



The Predictor

Iteration 8 Substep 1

July 2001

A NEWSLETTER FOR THE NPARC USERS ASSOCIATION

From the Support Team

Version 4.0 of the NPARC Alliance flow solver (WIND), was officially released to the NPARC Alliance user community in June 2001. Version 4.0 can be downloaded via IVMS by registered users using their IVMS userid and password. If you have forgotten your IVMS password, please contact the NPARC support team to establish a new password.

To become a registered user and receive the NPARC flow simulation software system, a Memorandum of Agreement (included at the end of the newsletter) must be completed and approved by the US Air Force at AEDC.

The annual NPARC planning workshop was held at AEDC the last days of April. For more details of the workshop, please see the adjacent article "The NPARC Alliance of the Future". The AEDC Distributed Center also hosted a WIND training session for DoD or DoD sponsored users. If you missed the training session, all the material used in the session can be found on the NPARC Alliance home page under a TRAINING link. Feel free to review the slides at your own pace. If you have any questions, please contact

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the support team at the email address below for more details.

For support questions, the NPARC support team can be contacted via:

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phone:

(931)-454-7455

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<http://www.arnold.af.mil/nparc>

The NPARC Alliance of the Future

This year's workshop was somewhat different from previous workshops, in which the focus was on identifying the requirements and schedule for development, validation and support of the structured CFD solver, Wind. While the structured CFD code supported by the Alliance will

continue to be upgraded and maintained, the amount of time required to invest in Wind is decreasing. At the same time, the major partners and contributors to the NPARC Alliance have additional CFD issues that must be addressed. The primary issue that is driving CFD investment is productivity. Productivity is being addressed at each organization in two important ways: Unstructured grid solver technology and a systems approach to CFD simulations. This meeting focused on how the Alliance members can work together to advance the current capabilities in each organization and the U.S. aerospace community.

Over the past two years, each organization has been pursuing unstructured grid technology in a loosely coordinated effort. The NPARC partners and contributors have been participating in an Unstructured Grid Consortium, spearheaded by the Boeing Company. This consortium is attempting to identify the needs of the CFD community relative to unstructured

grid generation and to provide a focal point for development of APIs for interfacing between various components of the grid generation process. In addition, each organization has shared information on experience with various unstructured grid solvers. As a result of this meeting, the NPARC Alliance will begin working toward formally supporting an existing unstructured grid solver methodology.

Some of the NPARC Alliance members have also been pursuing methods for improving application productivity through the development of a computational system or framework. The key to this approach is to define a software architecture to allow control of various modules of the computational process and communication between these different modules. At one level, this would entail coordination between the grid generation, solver and post-processing components to improve usability and productivity. This approach is also applicable to macro-processes such as store separation and aeroelasticity simulations.

The attendees agreed in principal to work together on these important capabilities. A second meeting is planned for late summer to finalize the plans and policies to reflect this position.

Improvements and Enhancements in Version 4.0

The NPARC Alliance is pleased to announce that Wind 4.0 is officially available.

In addition to bug fixes, major enhancements from Wind 3.0 to Wind 4.0 include:

- Option to read in/out CGNS files
- Direct worker-to-worker communication for faster parallel processing
- Zonal rotating frame-of-reference and circumferential averaging for turbomachinery simulations
- Double fringe for overlapped grids to improve solution accuracy
- Zonal specifications of species reactions to reduce computations
- Spalart's Detached Eddy Simulation (DES) turbulence model
- Non-reflecting outflow and two more compressor face BC models
- Wall functions modified for chemistry

There have also been several minor upgrades including:

- Turbulence models can be specified on a zone-by-zone basis
- Time history can be redirected to the list file
- Can specify a reference Mach number for transition
- Can control the print frequency of the residual, etc.
- All library version numbers are printed
- Can restart a solution with a modified zonal grid size
- Reverse bleed boundaries are now allowed
- "Make" system improved
- PC version can be run under Cygwin (www.cygwin.com) using the standard Unix scripts

There was a change to the ADF core routines so you must download all tools which read/write CGD or CFL files. New CGD or CFL files cannot be read by old tools or older versions of Wind. Old files are compatible with the new software.

You may download several tools at once by going to the "Tools Makefiles" project under IVMS. The files "tools.login", "tools.profile", and "INSTALL.tools" are not yet available due to some difficulties with IVMS. If you have installed the tools before, you may use the existing versions of these files. Otherwise contact NPARC Support and the files will be emailed to you. Also note that currently, the tools do not read CGNS files, so it is not recommended that the CGNS option in Wind be used, unless you are using another program for post-processing.

The PC version of Wind 4.0 is available also, but the most recent PC versions of the utilities have not been compiled as of now. Therefore, CFL files created with the PC version of 4.0 would not be compatible with tools such as CFPOST. Please keep checking, we will have the tools available as soon as possible.

Several upgrades have resulted in a changes to the default behavior of Wind. To run the code with the same defaults as in Version 3.0, insert the following lines in your DAT file:

```
COUPLING MODE LOW
CROSSFLOW 2.0 (affects 2D only)
TEST 106 1 (original dt calculation)
TEST 61 2 (double book corner BCs)
```

Changes with WIND tools

1. The Wind Chemistry Manager has been added to the list of tools supported by the NPARC Alliance. This program provides a graphical interface for creating and modifying the .chm files which are used by Wind to govern the chemistry of reacting flows.
2. 'thplt'- the new time history plotting program- has been added to the list of tools. This code is for use with the new and improved time history facility in

Wind (described above).

3. Several problems that were causing GMAN and other tools to be unstable on Linux platforms have been fixed.
4. Various bugs in the Common File Class Library have been found and fixed.
5. The Wind tools development environment has been enhanced to reduce the number of unnecessary libraries linked into the codes. Thus, for example, non-graphical utilities no longer require the presence of X Windows libraries to function.

If you are a registered user of the WIND software and have forgotten your IVMS userid and/or password, please contact nparc support at nparc-support@info.arnold.af.mil.

What To Expect in Wind Version 5.0

While it has only been a few months (as of this writing) since the Wind developers finally made the official release of version 4.0, work has been proceeding on version 5.0 ever since February 2001. The result is a much-enhanced code, with even more to come before it makes its official debut in early 2002. Following is a list of major enhancements, additional minor capabilities, and noteworthy bug fixes:

New major capabilities

1. Added the HLLE scheme from NXAIR (AEDC's store separation code). Preliminary support for HLLE with multiple species has been added as well.
2. Arbitrary inflow and freestream

boundary conditions can now be used with the full range of chemistry options. Previously, the code was limited to supersonic or frozen inflow conditions.

3. Sequencing can now be done on any sized grid, provided that the final sequenced gridline has at least five points.
4. Total conditions may now be held for perfect gas with any inflow boundary condition supported by BCFREE (HOLD keyword). Within ARBITRARY INFLOW blocks, IJK_RANGES can have different values from UNIFORM inflows in the same zone (but all IJK_RANGES in that zone have the same behavior).
5. Wind (and its associated tools) should compile and run "out of the box" on Compaq Alpha systems running Tru64 Unix.
6. Wind has also been ported (again) to IBM's RS6000 family of systems.

New minor capabilities

1. The method of selecting the right hand side algorithm has been restructured so that there is a distinction between the extrapolation method/order and the means by which the extrapolated values are used to formulate a flux. In conjunction with this change, the syntax of the RHS keyword has changed (though backwards compatibility remains for most variations).
2. One result of the above change is that the HLLE and van Leer schemes can now make use of all the higher order methods (including higher order zone coupling) that were previously limited to Roe schemes.
3. The calculation of laminar viscosity is now completely consistent throughout the code. There is now only one routine (besides the keyword changes)

that needs modification in order to implement an additional viscosity model.

4. Moving grid capability has been added for multi-species flows.
5. The time history capability has been significantly upgraded to include restart, parallel, and unstructured grid capabilities. In addition, virtually any flow variable can be tracked.

Bug fixes

1. Removed some overlap where the internal designations of some of the van Leer scheme variations were also used for the Lax-Friedrichs scheme (proprietary Boeing unstructured scheme).
2. Boundaries on the interior of grids are now treated in the same manner as boundaries on grid edges. This capability was originally intended to be implemented in version 4.0, but problems with the implementation prevented it from being included in that release.
3. The calculation of the last chemical species is now consistent throughout the code, and does not allow for negative values. It is also done using double precision variables, to minimize round-off error.
4. Numerous other problems relating to reacting flow were fixed, resulting in the code being significantly more stable than previous versions.
5. Several problems with the algorithm that imposed total conditions at inflows have been found and corrected, resulting in improved stability.
6. Several problems have been fixed in the Newton iteration procedure which enable it to be used on large grids (more than 64 zones) and prevent corrupted solutions in shared mode parallel computations with indirect I/O.
7. Moving grids with inviscid walls

now behave correctly.

The result of all of this is that WIND has taken still more large steps toward being the code that the NPARC Alliance envisioned back when we started this effort four years ago. More work is needed (it always is), but the additional capabilities are significant improvements on a code that already has a versatility that is hard to match anywhere.

Frequently Asked Questions?

The following are some of the more frequently asked questions of the user support team.

I noticed that depending on the assignment mode setting the Wind job file runs with NHOSTS+1 processors (for shared mode) and NZONES+1 processors (for dedicated mode). For the MPI version of WIND what is the recommended format for the multi-processor control (MPC) file, i.e. should users use the shared mode (specifying the number of processors minus 1 that they want to use) or should they use dedicated mode.

Also, when using the MPI version is it necessary to use NZONES+1 processors or could I modify the scripts such that only NZONES processors are used? I assumed that the addition of the extra processor is only required for the PVM version of the code.

It is better to use ASSIGNMENT MODE DEDICATED. SHARED mode has some pernicious problems which show up every once in a while. We haven't been able to figure out what's happening (yet), but it results

in corrupted files and bizarrely wrong solutions. You should avoid SHARED mode if possible.

The +1 on the number of processes which are created is due to the need to allocate a master process. Thus, you really do need it in order to do the actual work of solving zones on the number of processors that you are asking for. The master process should not (and from my experience, does not) put very much load on the system, especially when you are using ROUTE DIRECT and I/O DIRECT.

I noticed that the cfd.login and tools.login scripts add the WIND application and tools executable paths to the beginning of the path. This can cause some problems in our system environment. Do you know if this is absolutely necessary or could the executable paths be added to the end of the path?

If you're planning on running Wind and related utilities, and adding the Wind directories to the beginning of the path causes problems, then that would tend to imply that there are conflicting file names. If that's the case, then you can pretty much count on problems running Wind if the Wind-related directories are not at the beginning of the path. Otherwise, it doesn't matter; you can put them anywhere in the path.

Memorandum of Agreement
AEDC Software Release
U.S. Government

Date:

1. On behalf of the U.S. Government agency listed below, I request release of the following US Air Force software package (computer programs, system description, and documentation):

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Distribution format and media:

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The requested software package will be used as follows:

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2. I understand that the requested software package contains technical data whose export is restricted by the Arms Export Control Act (Title 22, U.S.C., Sec 2751, *et seq*) or Executive Order 12470, and that violations of these export laws are subject to severe criminal penalties. Further dissemination of this software is controlled under DoDD 5230.25 and AFI 61-204, and is limited to object or executable code.

Requester

Signature:
Printed Name:
Requesting Organization:
Address:
City, State and ZIP Code:

Requester: Technical Contact

Name:
Phone Number:
E-Mail Address:

AEDC OPR Certification / Verification

Name, Initials, and Date:

AEDC Software Release Authority

Signature:
Printed Name:
Test Operations Directorate
Arnold AFB. TN 37389-9010

Memorandum of Agreement
AEDC Software Release

U.S. Commercial & Educational and Canadian Organizations

Date:

1. I/we the undersigned, on behalf of the Requesting Organization listed below (hereafter referred to as the "Requester"), request release of the following US Air Force software package (computer programs, system description, and documentation, collectively, the "Package"):

Distribution format and media (default - electronic dissemination via Internet, FTP, etc.)

The requested software package will be used as follows:

2. I/we understand that the Package may be subject to limited rights or other restrictions or constraints. In consideration therefore, the Requester agrees:
 - a) The Requester shall not knowingly release or disclose the Package to third parties (other than the Requesting Organization).
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 - c) That any restrictive markings on the Package shall be included on all copies, modifications, and derivative works, or any parts or options thereof, in any form, manner or substance, which are produced by the Requester including but not limited to incorporation of the Package into any other data, technical data, computer software, computer software documentation, computer programs, source code, or firmware, or other information of like kind, type or quality. In all such events, Requester shall clearly denote where such Package derived data initiates and concludes by use of annotations or other standard markings.
3. The Requester and the Software Release Authority agree that:
 - a) No guaranties, representations, or warranties either express or implied shall be construed to exist in any language, provision, or term contained in these materials or in any other documentation provided herewith (all such items are collectively referred to as the "Agreement"), and furthermore, the releasing organization disclaims and the Requester waives and excludes any and all warranties of merchantability and any and all warranties of fitness for any particular purpose.
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4. The Requester's use of the Package shall not prevent the Government from releasing the Package at any point in the future.
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6. The Requester may use the released Package in a contract with the Government, but understands that the Government shall not pay the Requester for rights of use of such Package in performance of Government contracts or for the later delivery to the Government of such Package. The Requester may be entitled to compensation for converting, modifying, or enhancing the Package into another form for reproduction and delivery to the Government, if authorized under a contract with the Government.
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8. I/we understand that the Package received is intended for domestic use (US and Canada) only. It will not be made available to other foreign owned or controlled corporations, or other foreign governments; nor will it be used in any contract with another foreign government.
9. The Requester and the Software Release Authority intend that all agreements under this Memorandum of Agreement shall be governed by the laws of the United States of America.
10. The undersigned Requester has the authority to bind the requesting organization to the terms of this Agreement.

Requester

Signature:
Printed Name:
Requesting Organization:
Address:
City, State and ZIP Code:

Requester: Technical Contact

Name (if different from Requester):
Phone Number:
E-Mail Address:

AEDC OPR: Export-Control Info

Export Control Number & Expiration Date::
Data or Document Custodian's Name:
Phone Number:
E-Mail Address:

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Signature:
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Test Operations Directorate Arnold AFB TN 37389-9010