An iterative solution framework based on the Block-Based PREconditioner for Square Blocks PRESB: robustness, efficiency and scalability

EMTF, September 27, 2023

Michael Weiss,[1]
M. Neytcheva[2] & T. Kalscheuer[2]

[1] Leibniz Institute for Applied Geophysics, Hanover, Germany
[2] Uppsala University, Uppsala, Sweden

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Background · Method · Robustness · Efficiency & Scalability · Conclusions & Outlook

Linear system of equations derived from partial differential equations

Heat conservation equation: $\rho c_p \frac{\partial T}{\partial t} = -\frac{\partial}{\partial x_i}\left(-k\frac{\partial T}{\partial x_i}\right) + H$

Seismic wave propagation: $\rho \frac{\partial \mathbf{u}}{\partial t^2} = (\lambda + 2\mu)\nabla(\nabla\cdot\mathbf{u}) - \mu\nabla\times\nabla\times\mathbf{u} + \boldsymbol{f}$

Linear system of equations:

$$\mathbf{Ax} = \mathbf{b}$$

Navier-Stokes equation: $\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla P + \mu\nabla^2\mathbf{u} + \boldsymbol{f}$

Controlled-source electromagnetics: $\nabla\times\left(\frac{1}{\mu}\nabla\times\mathbf{E}\right) - \left(i\omega\sigma + \omega^2\varepsilon\right)\mathbf{E} = i\omega\mathbf{J}_s$

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Solution techniques for linear systems of equations

Direct solvers

- Very robust and easy to use
- Time and memory complexities of sparse direct solver are $\mathcal{O}(N^2)$ and $\mathcal{O}(N^{4/3})$ in 3D
- Scalability is non-optimal

⇒ Use computer clusters to avoid memory bottle neck

Iterative solvers

- Lack robustness
- Only need storage for non-zero entries of system matrix and several additional vectors
- Scalable matrix-vector multiplications and vector operations

⇒ Ensure robustness and improve convergence rate using appropriate preconditioning techniques

Motivation

- Increasingly larger data sets
  - ⇒ Leads to larger computational models
  - ⇒ Large-scale problems with huge number of degrees of freedom
  - ⇒ Require vast amounts of computational resources

- Iterative solution methods as solution
  - ⇒ Reduce computational costs (time and memory requirements)
  - ⇒ Enable modelling of large data sets

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Linear system of equations for CSEM

Complex-valued notation

$$(\mathbf{K} + i\mathbf{M}_\sigma - \mathbf{M}_\varepsilon)\,\mathbf{e} = \mathbf{b},$$

and real-equivalent two-by-two block system formulations

$$\begin{bmatrix} \mathbf{K}-\mathbf{M}_\varepsilon & -\mathbf{M}_\sigma \\ \mathbf{M}_\sigma & \mathbf{K}-\mathbf{M}_\varepsilon \end{bmatrix} \begin{bmatrix} \mathbf{e_R} \\ \mathbf{e_I} \end{bmatrix} = \begin{bmatrix} \mathbf{b_R} \\ \mathbf{b_I} \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} \mathbf{M}_\sigma & \mathbf{K}-\mathbf{M}_\varepsilon \\ \mathbf{K}-\mathbf{M}_\varepsilon & -\mathbf{M}_\sigma \end{bmatrix} \begin{bmatrix} \mathbf{e_R} \\ \mathbf{e_I} \end{bmatrix} = \begin{bmatrix} \mathbf{b_I} \\ \mathbf{b_R} \end{bmatrix}$$

Using $\hat{\mathbf{e}}_I = -\mathbf{e}_I$ one obtains

$$\begin{bmatrix} \mathbf{M}_\sigma & -(\mathbf{K}-\mathbf{M}_\varepsilon) \\ \mathbf{K}-\mathbf{M}_\varepsilon & \mathbf{M}_\sigma \end{bmatrix} \begin{bmatrix} \mathbf{e_R} \\ \hat{\mathbf{e}}_I \end{bmatrix} = \begin{bmatrix} \mathbf{b_I} \\ \mathbf{b_R} \end{bmatrix}$$

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PREconditioning for Square Blocks

More generally:

$$\mathcal{A} = \begin{bmatrix} \mathbf{A} & -b\,\mathbf{B}_2 \\ a\,\mathbf{B}_1 & \mathbf{A} \end{bmatrix},$$

subject to assumptions of matrix **A** being symmetric positive semi-definite and scalars a and b being of the same sign.
Then, PRESB short for *PREconditioning for Square Blocks* (e.g. Axelsson et al., 2016) of form

$$\mathcal{P} = \begin{bmatrix} \mathbf{A} & -\mathbf{B}_2 \\ \mathbf{B}_1 & \mathbf{A} + \sqrt{ab}(\mathbf{B}_1 + \mathbf{B}_2) \end{bmatrix}$$

is an efficient preconditioner for the above general systems due to the following properties

- $\lambda(\mathcal{P}^{-1}\mathcal{A}) \in [0.5, 1]$
- independent of mesh discretisation and material properties

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Iterative algorithm

Precondition the system

$$\begin{bmatrix} \mathbf{M}_\sigma & -(\mathbf{K}-\mathbf{M}_\varepsilon) \\ \mathbf{K}-\mathbf{M}_\varepsilon & \mathbf{M}_\sigma \end{bmatrix} \begin{bmatrix} \mathbf{e_R} \\ -\mathbf{e_I} \end{bmatrix} = \begin{bmatrix} \mathbf{b_{s_I}} \\ \mathbf{b_{s_R}} \end{bmatrix}$$

with PRESB

$$\mathbf{P} = \begin{bmatrix} \mathbf{M}_\sigma & -(\mathbf{K}-\mathbf{M}_\varepsilon) \\ \mathbf{K}-\mathbf{M}_\varepsilon & \mathbf{M}_\sigma + 2(\mathbf{K}-\mathbf{M}_\varepsilon) \end{bmatrix}$$

and solve it iteratively using the Generalized Conjugate Residual (GCR) method

Algorithm 1: GCR method

Input: $\mathbf{C_{RI}}, \mathbf{b}, \mathbf{H}, \mathbf{M}_\sigma$, tol
Output: $\mathbf{e}$
Let $\mathbf{x}_0$ be the initial guess. Set $\mathbf{r}_0 = \mathbf{b} - \mathbf{C_{RI}}\mathbf{x}_0$
for $i = 0, \ldots m$ **do**
  Solve system with P to compute $\mathbf{p}_i$
  $\mathbf{q}_i \leftarrow \mathbf{C_{RI}}\mathbf{p}_i$
  $\mathbf{q}_i \leftarrow \mathbf{q}_i - {}_{j=0}^{i-1} \mathbf{q}_j \frac{(\mathbf{q}_i,\mathbf{q}_j)}{(\mathbf{q}_j,\mathbf{q}_j)}$
  $\mathbf{p}_i \leftarrow \mathbf{p}_i - {}_{j=0}^{i-1} \mathbf{p}_j \frac{(\mathbf{q}_i,\mathbf{q}_j)}{(\mathbf{q}_j,\mathbf{q}_j)}$
  $al_i \leftarrow \frac{(\mathbf{r}_i,\mathbf{q}_i)}{(\mathbf{q}_i,\mathbf{q}_i)}$
  $\mathbf{x}_{i+1} \leftarrow \mathbf{x}_i + al_i\mathbf{p}_i$, $\mathbf{r}_{i+1} \leftarrow \mathbf{r}_i - al_i\mathbf{q}_i$
  if $\frac{||\mathbf{r}_{i+1}||_2}{||\mathbf{b}||_2} < tol$ **then** Stop
end

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Iterative algorithm & applying PRESB

Applying PRESB requires solving

$$\mathbf{P} \begin{bmatrix} \mathbf{w_1} \\ \mathbf{w_2} \end{bmatrix} = \begin{bmatrix} \mathbf{f_1} \\ \mathbf{f_2} \end{bmatrix},$$

which consists of the algorithm:

Algorithm 2: Solve system with P

Set $\mathbf{H} = \mathbf{M}_\sigma + (\mathbf{K} - \mathbf{M}_\varepsilon)$
Solve $\mathbf{Hg} = \mathbf{f_1} + \mathbf{f_2}$
Compute $\mathbf{M}_\sigma\mathbf{g}$ and $\mathbf{f_1} - \mathbf{M}_\sigma\mathbf{g}$
Solve $\mathbf{Hh} = \mathbf{f_1} - \mathbf{M}_\sigma\mathbf{g}$
Compute $\mathbf{w_1} = \mathbf{g} + \mathbf{h}$ and $\mathbf{w_2} = -\mathbf{h}$

Matrix $\mathbf{H}$: $\mathcal{H}_0(\mathrm{curl}, \Omega)$ problem

- Efficiently solvable using the auxiliary-space approach (Kolev and Vassilevski, 2009)
- The auxiliary-space Maxwell solver (AMS) in hypre (Falgout and Yang, 2002) based on it
  - ⇒ AMS used to precondition GCR algorithm (inner solver)
- Alternative solver for system $\mathbf{H}$ is direct solver MUMPS (Amestoy et al., 2000)

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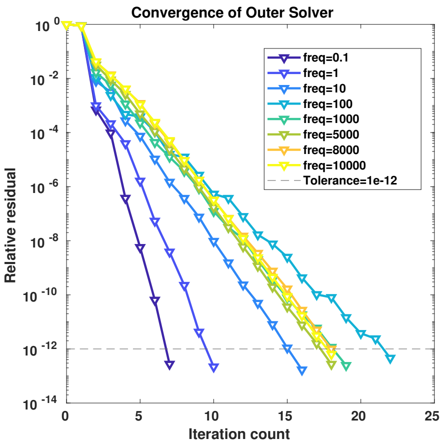
Implementation

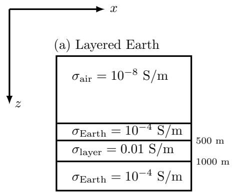
⇒ Iterative framework implemented in a stand-alone Fortran code (Weiss et al., 2023) and in the Python toolbox custEM (Rochlitz et al., 2019)

⇒ Parallelised using Message Passing Interface (MPI)

⇒ Utilising open-source libraries PETSc with access to hypre and MUMPS

Robustness with respect to frequency





Numerical parameters:

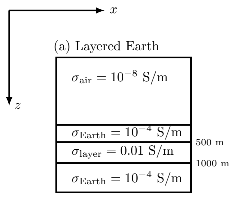
- Domain size: $30 \times 30 \times 30$ km^3
- Grounded cable extending from $(-100, 0, 0)$ to $(100, 0, 0)$ with source moment of 100 Am
- DOF: 980,100
- Run with two MPI processes
- Outer stopping criterion is 10^{-12} and inner tolerance is 10^{-3}

Robustness with respect to frequency

Inner solver	Iterative solver: AMS-GCR			Direct solver: DMUMPS		
freq [Hz]	N_{it}^{outer}	time [s]	mem [GB]	N_{it}^{outer}	time [s]	mem [GB]
0.1	7	**40.0**	**4.3**	6	121.8	14.1
1	10	**56.7**	**4.4**	9	147.3	14.1
10	16	**79.3**	**4.4**	15	145.3	14.0
100	22	**93.5**	**4.5**	18	157.2	14.1
1000	19	**70.2**	**4.4**	17	166.7	14.0
5000	18	**62.8**	**4.4**	17	153.0	14.0
8000	18	**96.8**	**4.4**	18	157.8	14.2
10,000	18	**460.7**	**4.4**	18	168.7	14.1

$\Downarrow$

Deterioration of inner preconditioned iterative solver!



Numerical parameters:

- Domain size: 30 × 30 × 30 km^3
- Grounded cable extending from (−100, 0, 0) to (100, 0, 0) with source moment of 100 Am
- DOF: 980,100
- Run with two MPI processes
- Outer stopping criterion is 10^{-12} and inner tolerance is 10^{-3}

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Robustness of solver with respect to problem size

	frequency [Hz]							
	0.1		10		1000		8000	
#DOF	N_{it}^{outer}	time[s]	N_{it}^{outer}	time[s]	N_{it}^{outer}	time[s]	N_{it}^{outer}	time[s]
980,100	**7**	42.2	**16**	79.3	**19**	70.2	**18**	96.8
3,641,400	**8**	152.9	**15**	286.4	**18**	272.6	**19**	310.2
6,879,600	**8**	343.4	**16**	646.5	**18**	521.8	**18**	790.5

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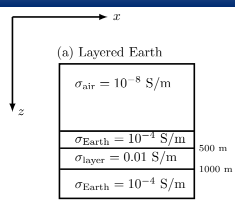
Simulation time increases approximately linearly with problem size



Numerical parameters:

- Domain size: 30 × 30 × 30 km^3
- Grounded cable extending from (−100, 0, 0) to (100, 0, 0) with source moment of 100 Am
- DOF: 980,100
- Run with two MPI processes
- Outer stopping criterion is 10^{-12} and inner tolerance is 10^{-3}

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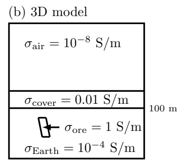
Robustness of solver with respect to material properties



relative dielectric permittivity of air, cover, host rock and ore body	$\varepsilon_r^{\text{air}} = 1$, $\varepsilon_r^{\text{cover}} = 20$, $\varepsilon_r^{\text{host rock}} = 5$, $\varepsilon_r^{\text{ore body}} = 1$			
relative magnetic permeability of ore body	$\mu_r = 1$		$\mu_r = 10$	
frequency [Hz]	$N_{\text{it}}^{\text{outer}}$	time[s]	$N_{\text{it}}^{\text{outer}}$	time[s]
0.1	9	590.4	11	691.6
10	16	282.3	16	279.8
100	23	278.5	24	285.1
8000	18	341.0	18	322.4

Numerical parameters:

- Domain size: 30 × 30 × 36 km^3
- Grounded cable extending from $(-79, 0, 0)$ to $(52, 0, 0)$ with source moment of 100 Am
- DOF: 2,033,986
- Run with two MPI processes
- Outer stopping criterion is 10^{-12} and inner tolerance is 10^{-3}

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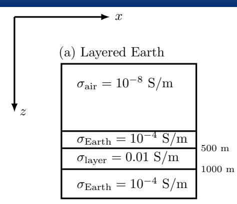
Time and memory requirements for iterative and direct solution methods



	Iterative Method: GCR				Direct Solver: ZMUMPS	
Inner solver	Preconditioned GCR		DMUMPS		-	
#DOF	time[s]	mem[GB]	time[s]	mem[GB]	time[s]	mem[GB]
980,100	93.5	4.4	157.2	14.1	166.8	9.0
3,641,400	368.4	16.4	1625.0	74.8	1874.1	55.5
6,879,600	661.0	30.1	-	out of memory	-	out of memory

Numerical parameters:

- Domain size: 30 × 30 × 30 km^3
- Grounded cable extending from $(-100, 0, 0)$ to $(100, 0, 0)$ with source moment of 100 Am
- DOF: 980,100
- Run with two MPI processes
- Outer stopping criterion is 10^{-12} and inner tolerance is 10^{-3}

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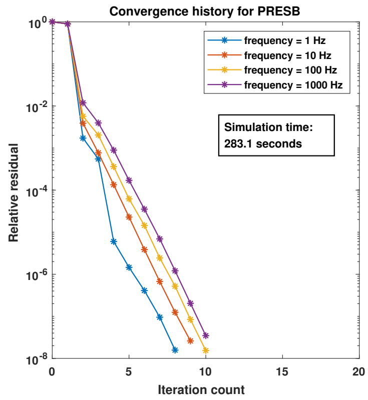
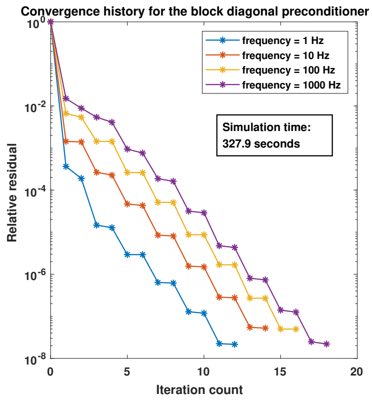
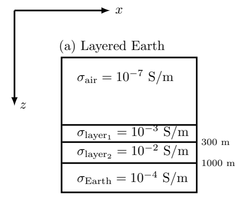
PRESB vs block diagonal preconditioner (Grayver and Bürg, 2014)





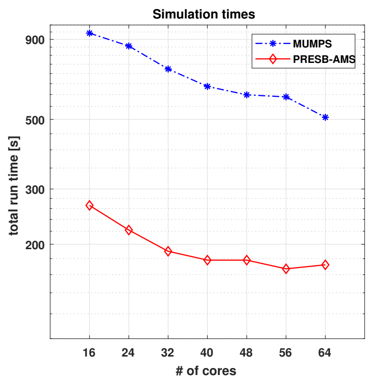


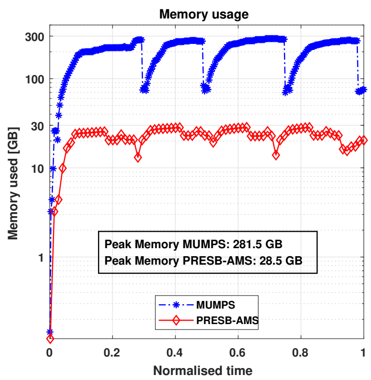
Numerical parameters:

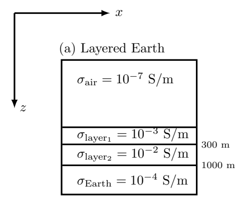
- Domain size: $200 \times 200 \times 200$ km^3
- Crooked loop example (Rochlitz et al., 2019)
- DOF: 13,447,978
- Run with 56 MPI processes
- Outer stopping criterion is 10^{-8} and inner tolerance is 10^{-3}

Background Method Robustness **Efficiency & Scalability** Conclusions & Outlook

Scalability and resource comparison





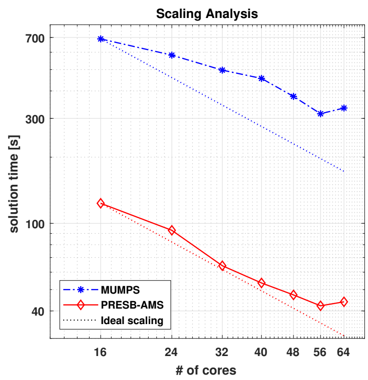


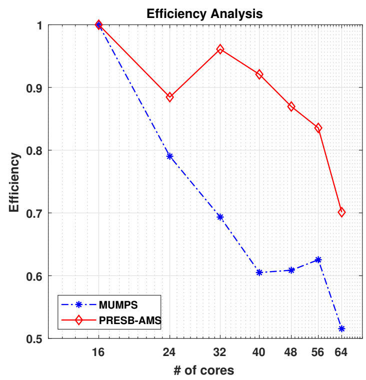
Numerical parameters:

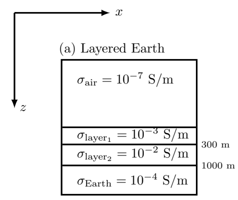
- Domain size: $200 \times 200 \times 200$ km^3
- Crooked loop example (Rochlitz et al., 2019)
- DOF: 13,447,978
- Run with variable MPI processes
- Outer stopping criterion is 10^{-8} and inner tolerance is 10^{-3}

Background ○○○ | Method ○○○○○ | Robustness ○○○○ | **Efficiency & Scalability** ○○○● | Conclusions & Outlook ○

Scalability and efficiency analysis







Numerical parameters:

- Domain size: $200 \times 200 \times 200$ km^3
- Crooked loop example (Rochlitz et al., 2019)
- DOF: 13,447,978
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- Outer stopping criterion is 10^{-8} and inner tolerance is 10^{-3}

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Conclusions & outlook

Iterative framework based on PRESB and AMS

- ⇒ Robust and highly efficient
  - ⇒ ≈ 3 times faster
  - ⇒ Requires about one order of magnitude less memory
- ⇒ Suited for large-scale problems
- ⇒ User friendly: Two simple switches in custEM

Future developments

- ⇒ Potential as forward operator for inversion
- ⇒ Strategies for dealing with multiple right-hand sides

```
# ########################################################################## #
# # # # #                         example 2                          # # # # #
# ########################################################################## #
# # # # #                    computation script                      # # # # #
# ########################################################################## #

from custEM.core import MOD
from custEM.misc.synthetic_definitions import example_2_loop_tx
import time
import dolfin as df


# specify frequencies
frequencies = [1e0, 1e1, 1e2, 1e3]

# ######################### run p1 computations ############################ #
meshes = ['example_2_mesh_fine']

for mesh in meshes:   # coarse, intermediate and fine meshes
    # Initialize MODel
    tic=time.perf_counter()
    M = MOD('p1', mesh, 'E_t', p=1, overwrite_results=True,
            m_dir='./meshes', r_dir='./results')

    # define frequency and condcutivities
    M.MP.update_model_parameters(frequencies=frequencies,
                                 sigma_ground=[1e-3, 1e-2, 1e-4],system_it=True)

    # let FEniCS set up the variational formulations
    M.FE.build_var_form()  # in this example, the Tx information is passed
                            # automatically with the mesh parameters JSON file

    toc=time.perf_counter()
    if df.MPI.comm_world.rank==0:
      print(f"Initialse model, update model and build variational form in \
            {toc - tic:0.4f} seconds")


    # call solver and convert H-fields
    tic=time.perf_counter()
    M.solve_main_problem(solver='PRESB',sym=True)
    #M.solve_main_problem(solver='MUMPS')
    toc=time.perf_counter()
    if df.MPI.comm_world.rank==0:
      print(f"Solve system in {toc - tic:0.4f} seconds")
```

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References

References

Amestoy, P. R., Duff, I. S., and L'excellent, J.-Y. (2000). Multifrontal parallel distributed symmetric and unsymmetric solvers. *Computer Methods in Applied Mechanics and Engineering*, 184(2-4):501–520.

Axelsson, O., Farouq, S., and Neytcheva, M. (2016). Comparison of preconditioned Krylov subspace iteration methods for PDE-constrained optimization problems. *Numerical Algorithms*, 73(3):631–663.

Falgout, R. D. and Yang, U. M. (2002). hypre: A library of high performance preconditioners. In *International Conference on Computational Science*, pages 632–641. Springer.

Grayver, A. V. and Bürg, M. (2014). Robust and scalable 3-D geo-electromagnetic modelling approach using the finite element method. *Geophysical Journal International*, 198(1):110–125.

Kolev, T. V. and Vassilevski, P. S. (2009). Parallel auxiliary space AMG for H (curl) problems. *Journal of Computational Mathematics*, pages 604–623.

Rochlitz, R., Skibbe, N., and Günther, T. (2019). custEM: Customizable finite-element simulation of complex controlled-source electromagnetic data. *Geophysics*, 84(2):F17–F33.

Weiss, M., Neytcheva, M., and Kalscheuer, T. (2023). Iterative solution methods for 3D controlled-source electromagnetic forward modelling of geophysical exploration scenarios. *Computational Geosciences*, 27:81–102.

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Acknowledgements

This work was partly funded by Uppsala's Center for Interdisciplinary Mathematics (CIM) and by the Germany Ministry for Education and Research (BMBF) as part of the DESMEX II project in the framework of the research and development program Fona-r4 under grant 033R130DN.

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