

MInDes 用户手册

Material Intelligence Design User Manual

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相图、相变及材料智能设计与制备科学中心,

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版本 V 0.1

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This document is based on the work *The Not So Short Introduction to L^AT_EX 2_ε (Or L^AT_EX 2_ε in 139 minutes)* by Tobias Oetiker, Hubert Partl, Irene Hyna and Elisabeth Schlegl. This modified version was created by Zihang Wang.

Changes made to the original document include (but are not limited to): updating typesetting, revising sections, and adding new content relevant to this user manual.

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前言

MInDes 是一款相場模拟软件包。本文将简要介绍 MInDes 的使用，包括软件功能介绍，UI 介绍，输入文件的编写等部分。

本软件的开源版本可以在 GitHub 主页[MIDGroup: //MInDes](https://github.com/MIDGroup/MInDes)中找到。

MInDes 开发组
MIDGroup

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第一章 软件介绍

1.1 关于软件包

MInDes 采用 C++ 高级程序语言搭建了基本程序框架。程序底层设置了必要的数据（函数）类型、运算方法、数据网格结构、程序核心循环、各物理场求解器和并行框架。程序中层是对接各求解器的接口模块，由研究人员进行模型、程序功能模块、数据库的二次开发设计。程序表层将在可视化界面上处理 MInDes 的输入（.mindes）、输出（.log、.vts、.dat 和.txt 等）等。MInDes 支持 windows、linux 多平台，支持使用 OpenMP 进行并行运算，未来将支持 CUDA 等并行库加速计算，使用差分法、傅里叶谱方法、格子玻尔兹曼法等对各物理场进行求解。

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MInDes 软件开发自 2023 年始，是中南大学相图、相变及材料智能设计与制备实验室（领导者：杜勇教授，长江学者、杰出青年）的在读博士黄奇（2018 年-2024 年）在其博士期间的主要成果 MID-MESO 程序库的框架基础上修改完善而来。多年后续开发期间，许多科研工作者对此进行了贡献：

黄奇（邮箱：qihuang0908@163.com）、王梓航（邮箱：w.zihang@qq.com）

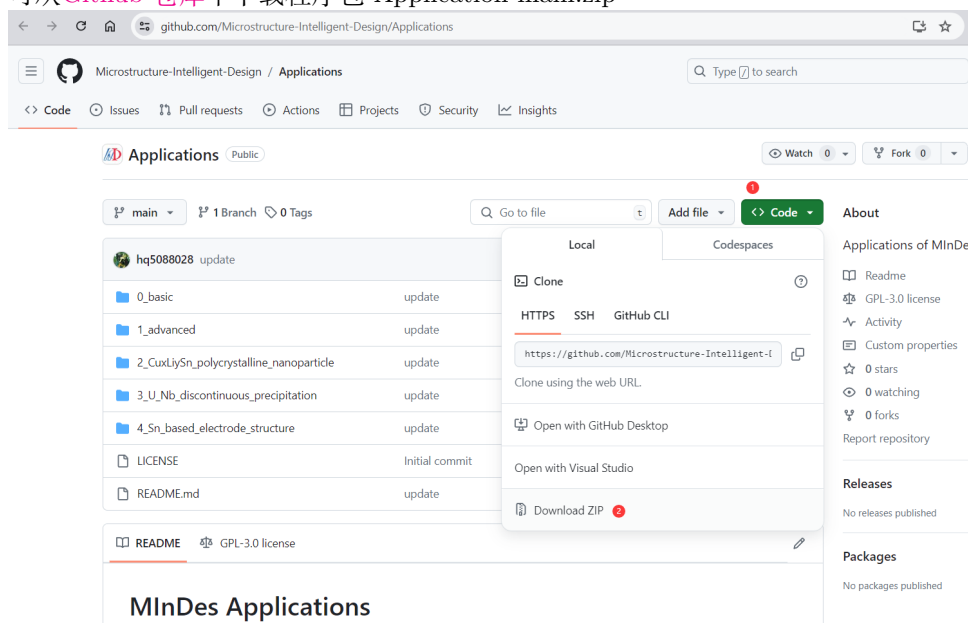
第二章 MInDes 的配置，安装

2.1 运行环境

本程序包可在 Windows 64 位环境下以及 Linux 发行版 Ubuntu 上运行。运行时建议将系统更新至最新的版本。

2.2 软件安装与初次运行

以下将以 Windows 10 操作系统为例演示程序包的安装
可从 [Github 仓库](#) 中下载程序包 Application-main.zip:



随后将程序包解压缩，可得到以下文件：

Name	Date modified	Type	Size
0_basic	28/05/2024 11:41	File folder	
1_advanced	28/05/2024 11:41	File folder	
2_CuxLiSn_polycrystalline_nanoparticle	28/05/2024 11:41	File folder	
3_U_Nb_discontinuous_precipitation	28/05/2024 11:41	File folder	
4_Sn_based_electrode_structure	28/05/2024 11:41	File folder	
LICENSE	28/05/2024 11:41	File	35 KB
README.md	28/05/2024 11:41	Markdown Source...	2 KB

其中基本的输入文件位于文件夹 *0_basic* 中，其余应用案例位于后续文件夹中。此处以 *2_CuxLiSn_polycrystalline_nanoparticle* 为例。

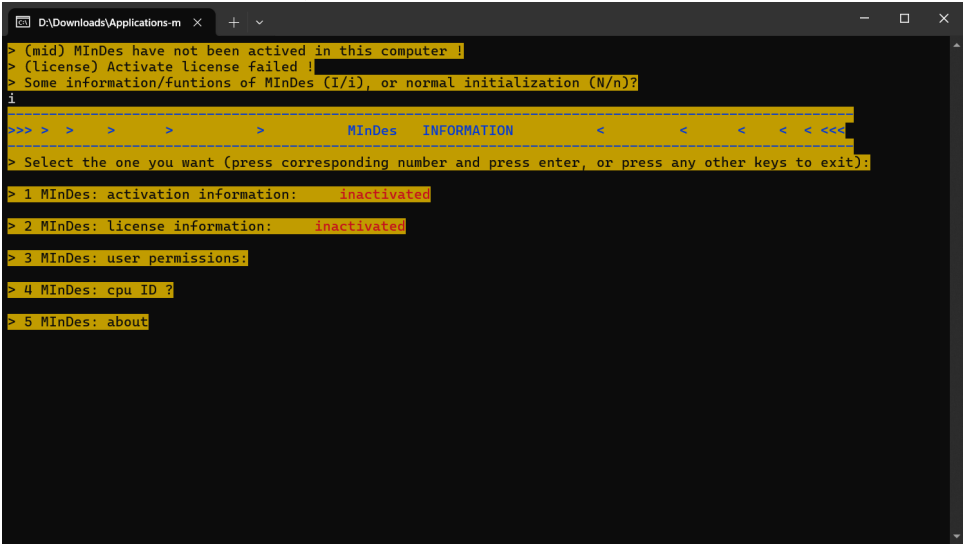
Name	Date modified	Type	Size
infile	28/05/2024 11:41	File folder	
libfftw3-3.dll	28/05/2024 11:41	Application extens...	2,650 KB
libfftw3f-3.dll	28/05/2024 11:41	Application extens...	2,708 KB
libfftw3l-3.dll	28/05/2024 11:41	Application extens...	1,219 KB
MInDes	28/05/2024 11:41	File	7,119 KB
MInDes.exe	28/05/2024 11:41	Application	1,361 KB

自上而下分别为：infile：输入文件所在文件夹；libfftw*.dll：软件运行依赖；MInDes：Linux 系统执行程序；MInDes.exe：Windows 系统执行程序。

于对应系统中运行可执行程序，即可进入软件配置界面：

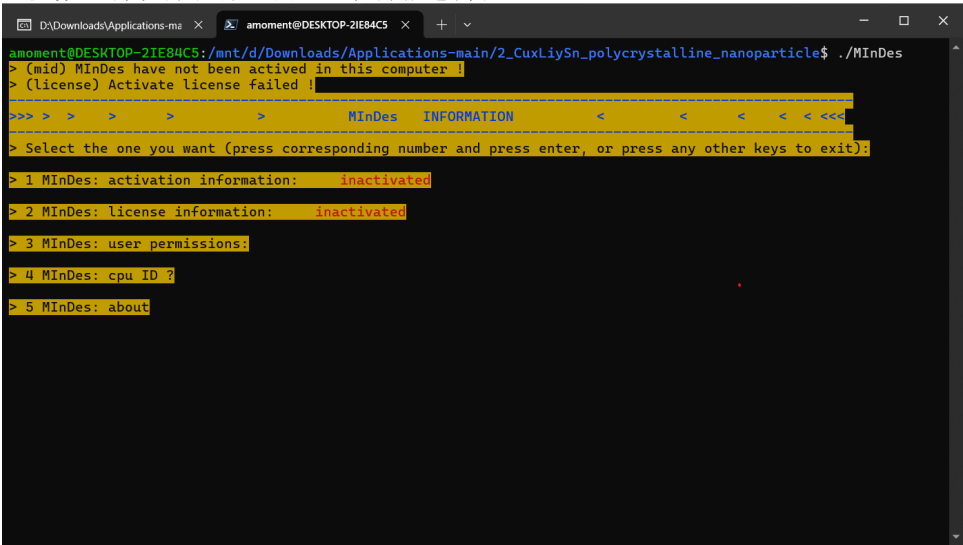
• Windows 环境下：

运行软件后键入 i 并回车，即可进入软件信息界面。



• Linux 环境下：

无参数运行软件后将直接进入软件信息界面。



于此界面下，可以查看：（1）激活信息；（2）许可证信息；（3）查看当前软件权限；（4）获取 CPU ID；（5）查看软件概况（如下图）。

[illegible]

第三章 MInDes 使用及示例

第四章 MInDes 输入文件 (infile)

第五章 MInDes 输出结果

第六章 MInDes 常见问题

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Version 1.3, 3 November 2008

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