the speed of the code
matmul.f90:1:1 [PWR003] (level: L1): Explicitly declare pure functions
matmul.f90:1:1 [PWR008] (level: L1): Declare the intent for each procedure parameter
matmul.f90:1:1 [PWR070] (level: L1): Declare array dummy arguments as assumed-shape arrays
matmul.f90:2:3 [PWR071] (level: L2): Disable implicit declaration of variables
matmul.f90:3:3 [PWR071] (level: L2): Prefer real(kind=kind_value) for declaring consistent floating types
matmul.f90:3:3 [PWR071] (level: L3): Avoid non-consecutive array access to improve performance
matmul.f90:7:5 [RMK010] (level: L3): The vectorization model states the loop is not a SIMD opportunity due to strided memory accesses
matmul.f90:15:7 [RMK010] (level: L3): The vectorization model states the loop is not a SIMD opportunity due to strided memory accesses

\$ codee checks --verbose -- gfortran matmul.f90

CHECKS REPORT

<...>

<...>

matmul.f90:1:1 [PWR007] (level: L2): Disable implicit declaration of variables

Suggestion: Add IMPLICIT NONE in the specification part of the procedure 'matmul' Documentation: https://github.com/codee-com/open-catalog/tree/main/Checks/PWR007 AutoFix: codee rewrite --modernization implicit-none --in-place matmul.f90:matmul -- gfortran matmul.f90

Detailed information on each check



5. Autofix

MLD

\$ codee rewrite --modernization implicit-none --in-place matmul.f90:matmul -- gfortran matmul.f90

```
Results for file '/home/user/matmul.f90':

Successfully applied AutoFix to the procedure at 'matmul.f90:1:1' [using insert implicit none]:

[INFO] Inserted implicit none:

- matmul.f90:1:1
```

Successfully updated matmul.f90

```
$ git diff matmul.f90
```

```
subroutine matmul(n, A, B, C)
```

```
+ ! Codee: Made all variable declarations explicit (2024-08-02 13:04:38)
```

- implicit none
- + integer :: i
- + integer :: j
- + integer :: k
- + integer :: n

```
double precision, dimension(n, n), intent(in) :: A, B
double precision, dimension(n, n), intent(out) :: C
```

Focus the Analysis: Select a subset of checks (I)

Common options:

--check-id <id>[,<id>]*
Focus on specific checks

--target-arch <arch> Focus on multiple checks

--list-available-checkers List all available checks

Focus the Analysis: Select a subset of checks (II)

\$ codee checks --target-arch cpu,gpu -- gfortran matmul.f90

< . . . >

CHECKS REPORT

matmul.f90:6:3 [PWR039] (level: L1): Consider loop interchange to improve the locality of reference and enable vectorization matmul.f90:1:1 [PWR068] (level: L1): Encapsulate external procedures within modules to avoid the risks of calling implicit interfaces matmul.f90 [RMK015] (level: L1): Tune compiler optimization flags to increase the speed of the code matmul.f90:1:1 [PWR003] (level: L1): Explicitly declare pure functions matmul.f90:1:1 [PWR008] (level: L1): Declare the intent for each procedure parameter matmul.f90:1:1 [PWR070] (level: L1): Declare array dummy arguments as assumed-shape arrays matmul.f90:1:1 [PWR007] (level: L2): Disable implicit declaration of variables matmul.f90:13:3 [PWR050] (level: L2): Consider applying multithreading parallelism to forall loop matmul.f90:2:3 [PWR071] (level: L2): Prefer real(kind=kind_value) for declaring consistent floating types matmul.f90:3:3 [PWR071] (level: L2): Prefer real(kind=kind_value) for declaring consistent floating types matmul.f90:13:3 [PWR055] (level: L3): Consider applying offloading parallelism to forall loop matmul.f90:13:3 [PWR035] (level: L3): Avoid non-consecutive array access to improve performance matmul.f90:7:5 [RMK010] (level: L3): The vectorization cost model states the loop is not a SIMD opportunity due to strided memory... matmul.f90:15:7 [RMK010] (level: L3): The vectorization cost model states the loop is not a SIMD opportunity due to strided memory...

Focus the Analysis: Select a subset of checks (III)

\$ codee checks --verbose --target-arch cpu,gpu -- gfortran matmul.f90

CHECKS REPORT

<...>

matmul.f90:13:3 [PWR055] (level: L3): Consider applying offloading parallelism to forall loop Suggestion: Use 'rewrite' to automatically optimize the code Documentation: https://github.com/codee-com/open-catalog/tree/main/Checks/PWR055 AutoFix (choose one option): * Using OpenMP (recommended): codee rewrite --offload omp-teams --in-place matmul.f90:13:3 -- gfortran matmul.f90 * Using OpenACC: codee rewrite --offload acc --in-place matmul.f90:13:3 -- gfortran matmul.f90 * Using OpenMP and OpenACC combined: codee rewrite --offload omp-teams,acc --in-place matmul.f90:13:3 -- gfortran matmul.f90

<...>

Focus the Analysis: Select a subset of checks (IV)

\$ codee rewrite --offload omp-teams --in-place matmul.f90:13:3 -- gfortran matmul.f90

Results for file 'matmul.f90':

Successfully applied AutoFix to the loop at 'matmul.f90:matmul:13:3' [using offloading]:

[INFO] matmul.f90:13:3 Parallel forall: variable 'C'

[INFO] matmul.f90:13:3 Loop parallelized with teams using OpenMP directive 'target teams distribute parallel for' Fine-tuning suggestions for better performance [using offloading]:

[TODO] Consider optimizing data transfers of arrays by adding the proper array ranges in data mapping clauses Documentation: https://github.com/codee-com/open-catalog/tree/main/Glossary/Offloading-data-transfers.md

```
$ git diff matmul.f90
```

```
! Accumulation
```

- + ! Codee: Loop modified by Codee (2024-08-02 13:35:36)
- + ! Codee: Technique applied: offloading with 'omp-teams' pragmas
- + ! Codee: Offloaded loop: begin

+ ! TODO (Codee): Consider optimizing data transfers of arrays by adding the proper array ranges in data mapping clauses

+ !\$omp target teams distribute parallel do shared(A, B, n) map(to: n, A, B) private(j) map(tofrom: C) schedule(static)

```
do i = 1, n
    do j = 1, n
    do k = 1, n
    @@ -17,4 +22,5 @@ subroutine matmul(n, A, B, C)
        end do
    end do
    end do
+ ! Codee: Offloaded loop: end
end subroutine matmul
```

codee

Use --compiler-driven-mode to generate pragmas optimized for the target compiler

Focus the Analysis: Select a subset of checks (V)

\$ codee checks -- gfortran matmul.f90

CHECKS REPORT

matmul.f90:6:3 [PWR039] (level: L1): Consider loop interchange to improve the locality of reference and enable vectorization
matmul.f90:1:1 [PWR068] (level: L1): Encapsulate external procedures within modules to avoid the risks of calling implicit interfaces
matmul.f90 [RMK015] (level: L1): Tune compiler optimization flags to increase the speed of the code
matmul.f90:1:1 [PWR003] (level: L1): Explicitly declare pure functions
matmul.f90:1:1 [PWR008] (level: L1): Declare the intent for each procedure parameter
matmul.f90:1:1 [PWR070] (level: L1): Declare array dummy arguments as assumed-shape arrays
matmul.f90:1:1 [PWR007] (level: L2): Disable implicit declaration of variables
matmul.f90:2:3 [PWR071] (level: L2): Prefer real(kind=kind_value) for declaring consistent floating types
matmul.f90:3:3 [PWR071] (level: L2): Prefer real(kind=kind_value) for declaring consistent floating types
matmul.f90:13:3 [PWR035] (level: L3): Avoid non-consecutive array access to improve performance
matmul.f90:7:5 [RMK010] (level: L3): The vectorization model states the loop is not a SIMD opportunity due to
strided memory accesses
matmul.f90:15:7 [RMK010] (level: L3): The vectorization model states the loop is not a SIMD opportunity due to
strided memory accesses

\$ codee checks --check-id PWR007 -- gfortran matmul.f90

CHECKS REPORT

matmul.f90:1:1 [PWR007] (level: L2): Disable implicit declaration of variables

Focus the Analysis: Select a subset of code

- \$ codee checks matmul.f90 -- gfortran matmul.f90
 Filter by file
- \$ codee checks matmul.f90:matmul -- gfortran matmul.f90
 Filter by function
- \$ codee checks matmul.f90:13 -- gfortran matmul.f90
 Filter by loop
- \$ codee checks matmul.f90:7,13 -- gfortran matmul.f90
 Filter by multiple elements

Main Takeaways

- **Simulation software** demands **maintainable** and **high-speed** Fortran/C/C++ code.
- <u>1. Modernize</u> your code to ensure <u>correctness</u>:
 - Update legacy code; e.g.: $F77 \rightarrow F2018$, $C++98 \rightarrow C++20$.
 - Ensure portability across compilers; no vendor-specific language extensions.
 - Leverage new language features; e.g.: Fortran modules, C++ smart pointers.
- <u>2. After that</u>, address <u>optimization</u>.
- **Customize the analysis** to your needs:
 - **Modernization:** codee --check-id <id> / codee --only-categories modern
 - **CPU optimization:** codee --target-arch cpu
 - **GPU optimization:** codee --target-arch gpu
- Look up the **Open Catalog** and leverage **Codee's autofix** capabilities to improve the code:
 - **Modernization autofix:** codee rewrite --modernization
 - (Optimization) CPU + OpenMP autofix: codee rewrite --multi omp-for

Hands-on Demos on Perlmutter @NERSC

- Live Demo #1: HIMENO modernization
- **Live Demo #2:** HIMENO optimization through CPU parallelism
- Live Demo #3: MATMUL optimization through GPU parallelism

Hands-on Labs on Perlmutter @NERSC

Step-by-step guides available at <u>docs.codee.com</u>:

- PI offloading to GPU at Perlmutter (<u>C/C++</u>)
- MATMUL offloading to GPU at Perlmutter (<u>C/C++</u>)
- COULOMB offloading to GPU at Perlmutter (<u>C/C++</u>)
- HIMENO modernization (<u>Fortran</u>)
- HIMENO optimization through CPU parallelism (Fortran)
- HIMENO optimization through GPU parallelism on NVIDIA/Cray Compilers (Fortran)



Automated Code Inspection for Modernization and Optimization

🚓 www.codee.com

- Subscribe: codee.com/newsletter/
- Spain
- 🕑 codee_com
- in /codee-com/